DLRBniCSx: An extension of FEniCSx-RBniCSx frameworks for Deep Learning based Reduced Basis methods

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Abstract

Model order reduction (MOR) or Reduced Basis (RB) methods for parameterised partial differential equations has found applications in various scientific areas. All these applications deal with different levels of complexity and require repeated high-fidelity model evaluation based on methods such as Finite Element Method (FEM) or Finite Volume Method (FVM). MOR is used to identify a low-fidelity model to accelerate exploration of solution manifold over parameter space. MOR methods rely on offline-online decoupling in order to split computations dealing with computationally expensive high-fidelity model and faster to evaluate low-fidelity model. On modern High Performance Computing (HPC) systems, it is important to consider implementation level decoupling for efficient utilisation of HPC resources. DLRBniCSx provides a simpler interface between different libraries for MOR operation execution on HPC systems.

Keywords: Reduced basis method, Scientific machine learning, High performance computing, Geometric parameters

1 Introduction

Parametrised Partial Differential Equation (PDE) systems are used in various engineering and physical applications. This includes applications in areas such as aerodynamics, geophysical flows, and thermomechanical modeling. For such applications, the parameters refer to geometric parameters which characterize the geometry (size and shape) of the domain, material parameters (such as viscocity, Lamé parameters, conductivity) or physical parameters (boundary conditions). In order to accelerate the exploration of solution manifold over parameter space, Model Order Reduction (MOR) or Reduced Basis (RB) methods are used. MOR methods rely on high-fidelity models based on classical numerical method such as Finite Element Method (FEM). In recent years, Deep Learning (DL) is used extensively for creating MOR based computationally cheaper alternative.

The geometric parameters require different considerations as it involves computations of parametrised PDE solutions on different domains and as a consequence mesh deformation. For this purpose, a separate library MDFEniCSx (Section 2) was developed and used as a dependency of DLRBniCSx (Section 3) for geometrically parametrised problems.

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2 MDFEniCSx

We present MDFEniCSx, a framework for mesh deformation techniques used in multiphysics applications, such as Fluid Structure Interaction (FSI), and geometrically parametrised problems for Model Order Reduction (MOR) (Hesthaven et al. [2015], Shah et al. [2021]). MDFEniCSx provides a set of abstraction layers/ interfaces for applying mesh deformation utilising the modern FEniCSx design Baratta et al. [2023]. Specifically, we focus on specifying mesh deformation field on the external boundaries of the domains, internal interfaces, and deformation on a part of a boundary. This specified mesh deformation is then propagated inside the domain to allow computations on the deformed mesh.

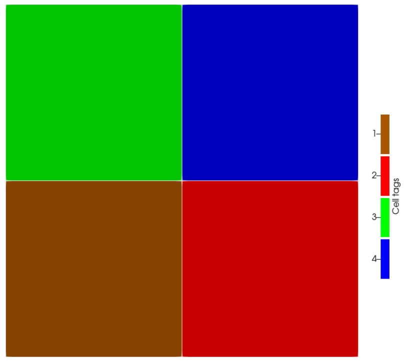
MDFEniCSx currently supports Harmonic mesh motion as well as Linear Elastic mesh motion (Figure 1). The key-feature of the interface provided in MDFEniCSx is the ability to specify either displacement from the current position or to specify final position of the points after deformation. Another key-feature of the interface is the option to specify whether mesh should be restored to original configuration after performing computations on the deformed domain. These features allow easy and uniform interface for incremental as well as non-incremental versions of the Harmonic and Linear elastic mesh deformation.

3 DLRBniCSx

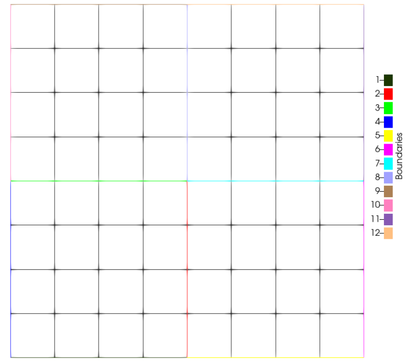
DLRBniCSx (Figure 2), a framework for deep learning based RB techniques, adds functionalities based on PyTorch Paszke et al. [2019] while, relying on FEniCSx for Finite Element Method (FEM) and RBniCSx Hesthaven et al. [2015] for Proper Orthogonal Decomposition (POD) and some auxilliary functions.

DLRBniCSx is divided into different modules (Figure 2). Activation function provides interface for activation functions with learnable/non-learnable parameters. The Custom dataset module provides interface for dataset scaling, serial computation as well as dataset partitioning for data-parallel computations. Wrappers provide interface for different functionalities such as checkpointing and setup for parallel training environment. Artificial Neural Network (ANN) module provides interface for random initialisation of ANN parameters. The training and validation routines provide CPU data-parallel as well as GPU data-parallel functionalities for ANN training.

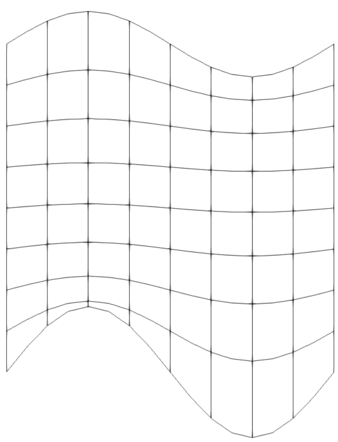
The structure of DLRBniCSx provides a simplified interface between CPU computations used for FEM-POD and GPU computations used for deep learning. In this manner, DLRBniCSx demonstrates the decoupling between CPU devices used for FEM and POD as well as GPU devices used for ANN training and inference. DLRBniCSx has been applied to applications such as thermomechanical modelling of blast furnace hearth walls (Shah et al. [2022a,b]) (Figure 3) as well as complex problems such as mixed formulation for the Poisson equation (saddle point problem) (Figure 4).



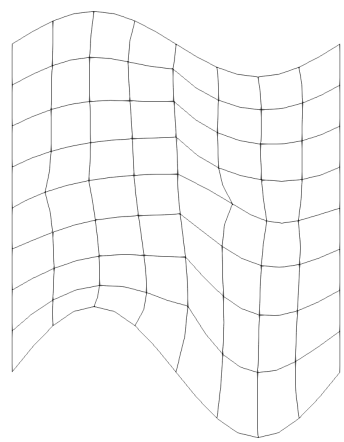
(a) Domain



(b) Domain and subdomain boundaries



(c) Harmonic mesh deformation



(d) Linear elastic mesh deformation

Figure 1: Harmonic and Linear elastic mesh deformation

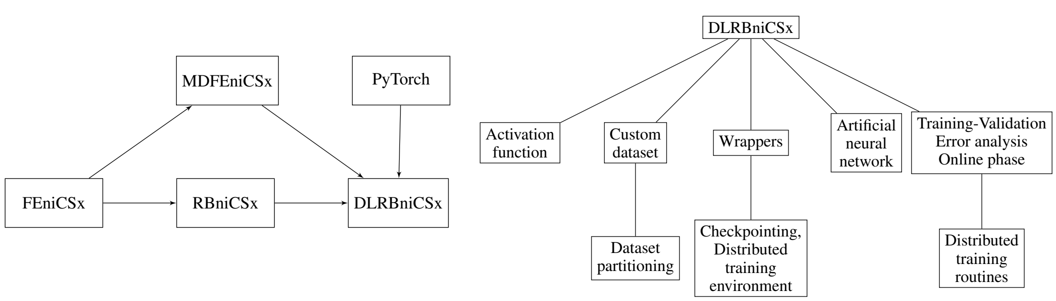
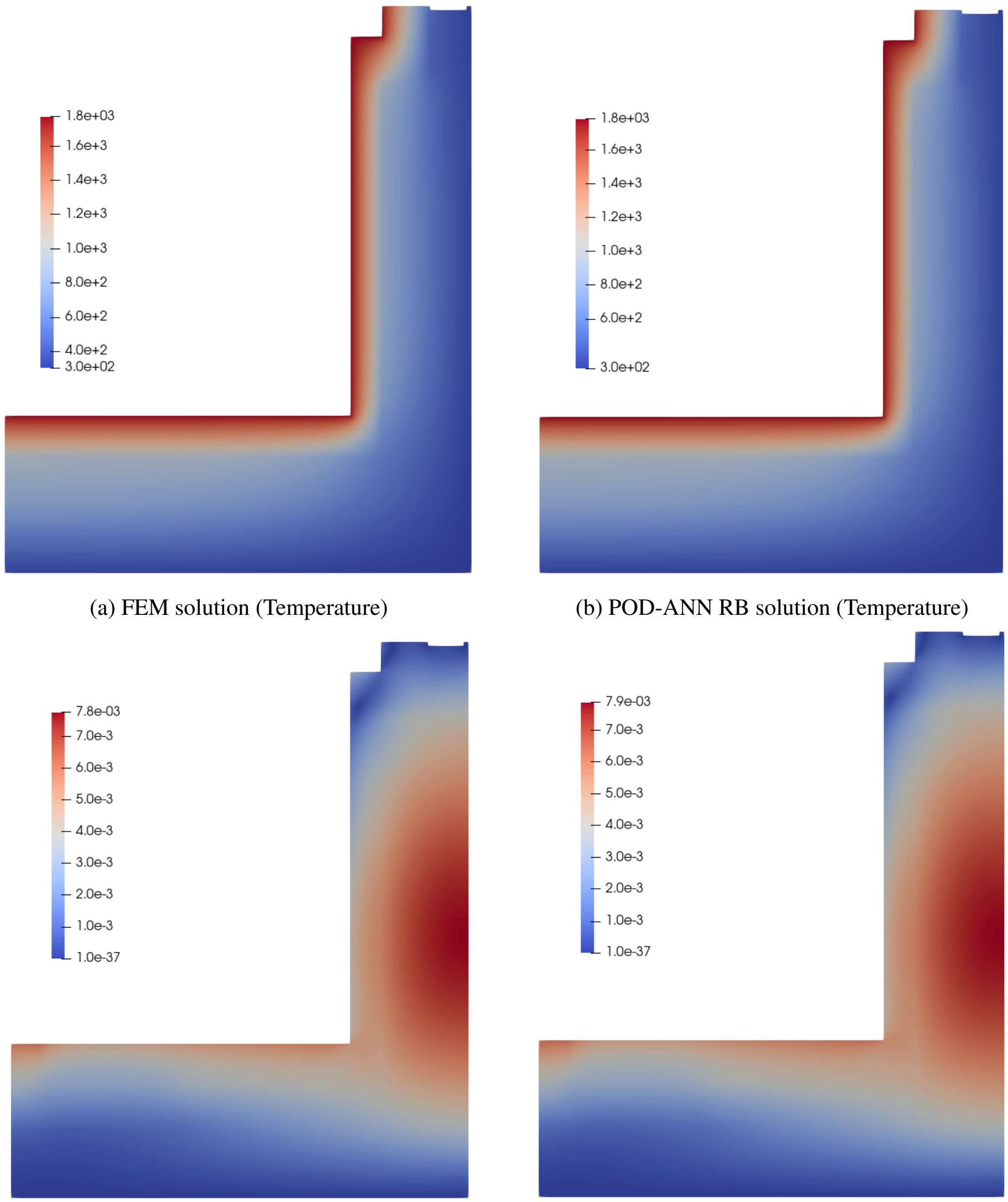


Figure 2: DLRBniCSx dependencies (left) and DLRBniCSx modules (right)



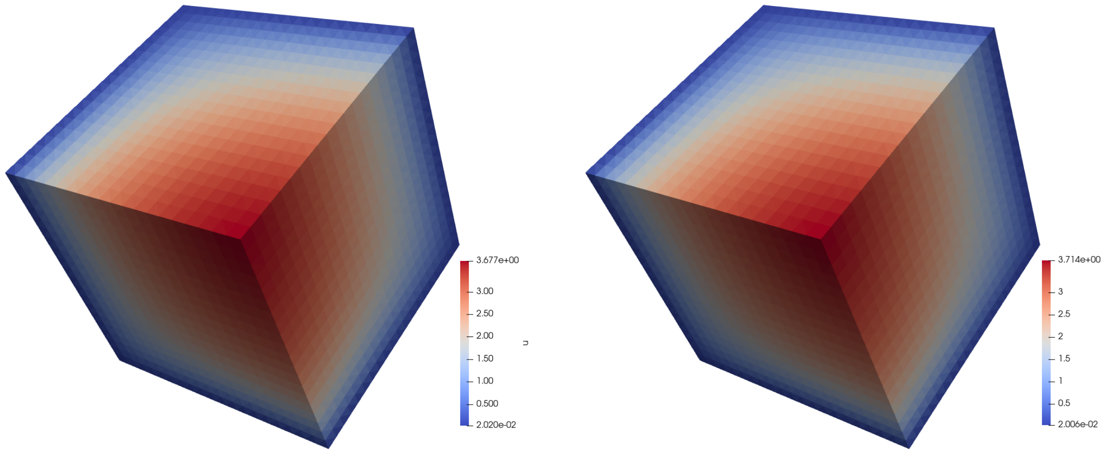
(a) FEM solution (Temperature)

(b) POD-ANN RB solution (Temperature)

(c) FEM solution (Displacement)

(d) POD-ANN RB solution (Displacement)

Figure 3: Thermomechanical model: Comparison of FEM and RB solution for temperature field (in K) and displacement field (in m)



(a) FEM solution

(b) POD-ANN RB solution

Figure 4: Mixed formulation for Poisson equation: Comparison of FEM and RB solutions

4 Conclusion and Future work

We proposed a new framework, DLRBniCSx, for reduced basis approach specifically focusing on modern software practices, implementation level decoupling between offline and online phase along with simple and clear interface between different libraries and modules.

While, DLRBniCSx currently supports proper orthogonal decomposition based reduced basis approaches, we plan to extend the framework to include data-driven techniques using Autoencoders and time-dependent problems. This extension will include Generative Artificial Intelligence (AI) techniques such as variational autoencoder and transformer neural network.

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