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A machine learning approach for efficient uncertainty quantification using multiscale methods

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ABSTRACT

Several multiscale methods account for sub-grid scale features using coarse scale basis functions. For example, in the Multiscale Finite Volume method the coarse scale basis functions are obtained by solving a set of local problems over dual-grid cells. We introduce a data-driven approach for the estimation of these coarse scale basis functions. Specifically, we employ a neural network predictor fitted using a set of solution samples from which it learns to generate subsequent basis functions at a lower computational cost than solving the local problems. The computational advantage of this approach is realized for uncertainty quantification tasks where a large number of realizations has to be evaluated. We attribute the ability to learn these basis functions to the modularity of the local problems and the redundancy of the permeability patches between samples. The proposed method is evaluated on elliptic problems yielding very promising results.

1. Introduction

Uncertainty quantification is an important task in practical engineering where some parameters are unknown or highly uncertain [7–9]. After selecting adequate priors for the uncertain parameters, simulations are performed for a large number of realizations. In the particular case of reservoir simulations, the problem is further aggravated where very fine details of the geological models are needed (large number of cells) for accurate description of the flow. One traditional approach to address this problem is to upscale the geological models [2]. Another more recent approach is to use multiscale methods [17, 14]. In these methods, the global fine scale problem is decomposed into many smaller local problems. The solution of these smaller local problems results in a set of numerically computed basis functions which are then used to build a coarse system of equations. After solving the coarse system, an interpolation is performed with the basis functions to obtain the fine scale solution.

We note that in multiscale methods, a large number of local problems are solved under the same boundary conditions to obtain the required basis functions. This process is repeated for each geological realization in uncertainty quantification tasks. Our aim is to exploit the redundancy that may arise in solving these local problems for several geological realizations by introducing a data-driven approach for estimating the basis functions efficiently. Specifically, we exploit the large number

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of local problem solutions that become available after a given number of full runs to construct a computationally cheap function that generates approximate solutions to local problems, i.e. approximate basis functions. In effect, what we propose is a type of hybrid surrogate model by embedding a data-driven approach into the multiscale numerical method. In this work, we focus on one multiscale method called the Multiscale Finite Volume method (MsFV) introduced by Jenny et al. [17]. However, the proposed approach can be applied to any multiscale method where the explicit construction of basis functions is performed such as in the more recent multiscale method based on restriction-smoothed basis functions (MsRSB) [22].

Aarnes and Efendiev [1] introduced a multiscale mixed finite element (MsMFE) method for porous media flows with stochastic permeability field where a set of precomputed basis functions is constructed based on selected set of realizations of the permeability field. These basis functions are then used to build a low-dimensional approximation space for the velocity field. We note that the cost of solving the upscaled problem (i.e. coarse scale) in [1] increases with the number of selected set of realizations. In contrast, in this manuscript we directly address the generation of basis functions via a "black box" surrogate modelling approach using machine learning. The generated basis functions are then directly employed in the multiscale formulation without any further modification. Another major difference is that our method directly benefits from increasing the number of realizations used to build the surrogate model without any increase in the computational cost of solving the coarse scale problems for new realizations.

This paper presents the first attempt to combine/embed machine learning techniques within multiscale numerical methods with very promising results. The motivation for our work comes from the observation that computational power and data storage capacity are ever increasing. This trend is likely to continue for some time and results in an increased ability to store and data-mine large volumes of simulation data. Another source of motivation comes from the renewed interest in machine learning among the research community, specially in the branch of deep learning to tackle AI-complete tasks such as computer vision and natural language processing. Neural network models are regarded as *universal function approximators* [12,13,5] with capacity to learn highly non-linear maps. Therefore, they seem to be suitable for our current application.

The rest of the paper is organized as follows: In section 2, we give a brief description of the multiscale finite volume method (MsFV) and neural networks (NN). In section 3, we present the methodology for the proposed approach for machine learning the basis. In section 4, we examine the effectiveness of the presented method for uncertainty quantification in two test cases. Finally, in section 5 we report the conclusions of this work along with a brief discussion of future directions.

2. Background

In this section we briefly describe the two main components of the proposed method: multiscale finite volume (MsFV) methods and neural networks (NN) for surrogate modelling. A number of variants of the MsFV method have been proposed since its introduction in [17]. In this manuscript, we employ the MsFV method as described in [20,21].

2.1. Multiscale finite volume method

We consider an elliptic equation describing the pressure field

$$-\nabla \cdot (\mathbf{K}\nabla p) = q \tag{1}$$

where p denotes the fluid pressure, q denotes fluid sources, and $\mathbf{K}$ denotes the permeability tensor. Discretizing Eq. (1) by the finite volume method results in a system of equations of the form $\mathbf{Ap} = \mathbf{q}$, which for some applications (such as reservoir simulation) tends to be extremely large. The MsFV method tackles this problem by constructing and solving a much coarser system of equations $\mathbf{A}_C\mathbf{p}_C = \mathbf{r}_C$, the solution of which is then used to obtain an approximation of $\mathbf{p}$ by interpolation. For this, it relies on a set of basis functions which are obtained by solving local problems. In this sense, the method slightly resembles the finite element method, except that the basis functions employed are not analytical functions but numerically computed functions.

The method begins with the definition of a pair of overlapping coarse grids, namely the *primal grid* and the *dual grid*, as shown in Fig. 1. In principle, the primal grid can be any coarse partition defined over the fine grid. Next, we define the *coarse nodes* as the fine cells at the centres of each primal cell. Lastly, the dual grid is defined by the lines connecting these coarse nodes. We denote the primal cells with $\Omega_i^C,\ i \in \{1, \cdots, N_C\}$, and the dual cells with $\Omega_j^D,\ j \in \{1, \cdots, N_D\}$.

A set of (partial) basis functions are obtained by solving the local problems

$$\begin{aligned} \nabla \cdot (\mathbf{K} \cdot \nabla \phi_j^i) &= 0 \quad \text{in } \Omega_j^D \\ \nabla \cdot_{\parallel} (\mathbf{K} \cdot \nabla \phi_j^i)_{\parallel} &= 0 \quad \text{on } \partial\Omega_j^D \\ \phi_j^i(\mathbf{x}_k) &= \delta_{ik} \quad k \in \{1, \cdots, N_C\}, \end{aligned} \tag{2}$$

where ϕ_j^i denotes the (partial) basis function on dual cell Ω_j^D (see Fig. 3a) associated with coarse node i, $\mathbf{x}_k$ denotes the coordinate of coarse node k, and $_{\parallel}\cdot_{\parallel}$ denotes the tangential component over the dual cell boundary $\partial\Omega_j^D$. In the 2D case, this means solving 1D problems over $\partial\Omega_j^D$, the solutions of which become the boundary conditions for the 2D problem on Ω_j^D.