Numer. Math. Theor. Meth. Appl.
doi: 10.4208/nmtma.OA-2021-0100

Vol. **14**, No. 4, pp. 862-892
November 2021

Generalized Rough Polyharmonic Splines for Multiscale PDEs with Rough Coefficients

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Received 12 June 2021; Accepted (in revised version) 5 July 2021

Abstract. We demonstrate the construction of generalized Rough Polyharmonic Splines (GRPS) within the Bayesian framework, in particular, for multiscale PDEs with rough coefficients. The optimal coarse basis can be derived automatically by the randomization of the original PDEs with a proper prior distribution and the conditional expectation given partial information on, for example, edge or first order derivative measurements as shown in this paper. We prove the (quasi)-optimal localization and approximation properties of the obtained bases. The basis with respect to edge measurements has first order convergence rate, while the basis with respect to first order derivative measurements has second order convergence rate. Numerical experiments justify those theoretical results, and in addition, show that edge measurements provide a stabilization effect numerically.

AMS subject classifications: 41A15, 34E13, 35B27

Key words: Generalized Rough Polyharmonic Splines, multiscale elliptic equation, Bayesian numerical homogenization, edge measurement, derivative measurement.

1. Introduction

Problems with a wide range of coupled temporal and spatial scales are ubiquitous in many phenomena and processes of materials science and biology. There has been amount of work concerning the design and analysis of numerical homogenization type methods for multiscale problems, such as asymptotic homogenization [22,37], numerical upscaling [1,10], heterogeneous multi-scale methods [11,12,24], multi-scale finite

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element methods [2,13,15], variational multi-scale methods [3,21,39], flux norm homogenization [4,34], rough polyharmonic splines (RPS) [36], generalized multi-scale finite element methods [7,8,14], localized orthogonal decomposition [20,27,38], etc. Numerical homogenization concerns the approximation of the high dimensional solution space of multiscale PDEs by a low dimensional approximation space with optimal error control, and furthermore, the efficient construction of such an approximation space, e.g., the localization of the basis on a coarse patch. Surprisingly, numerical homogenization has deep connections with Bayesian inference, kernel learning and probabilistic numerics [29,30,32,33]. The Bayesian homogenization approach [29] provides a unified framework for the construction of a proper coarse space with desired approximation and localization properties, and practically it corresponds to a variational problem with functional constraints, which is close to [27,39] in this sense.

In this paper, we generalize the so-called Rough Polyharmonic Splines (RPS) [36] within the Bayesian framework [29] for the following differential equation:

$$\begin{cases} \mathcal{L}u = g, & \text{on } \Omega, \\ \mathcal{B}u = 0, & \text{on } \partial\Omega, \end{cases} \tag{1.1}$$

where $\mathcal{L}$ and $\mathcal{B}$ are differential operators on Ω and $\partial\Omega$, such that $(\mathcal{L},\mathcal{B}) : \mathcal{H}(\Omega) \to \mathcal{H}_{\mathcal{L}}(\Omega) \times \mathcal{H}_{\mathcal{B}}(\partial\Omega)$, where $\mathcal{H}(\Omega), \mathcal{H}_{\mathcal{L}}(\Omega)$ and $\mathcal{H}_{\mathcal{B}}(\partial\Omega)$ are Hilbert spaces of generalized functions on Ω and $\partial\Omega$, such that $\mathcal{H}(\Omega) \subset L^2(\Omega) \subset \mathcal{H}_{\mathcal{L}}(\Omega)$. In this paper we consider the second order elliptic equation of divergence form with rough coefficients, such that $\mathcal{L} = -\operatorname{div}(\kappa(x)\nabla\cdot)$, $\mathcal{B} = \mathrm{Id}$, and Ω is a simply connected domain with piecewise smooth boundary $\partial\Omega$. The rough coefficient, $\kappa(x) \in L^\infty(\Omega)$ is uniformly elliptic on Ω, i.e., it is uniformly bounded from above and below by two strictly positive constants, denoted by $\kappa_{\min}$, $\kappa_{\max}$. $\kappa(x)$ may represent multiscale media with possibly high contrast ratio $\kappa_{\max}/\kappa_{\min}$ and fast oscillations with non-separable scales. For this example, we have $\mathcal{H}(\Omega) = H_0^1(\Omega)$, and $\mathcal{H}_{\mathcal{L}}(\Omega) = H^{-1}(\Omega)$. We use this assumption for the rest of this paper unless otherwise specified.

Under the Bayesian framework, the space of the generalized Rough Polyharmonic Splines (GRPS) can be identified by suitable choices of random noise and measurement functions. Point and volume measurements are used in [36] and [30], respectively. In this paper, we construct two new GRPS spaces based on the edge measurements and derivative measurements respectively. Such measurements are well motivated and necessary if there exists elongated structures such as cracks and channels in heterogeneous media. Rigorous proof for their approximation and localization properties are derived.

The paper is organized as follows: in Section 2, we first introduce the Bayesian homogenization framework and the variational formulation of numerical homogenization (coarse) basis, then we present the details for the construction of such basis. In Section 3, we provide the rigorous error analysis of the corresponding numerical homogenization method. Numerical examples are presented in Section 4 to validate the method. We conclude the paper in Section 5.