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Customized Coarse Models for Highly Heterogeneous Materials

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Abstract Using a toy model for subsurface flow in highly heterogeneous materials, we demonstrate a methodology for building customized coarse models from local eigenvalues problems in overlapping subdomains. We show that this methodology allows you to efficiently build accurate multiscale models with very few macroscale degrees of freedom for cases where classical computational homogenization methods break down. Such methods show great potential for modeling highly heterogeneous material where properties vary over very small length scales. Such problems are typical in many engineering applications, for example subsurface flow and composite materials.

Keywords Generalized Multiscale Finite Elements · Upscaling · Porous Media · Eigenvalue Problem

1 Introduction

We consider mathematical models represented by elliptic partial differential equations (PDEs) with high contrast coefficients that vary over small length scales relative to the macroscale dimension. Such models naturally arise in many engineering applications, for example composite materials or flow within porous media. In this paper we consider a toy model for porous media given by the scalar elliptic PDE

$$-\nabla \cdot (k(\mathbf{x})\nabla u(\mathbf{x})) = 1 \quad \forall \mathbf{x} \in \Omega := [0,1]^2 \tag{1}$$

subject to homogeneous Dirichlet boundary conditions $u(\mathbf{x}) = 0$ for all $\mathbf{x} \in \partial\Omega$. Here $u(\mathbf{x})$ denotes the pressure field and $k(\mathbf{x})$ is a spatially varying permeability field. For the numerical examples within this paper we take $k(\mathbf{x})$to be the random

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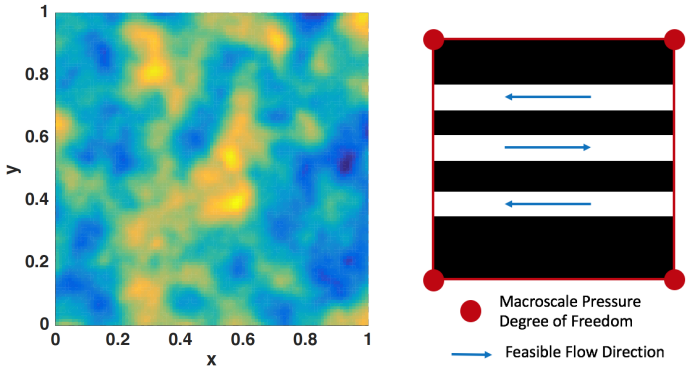

Fig. 1 (Left) Single realization of random field generated from a log-normal random field, characterized by a small correlation length and high contrast (colors plotted on a log scale) (Right) A block of rock with three high permeability channels, spanned by a single macroscale linear finite element.

field generated from a single sample of a log-normal random field, shown in Fig 1 (left).

Equation 1 can be solved using finite elements for which we seek the approximate solution $u_h \in V_h$ (the space of piece linear functions on a grid $\mathcal{T}_h$) which satisfies the variational equation

$$\int_\Omega k(\mathbf{x}) \nabla u_h \cdot \nabla v_h \, d\mathbf{x} + \int_\Omega v_h \, d\mathbf{x} = 0 \quad \forall v_h \in V_h. \tag{2}$$

Capturing the fine scale details, arising from the variations in $k(\mathbf{x})$ at the small length scales, is computationally expensive since we require a sufficiently small mesh size (h). It is therefore, natural to try and build efficient multiscale methods which upscales the microscale information to a coarse / lower dimensional finite element space V_H, which still captures the local microscale information of $k(\mathbf{x})$.

A natural question arises. What is a good choice of the coarse space V_H? It is easy to construct examples where the coarse model will provide a poor solution if V_H has insufficient degrees of freedom. For example, let V_H be the span of piecewise linear finite elements on a coarse grid characterized by a mesh size $H \gg h$. Consider a block of rock (Fig. 1 (right)) spanned by a single coarse linear finite element, which contains three channels of high permeability rock (white) surrounded by low permeability regions (black). One possible flow configuration is the fluid flows in one direction in two channels and the opposite direction in the third (as indicated by the arrows in Fig. 1 (right). For a single quadrilateral linear finite element the horizontal flow can only vary linearly in the vertical direction. Therefore this local switching of the flow is not a *mode* which is captured on the macroscale. For particular boundary conditions, such a coarse space would give non-representative results of the true microscale solution.

In such cases, additional degrees of freedom need to be added to V_H. Particularly in continuum mechanics this has led to the development of higher order continuum models, for example Cosserat or strain-gradient continuum[1,2]. Such models often provide accurate coarse scale descriptions of the microscale although their development often requires significant physical intuition and must be built

on a case-by-case basis. In this paper we describe a type of generalized multiscale method [3,4] whereby the macroscale model is custom built from a few local eigenmodes computed on overlapping subdomains. These coarse spaces have been shown to provide excellent preconditioners for two-level Schwarz method [5]. In this contribution we focus on their use as a multiscale method and provide step-by-step details an toy example of this exciting new multiscale method.

2 Customized Coarse Models for Highly Heterogeneous Models

Let V_h be the set of functions u spanned by the basis of piece-wise linear finite element functions $\{\phi_k(\mathbf{x})\}_{i=1}^{n:=\dim(\mathrm{V_h})}$ on a grid $\mathcal{T}_h$, which is characterized by the small grid size h. The indices k will denote the k^{th} degree of freedom, and so any function in V_h can be represented as $u = \sum_{k=1}^{n} u_k \phi_k(\mathbf{x})$. This converts the variational problem (2) to the system of linear equations

$$\mathbf{K}\mathbf{u} = \mathbf{f} \tag{3}$$

where $\mathbf{K}_{ij} = \int_\Omega k(\mathbf{x}) \nabla\phi_i \cdot \nabla\phi_j \, d\mathbf{x}$ is the stiffness matrix, $\mathbf{f}_i = \int_\Omega \phi_i \, d\mathbf{x}$ the load vector and $\mathbf{u} = [u_1, u_2, \ldots, u_n]^T$ the solution vector.

Starting with a non-overlapping partition of Ω into N subdomains made up of disjoint sets of elements $\Omega = \cup_{j=1}^{N} \Omega_j'$, the domains are overlapped by O layers to achieve an overlapping partition $\Omega = \cup_{j=1}^{N} \Omega_j$. The overlapping regions of a partition Ω_j are denoted by the set

$$\Omega_j^\circ := \{\mathbf{x} \in \Omega_j : \exists\, i \neq j \text{ such that } \mathbf{x} \in \Omega_i\}.$$

Furthermore the subset of indices k for which ϕ_k is supported in Ω_j is define by

$$\mathrm{dof}(\Omega_\mathrm{j}) := \{\mathrm{k} : 0 \leq \mathrm{k} \leq \mathrm{n} \text{ such that } \mathrm{supp}(\phi_\mathrm{k}) \subset \Omega_\mathrm{j}\}, \tag{4}$$

whilst those degrees of freedom *active* in Ω_j are denoted by the set

$$\overline{\mathrm{dof}}(\Omega_j) := \{k : 0 \leq k \leq n \text{ such that } \mathrm{supp}(\phi_\mathrm{k}) \cap \Omega_\mathrm{j} \neq \emptyset\}. \tag{5}$$

The definition of each of these sets can perhaps be better understood with an example, as shown in Fig. 2.

The aim is to construct global multiscale basis functions from local eigenfunctions. These local eigenfunctions are functions $u \in V_h$ restricted to a partition Ω_j. It is therefore natural to define the function space

$$V_h(\Omega_j) := \{v|_{\Omega_j} : v \in V_h\}$$

and the further restriction to those finite element functions which are supported on Ω_j i.e.

$$V_{h,0}(\Omega_j) := \{v \in V_h(\Omega_j) : \mathrm{supp}(v) \subset \Omega_j\}.$$

Any function $u \in V_{h,0}(\Omega_j)$ can be extended to V_h by padding it with zeros. This extension operator is defined by $R_j^T : V_{h,0}(\Omega_j) \to V_h$, and therefore it's transpose $R_j : V_h \to V_{h,0}(\Omega_j)$ defines the restriction operator of any function $u \in V_h$ to $V_{h,0}(\Omega_j)$. In practice the extension operator is can be coded as a sparse matrix

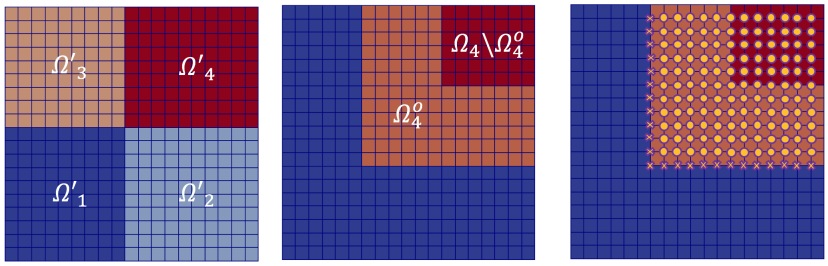

Fig. 2 (Left) Domain Ω split into $N = 4$ non-overlapping subdomains Ω'_j (Middle) Shows overlapping partition Ω_4 (red and orange) with the subregion Ω_4°, the overlapping region generated once Ω'_j are overlapped by 3 layers. (Right) circles mark $k \in \mathrm{dof}(\Omega_4)$ and crosses mark $k \in \overline{\mathrm{dof}}(\Omega_4) \backslash \mathrm{dof}(\Omega_4)$.

$\mathbf{R}_j^T$ of 0's and 1's which maps local degrees of freedom (nodal values) to the their global counterparts.

In constructing global multiscale basis functions from local eigenfunctions in overlapping subdomains it is important to carefully deal with those degrees of freedom which are supported by one more than subdomain. To patch, such overlapping functions together, global values at these shared nodes should be *some* average value of the values they take in each of the subdomains. To do this we construct a partition of unity operator.

Firstly we define the value $\xi_k := |\{j : k \in \mathrm{dof}(\Omega_\mathrm{j})\}|$ for each degree of freedom k, as the number of subdomains in which a degree of freedom k is supported. Suppose we have a set of functions $w^{(j)} = \sum_{k \in \overline{\mathrm{dof}}(\Omega_j)} w_k^{(j)} \phi_k \in V_h(\Omega_j)$ for each partition $j = 1 \dots N$, we define the local partition of unity operator

$$\Xi_j(w^{(j)}) := \sum_{k \in \mathrm{dof}(\Omega_\mathrm{j})} \frac{1}{\xi_k} w_k^{(j)} \phi_k|_{\Omega_j} \tag{6}$$

which maps $V_h(\Omega_j) \to V_{h,0}(\Omega_j)$. We then construct the global function over Ω, $\Phi \in V_h$ from the local functions as follows

$$\Phi(w^{(j)}) = \sum_{j=1}^{N} R_j^T \, \Xi_j(w^{(j)}) \tag{7}$$

In practice the partition of unity operator Ξ is implemented as a matrix operation $\mathbf{X}$ which acts on a vector of nodal values $\mathbf{w^{(j)}}$ i.e $\mathbf{X w^{(j)}}$, where $\mathbf{X}$ is a diagonal matrix with values $\mathbf{X}_{kl} = \xi_k^{-1}$ if $k = l$ and $k \in \mathrm{dof}(\Omega_\mathrm{j})$, otherwise $\mathbf{X}_{kl} = 0$.

For each subdomain $j = 1, \dots, N$ we calculate the first m eigenvalues $w^{(j)} \in V_{h,0}(\Omega_j)$ of the inner product

$$\int_{\Omega_j} k(\mathbf{x}) \nabla w^{(j)} \cdot \nabla v \, d\mathbf{x}, \tag{8}$$

which, written as matrix operator $\mathbf{K}_{\Omega_j}$ has eigenvectors $\mathbf{w}^{(j,i)}$for $i = 1, \dots, m$, associated with the m lowest eigenvalues. Once these eigenvectors are computed on each subdomain the coarse space can be constructed as

$$V_H := \mathrm{span}\{\mathrm{R_j^T} \Xi_\mathrm{j}(\mathrm{w}^{(\mathrm{j},\ell)}) : \ell = 1, \dots, \mathrm{m}; \mathrm{j} = 1, \dots, \mathrm{N}\}.$$

Fig. 3 Eigenvectors associated with lowest 5 eigenvalues for Ω_6 with $O = 5$

The mapping of coarse mode coefficients in V_H to the original fine scale space V_h can be encode by the mapping $\mathbf{R}_H^T$, a matrix of $\dim(\mathrm{V_h})$ by Nm, with columns $\mathbf{R}_j^T \mathbf{X}_j \mathbf{w}_j^{(i)}$for $j = 1, \ldots, N$ and $i = 1, \ldots, m$. Finally we reformulate the original variational problem (2) in the customized coarse space so that

$$\mathbf{K}_H \mathbf{U} = \mathbf{F} \tag{9}$$

where $\mathbf{K}_H = \mathbf{R}_H \mathbf{K} \mathbf{R}_H^T$, $\mathbf{U}$ is the solution vector which contains the coefficients of the coarse modes and $\mathbf{F}$ the load vector with entries $\mathbf{F}_{m(j-1)+i} = \mathbf{f}^T \mathbf{R}_j^T \mathbf{X}_j \mathbf{w}_j^{(i)}$.

Importantly the computation of the eigenvectors on each subdomain are independent, and the assembly of $\mathbf{K}_H$ and $\mathbf{F}$ require only nearest-neighbor (subdomain) communication. Therefore this coarse model can be assembled efficiently in parallel. In effect, we substitute one large solve for N independent (parallel) small eigenvalue problems and one inexpensive coarse solve.

3 Results & Concluding Remarks

In this section we test the methodology for our toy problem (2), for which we take the permeability field $k(\mathbf{x})$ as a single realization of a random field define by a log-normal distribution, as shown in Fig. 1 (left). The fine mesh $\mathcal{T}_h$ is defined on a uniform square grid with $h = 1/200$ (i.e. 40,000 elements and 36,601 degrees of freedom), the domain is split into $N = 16$ square non-overlapping domains Ω_j', each of 2,500 elements and then overlapped by O elements to form an overlapping partition Ω_j. Figure 3 shows the first 5 eigenvectors of the Ω_6 partition (i.e $\mathbf{w}^{(6,i)}$for $i = 1, \ldots, 5$, with $O = 5$). We note that the lowest eigenvalue is zero associated with a constant pressure in Ω_6. This will be the case for any subdomain for which Ω_j contains no degrees of freedom which lie on the constrained boundary of Ω. First we visually compare the fine scale solution $\mathbf{u}_h$ computed on the fine grid $\mathcal{T}_h$ (Fig. 3 (left))with the coarse approximation $\mathbf{U}_H$with an overlap of $O = 5$ and $m = 20$, Fig.3 (middle). Defining the error as $\varepsilon = \|\mathbf{u}_h - \mathbf{R}_H^T \mathbf{U}_H\|_2 / \|\mathbf{u}_h\|_2$, this coarse model with over 100 times less degrees of freedom computes the solution with $\varepsilon = 0.034$. Finally in Fig. 3 (right) we compare the error ε in the coarse model relative to the fine scale model for various sizes of overlap O and number of eigenvalues per patch m.

In this short paper we have demonstrated the power of using local spectral information to build bespoke multiscale function space along the same lines of the generalized multiscale finite element method [4,5]. This method allows you to construct coarse models with a fraction of the degrees of freedom in comparison to the

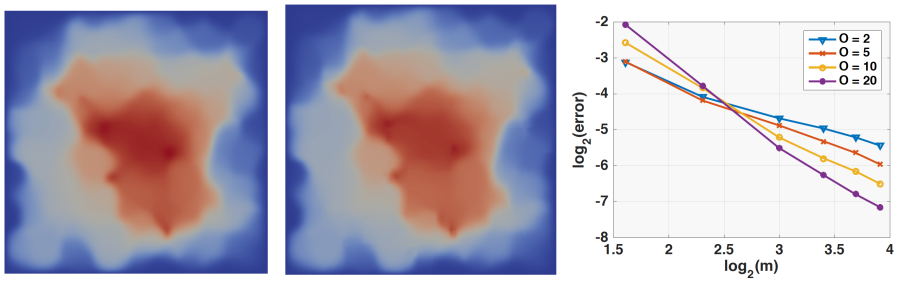

Fig. 4 (Left) Fine scale solution $\mathbf{u}_h$(Middle) Bespoke Coarse space solution $\mathbf{R}_H^T\mathbf{U}_H$ with $m = 20$ and $O = 5$ (Right)Plot of $\log(m)$ against $\log_2(\varepsilon)$ for various values of O.

fine scale counterpart, but still achieve accurate solutions with microscale information. For the particular toy model presented the degrees of freedom are reduced by a factor of over 100, to achieve a solution within 3% of the fine scale solution. These methods show particular promise for applications in which material parameters (coefficients of the PDE) vary over a range length scales, have a complex distribution and/or demonstrate high contrast. For such cases, the macroscale relevant modes can be unclear, and it is natural to use the local eigenfunctions on the subdomains to hand pick your coarse space.

We have not demonstrated the computational savings of this method since we test the methodology on small toy problems (e.g. $\sim 3.6 \times 10^4$ degrees of freedom). For such cases, even the fine scale problem and can easily be solved on a single processor with a good direct solver. We observed a factor 2 - 3 speed up for a error of 3%. Once we push the applications of this method to 3D problems with large number of degrees of freedom (e.g. $\dim(\mathrm{V_h}) > 10^7$) it is easy to postulate the method's potential. In effect, we substitute one large solve for N independent (parallel) small eigenvalue problems and one inexpensive coarse solve. Further gains can be expected for high contrast materials (e.g. composites materials) which display significant periodicity, since in such cases only representative local eigenproblems need be solved. In the short term the application of these methods to 3D linear elasticity (a vector-valued elliptic PDE) will be explored.

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