Interplay of Theory and Numerics for Deterministic and Stochastic Homogenization

Abstracts

Coupling reduced basis and numerical homogenization methods for solving quasilinear elliptic problems

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We study finite element (FE) discretizations of quasilinear second-order elliptic problems of the form

(1)
$$-\nabla \cdot (a^{\varepsilon}(x, u^{\varepsilon}(x)) \nabla u^{\varepsilon}(x)) = f(x) \text{ in } \Omega, \qquad u^{\varepsilon}(x) = 0 \text{ on } \partial\Omega,$$

where Ω is a bounded convex polyhedron in \mathbb{R}^d with $d \leq 3$. The $d \times d$ tensor $a^{\varepsilon}(x, s)$, assumed to be uniformly elliptic and bounded, is allowed to vary on a very small spatial scale denoted by ε . We note that the homogenization of this problem has been studied in [8],[9], where it is shown that the homogenized equation is of the same quasilinear type as the original equation, with $a^{\varepsilon}(x, u^{\varepsilon}(x))$ replaced by a homogenized tensor $a^0(x, u^0(x))$ depending nonlinearly on a homogenized solution u^0 . We are interested in the following two problems:

- derive an efficient numerical homogenization of (1) (i.e., a numerical method that approximate the homogenized solution u^0 without the a priori knowledge of $a^0(x, u^0(x))$),
- control the error of the approximation process, i.e., derive an a priori error analysis.

Notations. We consider a macro finite element (FE) space $S_0^{\ell}(\Omega, \mathcal{T}_H)$ made of piecewise polynomial of degree ℓ defined on a family of (macro) partition \mathcal{T}_H of Ω in simplicial or quadrilateral elements K of diameter H_K ($H \gg \varepsilon$ is allowed). We then define a quadrature formula (QF) $\{x_{K_j}, \omega_{K_j}\}_{j=1}^J$ on each $K \in \mathcal{T}_H$ given by an affine transformation of a QF from a reference element \hat{K} . For each $K \in \mathcal{T}_H$ and $x_{K_j} \in K, j = 1, \ldots, J$, we define a sampling domain $K_{\delta_j} = x_{K_j} + (-\delta, \delta)^d$, $(\delta \geq \varepsilon)$ and we consider a micro FE space $S^q(K_{\delta_j}, \mathcal{T}_h) \subset W(K_{\delta_j})$ with simplicial or quadrilateral FEs and piecewise polynomial of degree q (\mathcal{T}_h is a conformal and shape regular family of triangulation \mathcal{T}_h). The space $W(K_{\delta_j})$ is either the Sobolev space $W(K_{\delta_j}) = W_{per}^1(K_{\delta_j}) = \{z \in H_{per}^1(K_{\delta_j}); \int_{K_{\delta_j}} zdx = 0\}$ or $W(K_{\delta_j}) =$ $H_0^1(K_{\delta_j})$.

The numerical homogenization method. We work in the framework of the finite element heterogeneous multiscale method (FE-HMM) [1, 10, 4] and consider the following micro-macro FEM [5]: Find $u^H \in S_0^{\ell}(\Omega, \mathcal{T}_H)$ such that

$$B_H(u^H; u^H, w^H) = F(w^H), \qquad \forall w^H \in S_0^{\ell}(\Omega, \mathcal{T}_H),$$

where

$$B_H(u^H; v^H, w^H) = \sum_{K \in \mathcal{T}_H} \sum_{j=1}^J \frac{\omega_{j,K}}{|K_{\delta_j}|} \int_{K_{\delta_j}} a^{\varepsilon}(x, u^H_{K_j}) \nabla v^h_{K_j}(u^H_{K_j}) \cdot \nabla w^h_{K_j}(u^H_{K_j}) dx,$$

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and $v_{K_j}^h(s)$ is sol. of the micro pblm $v_{K_j}^h(s) - v_{lin}^H \in S_h(K_{\delta_j}, \mathcal{T}_h)$

$$\int_{K_{\delta_j}} a^{\varepsilon}(x,s) \nabla v_{K_j}^h(s) \cdot \nabla z^h dx = 0 \quad \forall z^h \in S_h(K_{\delta_j},\mathcal{T}_h),$$

and similarly for $w_{K_j}^h(s)$). Here we use the short-hand notation $u_{K_j}^H = u^H(x_{K_j})$. **The Newton method.** A practical computation of a macroscopic numerical solution relies on a Newton method: consider a sequence $\{u_k^H\}$ such that

$$\partial B_H(u_k^H; u_{k+1}^H - u_k^H, w^H) = F_H(w^H) - B_H(u_k^H; u_k^H, w^H) \ \forall w^H \in S_0^\ell(\Omega, \mathcal{T}_H),$$

where the Fréchet derivative ∂B_H is given by

$$\partial B_{H}(z^{H}; v^{H}, w^{H}) := B_{H}(z^{H}; v^{H}, w^{H})$$

+
$$\sum_{K \in \mathcal{T}_{H}} \sum_{j=1}^{J} \omega_{K_{j}} \frac{d}{ds} a^{0}_{K_{j}}(s)|_{s=z^{H}(x_{K_{j}})} v^{H}(x_{K_{j}}) \nabla z^{H}(x_{K_{j}}) \cdot \nabla w^{H}(x_{K_{j}}).$$

For the implementation we consider $z_k^H = \sum_{i=1}^{M_{macro}} U_k^i \phi_i^H, U_k = (U_k^1, \dots, U_k^{M_{macro}})^T (B(z_k^H) + B'(z_k^H))(U_{k+1} - U_k) = -B(z_k^H)U_k + F.$

The local contribution to the stiffness matrix relies on the matrices
$$B_K(z_k^H)$$
 and $B'_K(z_k^H)$. This latter matrix involves the computation of $\frac{\partial}{\partial s}(B_{K,j}(s))$ that can be approximated by $\frac{\partial}{\partial s}(B_{K,j}(s)) \approx \frac{B_{K,j}(s+\sqrt{eps})-B_{K,j}(s)}{\sqrt{eps}}$. Hence, at each iteration of the Newton method, we have to solve $\mathcal{O}(M_{mac})$ micro problems, where M_{mac} represents the macroscopic degrees of freedom (DOF). Furthermore the a-priori estimates given in [5] indicate that the DOF in each micro problem have to increase as M_{mac} increases.

Reduced basis FE-HMM. In order to reduce the computational complexity of the FE-HMM, we suggest a reduced basis (RB) FE-HMM. The use of RB for numerical homogenization problems has first been proposed in [12] and analyzed for the FE-HMM for a class of linear elliptic problems in [3],[6]. The RB-FE-HMM method is based on offline and online stages. In the offline procedure, accurate micro solutions for the original problem on sampling domains are selected and computed. Theses micro problems are parametrized by the location of the cell problem in the domain Ω and (for nonlinear problems) by the value of the macroscopic solution at this location. We consider a compact subspace \mathcal{D} of $\Omega \times \mathbb{R}$ $(\mathcal{D}$ should be chosen such that $T_{\delta} \subset \Omega$, for all $(x_{\tau}, s) \in \mathcal{D}$). For any randomly chosen parameter we define the map $G_{x_{\tau}}$ from the physical sampling domain $T_{\delta} = x_{\tau} + (-\delta/2, \delta/2)^d$ centered at x_{τ} to the reference domain Y. A greedy algorithm allows to choose an optimal basis of micro functions

$$\hat{S}_N(Y) = \text{span}\{\hat{\xi}_{\mathcal{N},n}(y), n = 1, ..., N\}$$

that is computed with high accuracy for selected values of the parameters.

We note that a crucial ingredient for the Greedy algorithm are appropriate a posteriori error estimates for the construction of the basis of $\hat{S}_N(Y)$. As the precomputed microscopic functions depend nonlinearly on the macroscopic solution, we introduce a new a posteriori error estimator for the Greedy algorithm that guarantees the convergence of the online Newton method and the uniqueness of the method.

In the online stage, the micro problems are then computed in the sampling domains K_{δ_j} as defined above using the reduced basis space (a shifted and scaled version of $\hat{S}_N(Y)$). If one has an "affine" representation of the tensor $a^{\varepsilon}(x,s) =$ $a(x, x/\varepsilon, s) = \sum_{q=1}^{Q} \Theta_q(x, s) a_q(x/\varepsilon)$ then the online micro problems can be computed by solving a small $N \times N$ linear system (essentially pre-assembled in the onfline stage), where N is the dimension of $\hat{S}_N(Y)$ (N is usually small when the RB strategy applies). When the affine representation is not available an interpolation method [11] can be used to approximate the tensor in an affine form.

A priori error estimates in terms of macro, micro, modeling and reduced basis errors have been derived for the RB-FE-HMM applied to quasilinear homogenization problems have been derived in [7], generalizing results for quasilinear problems previously obtained for the FEM [2] and the FE-HMM [5].

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