Abstracts

Reduced basis techniques for multiscale methods

Assyr Abdulle

In this report, we consider reduced basis numerical homogenization methods for the numerical solution of *multiscale* partial differential equations (PDEs) in a domain $\Omega \in \mathbb{R}^d$, $1 \leq d \leq 3$. We will consider two classes of multiscale PDEs. First we consider quasilinear problems: find $u^\varepsilon \in H_0^1(\Omega)$ such that

$$\int_\Omega a^\varepsilon(x, u^\varepsilon)\nabla u^\varepsilon \cdot \nabla w dx = \int_\Omega f w dx \quad \forall\ w \in H_0^1(\Omega), \tag{1}$$

where $f \in L^2(\Omega)$, $a^\epsilon(x,u)$ is a $d \times d$ tensor of Carathéodory type, uniformly elliptic and bounded. Second, we consider Stokes problems in porous media: find $(\mathbf{v}^\varepsilon, p^\epsilon) \in (H_0^1(\Omega_\epsilon))^d \times L^2(\Omega_\epsilon)/\mathbb{R}$ such that

$$\begin{aligned} a(\mathbf{v}^\epsilon, \mathbf{w}) + b(\mathbf{w}, p^\epsilon) &= \int_\Omega \mathbf{f}\cdot\mathbf{w} dx \quad \forall \mathbf{w} \in (H_0^1(\Omega_\epsilon))^d, \\ b(\mathbf{v}^\epsilon, q) &= 0 \quad \forall q \in L^2(\Omega_\epsilon)/\mathbb{R}, \end{aligned} \tag{2}$$

where $\mathbf{f} \in (L^2(\Omega))^d$, $a(\mathbf{v},\mathbf{w}) = \int_{\Omega_\epsilon} \nabla\mathbf{v} : \nabla\mathbf{w} dx$, $b(\mathbf{v}, q) = -\int_{\Omega_\epsilon} q(\nabla\cdot\mathbf{v}) dx$. The multiscale nature of the above PDEs has different sources. For the quasilinear problems, the tensor $a^\varepsilon(x,u^\varepsilon)$ oscillates over a small length scale ϵ. For the Stokes problems, the presence of pore structures (solid parts) of size ϵ makes the fluid domain Ω_ϵ highly heterogeneous. Precisely $\Omega_\epsilon = \Omega \backslash \bigcup_{x\in(1/2+\mathbb{Z})^d} \epsilon(x + \varphi(Y_S; \epsilon x))$, where Y_S is a reference solid domain $\subset \bar{Y}$ with $Y = (-1/2, 1/2)^d$ and $\varphi(\cdot; x)$: $\overline{Y} \to \overline{Y}$ is a homeomorphism such that $\varphi(\cdot;x)|_{\partial Y}$ is an identity for every $x \in \overline{\Omega}$.

Homogenization. For both problems described above, a direct application of a finite element method (FEM) is computationally prohibitive as such a method needs a mesh size $h < \epsilon$ to converge. However, in many applications one is interested in the macroscale behavior of the solution. Such effective equations have been derived for the considered problems. They involve a macroscale partial differential operator. Under suitable assumptions on the data of the problem, it is possible to show that the family of micro solutions converge (usually in a weak sense, up to a subsequence extraction) towards the solution of the macroscale problem. For (1) the homogenized problem reads [11] : find $u \in H_0^1(\Omega)$ such that

$$\int_\Omega a(x,u)\nabla u \cdot \nabla w dx = \int_\Omega f w dx, \quad \forall\ w \in H_0^1(\Omega). \tag{3}$$

The effective equation is of the same type as the microscopic equation, but the oscillating tensor has been replaced by an averaged ϵ independent tensor. For (2) the homogenized problem reads [15, 10]: find $p \in H^1(\Omega)/\mathbb{R}$ such that

$$\int_\Omega a(x)\nabla p \cdot \nabla q dx = \int_\Omega a(x)\mathbf{f}\cdot\nabla q dx, \quad \forall\ q \in H^1(\Omega)/\mathbb{R}, \tag{4}$$

where $a(x)$ is a $d \times d$ conductivity tensor. The effective problem is of Darcy type, the domain does not contain "pore scales" anymore (it has been "homogenized"). For both problems, under suitable assumptions on the oscillatory data (respectively the pore structure), the effective conductivity tensor is recovered at a given point $x \in \Omega$ by solving "micro problems" (PDEs involving the original multiscale problem in a unit reference domain where x enters as a parameter).

A brief description of a numerical homogenization method. Given the problems (1) or (2), the goal is to find a numerical approximation of (3) or (4) involving *a priori unknown* homogenized coefficients ($a(x, u)$, or $a(x)$ for our problems). We describe the finite element heterogeneous multiscale method (FE-HMM) [3, 1, 13] (see [4, 7] for an analysis of problems (1),(2)). It relies on

1. A macroscopic FE solver for the effective (homogenized) problem *with a priori unknown data* $\{a^h(x_{K,j}, u(x_{K,j}))\}_{j=1}^J$ (quasilinear problem), $\{a^h(x_{K,j})\}_{j=1}^J$ (Stokes problem), defined on quadrature points $x_{K,j}$ on each macro element K of a macroscopic partition $\mathcal{T}_H$ of Ω;

2. A microscopic FE solver for "micro" problems based on the differential operators (1) or (2) with right-hand side involving the unit vectors $\{\mathbf{e}_1, \ldots, \mathbf{e}_d\}$ in $\mathbb{R}^d$ on sampling domains $K_{\delta_j} = x_{K,j} + \delta(-1/2, 1/2)^d$, $\delta \geq \epsilon$; the outcome of this step are d FE solutions $\xi^i_{x_{K,j}}, i = 1, \ldots, d$ for each quadrature point $x_{K,j}$ of each element $K \in \mathcal{T}_H$ (for the Stokes micro problems each micro function is a couple of velocity-pressure solutions).

3. A data recovery process in which the effective data $a^h(x_{K,j}, u(x_{K,j}))$, respectively $a^h(x_{K,j})$, at the point $x_{K,j}$ are computed using a suitable average involving the fine scale functions $\xi^i_{x_{K,j}}, i = 1, \ldots, d$ in each K_{δ_j} (for the Stokes problem only the micro velocity (vector) solution enter in the computation of $a^h(x_{K,j})$).

Reduced basis techniques for numerical homogenization. The main computational cost of the FE-HMM comes from the repeated solutions of micro problems around macro quadrature points. One can thus ask if the macroscopic dependence of the micro solutions could be "interpolated" in an appropriate way and if a reduced number of micro solutions could be precomputed and used to compute the effective data at the required quadrature nodes of the macro solver. This question has been addressed for numerical homogenization in the framework of the reduced basis (RB) method [12, 2, 5].

Observe that the effective data computed in the FE-HMM are parameter dependent. For Problem (1) the effective data depend on $x \in \Omega$, on the force field of the micro problems which involves any of the unit vector $\{\mathbf{e}_1, \ldots, \mathbf{e}_d\}$ in $\mathbb{R}^d$ and the value of the unknown (numerically) homogenized solution itself (cheap upper and lower bounds $[u_{low}, u_{up}]$ are available for this solution). For Problem (4) the effective data depend on a set of geometrical parameters $(\mu_1(x), \ldots, \mu_p(x)) \in \mathcal{D} \subset \mathbb{R}^d$ and on the force field of the micro problem $\{\mathbf{e}_1, \ldots, \mathbf{e}_d\}$ in $\mathbb{R}^d$.

A greedy algorithm allows to select (thanks to suitable a posteriori error estimators) among this parameter space an $N-$dimensional set of the parameters for which the corresponding micro functions differ most (measured in a Hilbert norm

corresponding to the PDE). For many problems N turns out to be small. The corresponding $N-$dimensional set of micro functions accurately computed span the reduced basis space. A separation between microscopic variables and parameters variables (either in the tensor for (1) or in the geometry for (4)), called an affine representation is crucial for the efficiency of the Greedy procedure (appropriate interpolation procedures [14] can be applied if this requirement is not satisfied). In an online stage, the precomputed basis (set once for all) is used at the macroscopic quadrature point to compute the actual value of the effective data. Thanks to the affine representation this amounts to solve (small) $N \times N$ linear system (essentially pre-assembled in the offline stage).

A priori error estimates in terms of macro, micro, modeling and reduced basis errors have been derived for the RB-FE-HMM applied to Problems (1) in [6]. An adaptive FE-HMM method for Problem (2) has been analyzed in [7] and reduced basis approximations have been presented in [8, 9].

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Kolmogorov widths and low-rank approximations of parametric elliptic PDEs

Markus Bachmayr
(joint work with Albert Cohen)

We consider parametric diffusion equations

$$-\operatorname{div}_x\big(a(x,y)\nabla u(x,y)\big) = f(x)\,, \quad x \in D \subset \mathbb{R}^m,\ y \in U := [-1,1]^d,$$

with $m, d \in \mathbb{N}$, where the coefficient a has the form $a(x,y) = \bar{a}(x) - \sum_{i=1}^d y_i \psi_i(x)$ and is assumed to satisfy a uniform ellipticity assumption, that is, there exist $0 < r \le R$ such that $0 < r \le a(x,y) \le R < \infty$ for $x \in D$ and $y \in U$. The weak form of this problem on $V := H_0^1(D)$ reads

$$\Big(\bar{A} - \sum_{i=1}^d y_i A_i\Big) u(y) = f\,,$$

where $f \in V'$ and $\bar{A}, A_i \colon V \to V'$, $i = 1, \dots, d$, are defined by

$$\langle \bar{A}u, v\rangle := \int_D \bar{a}\nabla u \cdot \nabla v \, dx\,, \quad \langle A_i u, v\rangle := \int_D \psi_i \nabla u \cdot \nabla v \, dx\,, \qquad u, v \in V\,.$$

Our aim is to study the performance of low-rank approximations of u of the form

$$\sum_{k=1}^n v_k(x)\, \phi_k(y)\,, \tag{1}$$

where the v_k and ϕ_k can be chosen arbitrarily to minimize the error for each n.

Approximations of the type (1) are used implicitly in reduced basis or POD methods and constructed explicitly in methods based on more general tensor decompositions. In all of these approaches, it is of crucial importance that the required number of terms n does not increase too rapidly with a decreasing error tolerance in approximating u. In the reduced basis context, where one is generally interested in uniform error estimates, the relevant measure for assessing the speed of convergence of (1) towards u is the Kolmogorov n-width of $u(U) \subset V$, which is defined for $n \in \mathbb{N}$ by

$$d_n\big(u(U)\big)_V := \inf_{\dim(W)=n} \sup_{y\in U} \min_{w\in W} \|u(y) - w\|_V\,,$$

where we consider u as a map $y \mapsto u(y)$ from U to V. The rank of a $v \in L^2(U,V)$ is defined as the rank of the induced Hilbert-Schmidt operator $\varphi \mapsto \int_U v(y)\,\varphi(y)\,dy$ from $L^2(U)$ to V.

First upper bounds for the n-widths can be obtained from polynomial expansions [1, 2], where the functions ϕ_k are selected from a given basis of tensor product polynomials. However, if the problem has additional structure, one can obtain stronger decay of n-widths when allowing arbitrary ϕ_k.