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Guaranteed upper–lower bounds on homogenized properties by FFT-based Galerkin method

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Abstract

Guaranteed upper–lower bounds on homogenized coefficients, arising from the periodic cell problem, are calculated in a scalar elliptic setting. Our approach builds on the recent variational reformulation of the Moulinec–Suquet (1994) Fast Fourier Transform (FFT) homogenization scheme by Vondřejc et al. (2014), which is based on the conforming Galerkin approximation with trigonometric polynomials. Upper–lower bounds are obtained by adjusting the primal–dual finite element framework developed independently by Dvořák (1993) and Więckowski (1995) to the FFT-based Galerkin setting. We show that the discretization procedure differs for odd and non-odd number of grid points. Thanks to the Helmholtz decomposition inherited from the continuous formulation, the duality structure is fully preserved for the odd discretizations. In the latter case, a more complex primal–dual structure is observed due to presence of the trigonometric polynomials associated with the Nyquist frequencies. These theoretical findings are confirmed with numerical examples. To conclude, the main advantage of the FFT-based approach over conventional finite-element schemes is that the primal and the dual problems are treated on the same basis, and this property can be extended beyond the scalar elliptic setting.

Keywords: Upper–lower bounds; Numerical homogenization; Galerkin approximation; Trigonometric polynomials; Fast Fourier Transform

1. Introduction

This work is dedicated to the determination of guaranteed upper–lower bounds on homogenized (effective) material coefficients originating from the theory of homogenization of periodic media. These bounds, which are essential for the development of reliable multi-scale simulations [1], are calculated with an FFT-based Galerkin approach, a method introduced by the authors in [2] as a variational reformulation of the fast iterative scheme proposed by Suquet and

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Moulinec in [3]. Since our objective is to develop a general methodology, we restrict our attention to scalar linear elliptic problems. Despite this limitation, we believe that our results are relevant to various FFT-based analyses of complex material systems e.g. [4–6, and references therein].

In this introduction, we briefly describe the basic framework of periodic homogenization leading to a cell problem, a variational problem that defines the homogenized matrix. We then discuss possible methods for its numerical treatment with an emphasis on FFT-based schemes and approaches and connect them to techniques for obtaining guaranteed bounds on the homogenized matrix. Finally, we introduce the structure of the paper.

1.1. Periodic cell problem

Using the notation introduced in Section 2, let us consider an open set $\Omega \subset \mathbb{R}^d$ with a Lipschitz boundary and a positive parameter $\varepsilon > 0$ denoting the characteristic size of microstructure. We search for the scalar quantity $u^\varepsilon : \Omega \to \mathbb{R}$, $u^\varepsilon \in H^1_0(\Omega)$, satisfying the variational equation

$$\int_\Omega \big(\boldsymbol{A}^\varepsilon(\boldsymbol{X})\nabla u^\varepsilon(\boldsymbol{X}), \nabla v(\boldsymbol{X})\big)_{\mathbb{R}^d} \,\mathrm{d}\boldsymbol{X} = F(v) \quad \forall v \in H^1_0(\Omega), \tag{1}$$

where $\big(\cdot,\cdot\big)_{\mathbb{R}^d} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ denotes the standard scalar product on $\mathbb{R}^d$. The linear functional $F : H^1_0(\Omega) \to \mathbb{R}$ covers both the prescribed source terms and various boundary conditions, and $\boldsymbol{A}^\varepsilon : \Omega \to \mathbb{R}^{d\times d}$ represents the symmetric, uniformly elliptic, and bounded matrix field of material coefficients, i.e. $\boldsymbol{A}^\varepsilon \in L^\infty(\Omega; \mathbb{R}^{d\times d}_{\mathrm{spd}})$. For the purpose of this work, we focus on periodic media, for which

$$\boldsymbol{A}^\varepsilon(\boldsymbol{X}) = \boldsymbol{A}\left(\frac{\boldsymbol{X}}{\varepsilon}\right) \quad \text{for } \boldsymbol{X} \in \Omega,$$

where the symmetric and uniformly elliptic matrix $\boldsymbol{A} : \mathbb{R}^d \to \mathbb{R}^{d\times d}$ is $\mathcal{Y}$-periodic with $\mathcal{Y} = \prod_{\alpha=1}^d \big(-\frac{Y_\alpha}{2}, \frac{Y_\alpha}{2}\big) \subset \mathbb{R}^d$ denoting the periodic cell, cf. (9). Hence, the coefficients $\boldsymbol{A}^\varepsilon$ develop finer oscillations with a decreasing microstructural parameter ε.

The unique solution to (1) exists thanks to the Lax–Milgram lemma, and thus it can be numerically approximated by, for example, the standard Finite Element Method (FEM). However, in order to obtain a satisfactory approximation, the element size must satisfy $h \ll \varepsilon|\mathcal{Y}| \ll 1$, which renders the direct approach infeasible due to excessive computational demands.

Alternatively, the complexity of (1) can be reduced by homogenization. It involves a limit process for $\varepsilon \to 0$, leading to the decomposition of the problem into the macroscopic and the microscopic parts. This limit passage can be performed by various techniques, such as formal asymptotic expansion [7], two-scale convergence methods [8,9], or periodic unfolding [10]. Irrespective of the method used, we find that the solutions u^ε converge weakly in $H^1_0(\Omega)$ to a limit state u_{H} described by the macroscopic variational equation

$$\int_\Omega \big(\boldsymbol{A}_{\mathrm{H}}\nabla u_{\mathrm{H}}(\boldsymbol{X}), \nabla v(\boldsymbol{X})\big)_{\mathbb{R}^d} \,\mathrm{d}\boldsymbol{X} = F(v) \quad \forall v \in H^1_0(\Omega).$$

Here, $\boldsymbol{A}_{\mathrm{H}} \in \mathbb{R}^{d\times d}_{\mathrm{spd}}$ represents the homogenized matrix of coefficients $\boldsymbol{A}^\varepsilon$ that is described by the microscopic variational formulation defined on the periodic cell $\mathcal{Y}$ only

$$\big(\boldsymbol{A}_{\mathrm{H}}\boldsymbol{E}, \boldsymbol{E}\big)_{\mathbb{R}^d} = \min_{v\in H^1_{\#,\langle 0\rangle}(\mathcal{Y})} \frac{1}{|\mathcal{Y}|}\int_{\mathcal{Y}} \big(\boldsymbol{A}(\boldsymbol{x})[\boldsymbol{E}+\nabla v(\boldsymbol{x})], [\boldsymbol{E}+\nabla v(\boldsymbol{x})]\big)_{\mathbb{R}^d} \,\mathrm{d}\boldsymbol{x}, \tag{2}$$

where $H^1_{\#,\langle 0\rangle}(\mathcal{Y})$ denotes the space of $\mathcal{Y}$-periodic functions with square integrable gradients and zero mean, cf. Section 2, and (2) must hold for any vector $\boldsymbol{E} \in \mathbb{R}^d$.

1.2. FFT-based homogenization methods

The numerical solution of the cell problem (2), particularly an approximation to the homogenized matrix $\boldsymbol{A}_{\mathrm{H}}$, can be carried out by various approaches such as Finite Differences [11–13], Finite Elements [14–16], Boundary Elements [17–19], or Fast Multipole Methods [20–22]. Here, we focus on FFT-based methods, efficient solvers developed for cell problems with coefficients $\boldsymbol{A}$ defined by general high-resolution images.