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 Dvorský (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 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, 5, 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

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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

\[
\int_{\Omega} \left( A^\varepsilon(X) \nabla u^\varepsilon(X), \nabla v(X) \right)_{\mathbb{R}^d} \, dX = F(v) \quad \forall v \in H^1_0(\Omega),
\]

where \( \left( \cdot, \cdot \right)_{\mathbb{R}^d} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d \) 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 \( A^\varepsilon : \Omega \to \mathbb{R}^{d \times d} \) represents the symmetric, uniformly elliptic, and bounded matrix field of material coefficients, i.e. \( A^\varepsilon \in L^\infty(\Omega; \mathbb{R}^{d \times d}) \).

For the purpose of this work, we focus on periodic media, for which

\[
\varepsilon \to 0 \quad \text{infeasible due to excessive computational demands.}
\]

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 \( u^\varepsilon \) converge weakly in \( H^1_0(\Omega) \) to a limit state \( u_H \) described by the macroscopic variational equation

\[
\int_{\Omega} \left( A_H \nabla u_H(X), \nabla v(X) \right)_{\mathbb{R}^d} \, dX = F(v) \quad \forall v \in H^1_0(\Omega).
\]

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

\[
\left( A_H E, E \right)_{\mathbb{R}^d} = \min_{v \in H^1_{0,0}(\mathcal{Y})} \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \left( A(x) |E + \nabla v(x)|^2, |E + \nabla v(x)|^2 \right)_{\mathbb{R}^d} \, dx,
\]

where \( H^1_{0,0}(\mathcal{Y}) \) 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 \( E \in \mathbb{R}^d \).

1.2. FFT-based homogenization methods

The numerical solution of the cell problem [2], particularly an approximation to the homogenized matrix \( A_H \), can be carried out by various approaches such as Finite Differences [11, 12, 13], Finite Elements [14, 15, 16], Boundary Elements [17, 18, 19], or Fast Multipole Methods [20, 21, 22]. Here, we focus on FFT-based methods, efficient solvers developed for cell problems with coefficients \( A \) defined by general high-resolution images.

The original FFT-based formulation proposed by Moulinec and Suquet in [3] is based on an iterative solution to the integral Lippmann-Schwinger equation corresponding to [2] by the Neumann series expansion.
Efficiency of the algorithm is achieved by approximating and evaluating the action of the integral kernel by the Fast Fourier Transform (FFT) algorithm in only $O(N \log N)$ operations, as both the data of the problem and its solution are defined on a regular periodic grid. A theoretical background to the original algorithm has been provided only recently by interpreting the method as a suitable Galerkin scheme and proving the convergence of approximate solutions to the continuous one. In particular, the work of Brisard and Dormieux \cite{23, 24} utilizes the Hashin-Shtrikman variational principles \cite{25} combined with pixel or voxel-wise constant basis functions. Our approach \cite{2} builds on standard variational principles and approximation spaces of trigonometric polynomials together with convergence results, which have been generalized for rough coefficients in \cite{26}. Besides, several improvements of the original solver, leading to faster convergence \cite{27, 28, 29, 30} or higher robustness \cite{31, 32}, have been proposed along with heuristic approaches to increase the accuracy of local fields based on the incorporation of the so-called shape functions \cite{32, 33} or modification of the integral kernel \cite{34}.

The present work is based on our recent study \cite{2}, which shows that the original Moulinec-Suquet scheme is equivalent to a Galerkin discretization of a weak solution to the cell problem \cite{2}, when the approximation space is spanned by trigonometric polynomials and a suitable numerical quadrature scheme is used to evaluate the linear and bilinear forms. We also demonstrated that the system of linear equations arising from the discretization can be efficiently solved with Krylov solvers, cf. \cite{29, 35}, and that the action of the system matrix can be efficiently evaluated by FFT. To minimize technicalities, the analysis was restricted to the primal formulation and to grids with odd number of points along each coordinate.

1.3. Upper and lower bounds on homogenized matrix

The theory of rigorous bounds on the homogenized matrix has been the subject of many studies in analytical homogenization theories. These techniques employ the primal-dual formulations of \cite{2} under limited — and often uncertain — information on the material coefficients $A$. Specific examples include the Voigt \cite{36}, Reuss \cite{37}, and Hashin-Shtrikman bounds \cite{38}; see the monographs \cite{39, 40, 41, 42} for a more complete overview. Because the bounds rely on limited data, their performance rapidly deteriorates for highly-contrasted media.

Relatively less attention has been given to the upper-lower bounds arising from an approximate solution to \cite{2} obtained by a numerical method. To our knowledge, the pioneering work relevant to FEM has been made by Dvóřák and Haslinger \cite{43, 44, 45}, who proposed a general framework for elliptic problems, developed unified primal-dual $p$-version solvers for the two-dimensional scalar equation, and applied them later to the optimal design of matrix-inclusion composites. Error estimates and convergence rates of homogenized properties are provided there together with a reformulation using stream functions which leads to a dual formulation with the same structure as the primal one in the two-dimensional scalar setting. In more general situations, mixed approaches are usually needed to approximate the dual formulation, as demonstrated by Więckowski \cite{46} for linear elasticity.

Let us note that FFT-based bounds on a homogenized properties have also been investigated independently in \cite{47, 48}, utilizing the Brisard-Dormieux approach \cite{23, 24}. In this case, however, the evaluation of guaranteed bounds involves an infinite sum that converges very slowly, and a truncation of the sum violates the structure of the guaranteed bounds; see \cite{2} Section 7 for a related discussion. This limitation is overcome here by a suitable integration rule developed in Section 6.

1.4. Content of the paper

The aim of this paper is twofold. First, we demonstrate that the FFT-Galerkin method is directly applicable to the Dvóřák-Haslinger setting \cite{43, 44, 45} and that it naturally generates primal and dual problems with the same structure. We then extend our results from \cite{2} to general grids by carefully treating the Nyquist frequencies. To this purpose, the paper is organized as follows.

Section 2 summarizes useful facts on periodic functions, the Fourier transform, and the Helmholtz decomposition, which also play a fundamental role in the continuous and discretized primal-dual formulations analyzed throughout the paper.

Section 3 provides a continuous formulation of the homogenization problem together with their main properties. Then the results by Dvóřák \cite{43, 44} are employed. In particular, an abstract duality result is
formulated here in order to cover both continuous and discrete problems, complemented with the theory for accurate upper-lower bounds based on conforming approximations to the homogenization problem.

Section 4 deals with the spaces of trigonometric polynomials [49], which are used to approximate the homogenization problem. Our exposition follows the developments presented in [2] for an odd number of grid points and extends it to the general case.

Section 5 is dedicated to discrete formulations arising from the Galerkin approximation with numerical integration. Here, the emphasis is again on the extension of results in [2] to general grids such that conforming approximations are obtained. The relations between the primal-dual formulations are investigated using the duality arguments from Section 3.1.

Section 6 contributes to methodology for the evaluation of the upper-lower bounds on homogenized properties; the details are provided for general matrix-inclusion composites.

Section 7 gathers several computational aspects with an emphasis on effective implementation.

In this section, we introduce our notation and recall some useful facts related to matrix analysis, Section 2.1, and to spaces of periodic functions and the Fourier transform, Section 2.2, used throughout the paper. Section 2.3 is dedicated to the Helmholtz decomposition of vector-valued periodic functions and its description by orthogonal projections, which will be essential for the duality arguments in both discrete and continuous settings.

Section 8 contains numerical examples that confirm the theoretical findings on the structure of the upper-lower bounds and differences between discretization using odd and even grids. Performance of the method is demonstrated with a real-world material described by a high-resolution image.

Section 9 summarizes the most interesting results, while Appendix A concludes the paper by proving the abstract duality result from Section 3.1.

Let us remark that throughout the paper, we attempt to make a systematic distinction among infinite-dimensional variables, their finite-dimensional approximations, and fully discrete (matrix) representations. Although this approach leads to a somewhat more involved notation, we have found it to be very helpful in understanding the theoretical basis of FFT-based homogenization algorithms as well as connections among the many variants of FFT-based algorithms available in the literature.

2. Notation and preliminaries

In this section, we introduce our notation and recall some useful facts related to matrix analysis, Section 2.1, and to spaces of periodic functions and the Fourier transform, Section 2.2, used throughout the paper. Section 2.3 is dedicated to the Helmholtz decomposition of vector-valued periodic functions and its description by orthogonal projections, which will be essential for the duality arguments in both discrete and continuous settings.

In general, number spaces are denoted with double-struck symbols, e.g., \( \mathbb{N}, \mathbb{Z}, \mathbb{R}, \) or \( \mathbb{C}, \) operators are denoted with calligraphic letters, e.g., \( \mathcal{I}, \mathcal{Q}, \mathcal{P}, \) or \( \mathcal{G}, \) and function spaces are denoted in the standard way, e.g., \( L_2^p(Y), C_0^\infty(Y; \mathbb{R}^d), \) or using a script font, e.g., \( \mathcal{U}, \mathcal{E}, \mathcal{H}, \) or \( \mathcal{F}. \)

2.1. Vectors and matrices

In the sequel, \( d \) is reserved for the dimension of the model problem, assuming \( d = 2, 3. \) To keep the notation compact, \( \mathcal{X} \) abbreviates the space of scalars, vectors, or matrices, i.e., \( \mathbb{R}, \mathbb{R}^d, \) or \( \mathbb{R}^{d \times d}, \) and \( \mathcal{X} \) is used for their complex counterparts, i.e., \( \mathbb{C}, \mathbb{C}^d, \) or \( \mathbb{C}^{d \times d}. \) Vectors and matrices are denoted by boldface letters, e.g., \( \mathbf{u}, \mathbf{v} \in \mathbb{R}^d \) or \( \mathbf{M} \in \mathbb{R}^{d \times d}, \) with Greek letters used when referring to their entries, e.g., \( \mathbf{M} = (M_{\alpha\beta})_{\alpha,\beta=1,..,d}. \)

Matrix \( \mathbf{I} = (\delta_{\alpha\beta})_{\alpha\beta} \) denotes the identity matrix where the symbol \( \delta_{\alpha\beta} \) is reserved for the Kronecker delta, defined as \( \delta_{\alpha\beta} = 1 \) for \( \alpha = \beta \) and \( \delta_{\alpha\beta} = 0 \) otherwise.

As usual, matrix-matrix product \( \mathbf{LM}, \) matrix-vector product \( \mathbf{Mu}, \) and outer product \( \mathbf{u} \otimes \mathbf{v} \) refer to

\[
(LM)_{\alpha\beta} = \sum_\gamma L_{\alpha\gamma} M_{\gamma\beta} \quad (Mu)_\alpha = \sum_\beta M_{\alpha\beta} u_\beta, \quad (u \otimes v)_{\alpha\beta} = u_\alpha v_\beta,
\]

where we assume that \( \alpha \) and \( \beta \) range from 1 to \( d \) for the sake of brevity. Moreover, we endow the spaces with the standard inner products and norms, e.g.,

\[
(v, v)_{\mathbb{C}^d} = \sum_\alpha u_\alpha \overline{v_\alpha}, \quad \|u\|_{\mathbb{C}^d}^2 = (u, u)_{\mathbb{C}^d}, \quad \|M\|_{\mathbb{C}^{d \times d}} = \max_{\mathbf{u} \neq \mathbf{0}} \frac{\|Mu\|_{\mathbb{C}^d}}{\|u\|_{\mathbb{C}^d}}.
\]
The set $\mathbb{R}_{spd}^{d \times d} \subset \mathbb{R}^{d \times d}$ denotes the space of symmetric positive definite matrices satisfying

$$M_{\alpha\beta} = M_{\beta\alpha} \quad \text{for all } \alpha, \beta, \quad (Mu, u)_{\mathbb{R}^d} > 0 \quad \text{for all } u \in \mathbb{R}^d \text{ such that } u \neq 0.$$ 

In this space, the trace operator, $\text{tr} M = \sum_\alpha M_{\alpha\alpha}$ for $M \in \mathbb{R}^{d \times d}$, becomes an equivalent norm to the Frobenius norm, as it equals to the sum of eigenvalues, cf. [50] Section 5.6. The Löwner partial order, cf. [51] Section 7.7, of symmetric positive definite matrices will be found useful, i.e. for $L, M \in \mathbb{R}_{spd}^{d \times d}$ we write

$$L \preceq M \quad \text{if} \quad (Lu, u)_{\mathbb{R}^d} \leq (Mu, u)_{\mathbb{R}^d} \quad \text{for all } u \in \mathbb{R}^d.$$ 

We also systematically use the inverse inequality property

$$L \preceq M \iff M^{-1} \preceq L^{-1} \quad \text{(4)}$$

for $L, M \in \mathbb{R}_{spd}^{d \times d}$, cf. [51] Corollary 7.7.4.(a).

### 2.2. Periodic functions and Fourier transform

We consider cells in the form $Y = \prod_\alpha \left(-\frac{Y_\alpha}{2}, \frac{Y_\alpha}{2}\right)$ for $Y \in \mathbb{R}^d$ such that $Y_\alpha > 0$. Then, a function $u : \mathbb{R}^d \to \mathbb{X}$ is $Y$-periodic if

$$u(x + \sum_\alpha Y_\alpha k_\alpha) = u(x) \quad \text{for all } x \in Y \text{ and all } k \in \mathbb{Z}^d.$$

The space $C_#(Y; \mathbb{X})$ collects all continuous $Y$-periodic functions $\mathbb{R}^d \to \mathbb{X}$. For $p \in \{2, \infty\}$,

$$L^p_#(Y; \mathbb{X}) = \left\{ u : Y \to \mathbb{X} : u \text{ is } Y \text{-periodic, measurable, and } \|u\|_{L^p_#(Y; \mathbb{X})} < \infty \right\} \quad \text{(5)}$$

denotes the Lebesgue spaces equipped with the norm

$$\|u\|_{L^p_#(Y; \mathbb{X})} = \begin{cases} \text{ess sup}_{x \in Y} \|u(x)\|_\mathbb{X} & \text{for } p = \infty, \\ \left( |Y|^{-1} \int_Y \|u(x)\|_\mathbb{X}^p \, dx \right)^{1/p} & \text{for } p = 2, \end{cases}$$

where $|Y| = \prod_\alpha Y_\alpha$ denotes the Lebesgue measure of the cell $Y$.

For the sake of brevity, we write $L^p_#(Y)$ instead of $L^p_#(Y; \mathbb{R}^d)$, and often shorten $L^2_#(Y; \mathbb{R}^d)$ to $L^2_#$ when referring to the norms and the inner product.

The Fourier transform of $u \in L^2_#(Y; \mathbb{X})$ is given by

$$\hat{u}(k) = \frac{1}{|Y|} \int_Y u(x) \varphi_{-k}(x) \, dx \in \mathbb{X} \quad \text{for } k \in \mathbb{Z}^d,$$

where the Fourier trigonometric polynomials,

$$\varphi_k(x) = \exp \left( 2\pi i \langle \xi(k), x \rangle_{\mathbb{R}^d} \right) \quad \text{for } x \in Y, k \in \mathbb{Z}^d,$$

form an orthonormal basis $\{\varphi_k\}_{k \in \mathbb{Z}^d}$ of $L^2_#(Y)$, i.e.

$$\langle \varphi_k, \varphi_m \rangle_{L^2_#(Y)} = \delta_{km} \quad \text{for } k, m \in \mathbb{Z}^d, \quad \text{(6)}$$

cf. [51] pp. 89–91. Thus, every function $u \in L^2_#(Y; \mathbb{X})$ can be expressed in the form

$$u(x) = \sum_{k \in \mathbb{Z}^d} \hat{u}(k) \varphi_k(x) \quad \text{for } x \in Y.$$
The space \( L^2_\#(\mathcal{Y}; \mathbb{R}^d) \) is also a Hilbert space with the inner product
\[
\langle u, v \rangle_{L^2_\#(\mathcal{Y}; \mathbb{R}^d)} = \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} (u(x), v(x))_{\mathbb{R}^d} \, dx = \sum_{k \in \mathbb{Z}^d} \langle \hat{u}(k), \hat{v}(k) \rangle_{\mathbb{C}^d},
\]
which can be expressed, thanks to Parseval’s theorem, in both original and Fourier spaces.

The mean value of function \( u \in L^2_\#(\mathcal{Y}; \mathbb{R}) \) over periodic cell \( \mathcal{Y} \) is denoted as
\[
\langle u \rangle = \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} u(x) \, dx = \hat{u}(0) \in \mathbb{R}
\]
and corresponds to the zero-frequency Fourier coefficient.

2.3. Helmholtz decomposition for periodic functions

Operator \( \oplus \) denotes the direct sum of mutually orthogonal subspaces, e.g. \( \mathbb{R}^d = U^{(1)} \oplus U^{(2)} \oplus \ldots \oplus U^{(d)} \) for vectors \( U^{(a)} = (\delta_{\alpha,b})_b \). By the Helmholtz decomposition [52] pages 6–7, \( L^2_\#(\mathcal{Y}; \mathbb{R}^d) \) admits an orthogonal decomposition
\[
L^2_\#(\mathcal{Y}; \mathbb{R}^d) = \mathcal{W} \oplus \mathcal{E} \oplus \mathcal{J} \tag{7}
\]
into the subspaces of constant, zero-mean curl-free, and zero-mean divergence free fields
\[
\mathcal{W} = \{ v \in L^2_\#(\mathcal{Y}; \mathbb{R}^d) : v(x) = \langle v \rangle \text{ for all } x \in \mathcal{Y} \}, \tag{8a}
\mathcal{E} = \{ v \in L^2_\#(\mathcal{Y}; \mathbb{R}^d) : \text{curl} \, v = 0, \langle v \rangle = 0 \}, \tag{8b}
\mathcal{J} = \{ v \in L^2_\#(\mathcal{Y}; \mathbb{R}^d) : \text{div} \, v = 0, \langle v \rangle = 0 \}. \tag{8c}
\]
Here, the differential operators curl and div are understood in the Fourier sense, so that
\[
(\text{curl} \, u)_{\alpha \beta} = \sum_{k \in \mathbb{Z}^d} 2\pi i (\xi_\beta(k) \hat{u}_\alpha(k) - \xi_\alpha(k) \hat{u}_\beta(k)) \varphi_k, \quad \text{div} \, u = \sum_{k \in \mathbb{Z}^d} 2\pi i (\xi(k), \hat{u}(k))_{\mathbb{C}^d} \varphi_k,
\]
cf. [52] pp. 2–3 and [49]. Furthermore, the constant functions from \( \mathcal{W} \) are identified with vectors from \( \mathbb{R}^d \).

Alternatively, the subspaces arising in the Helmholtz decomposition (8) can be characterized by the orthogonal projections introduced next.

**Definition 1.** Let \( G^\mathcal{W}, G^\mathcal{E}, \text{ and } G^\mathcal{J} \) denote operators \( L^2_\#(\mathcal{Y}; \mathbb{R}^d) \to L^2_\#(\mathcal{Y}; \mathbb{R}^d) \) defined via
\[
G^\bullet[v](x) = \sum_{k \in \mathbb{Z}^d} \hat{G}^\bullet(k) \hat{v}(k) \varphi_k(x) \quad \text{for } \bullet \in \{ \mathcal{W}, \mathcal{E}, \mathcal{J} \},
\]
where the matrices of Fourier coefficients \( \hat{G}^\bullet(k) \in \mathbb{R}^{d \times d} \) read
\[
\hat{G}^\mathcal{W}(k) = \begin{cases} I & \text{for } k = 0 \\ 0 & \text{for } k \in \mathbb{Z}^d \setminus \{0\} \end{cases}, \quad \hat{G}^\mathcal{E}(k) = \begin{cases} 0 \otimes 0 & \text{for } k = 0 \\ \frac{\xi(k) \otimes \xi(k)}{(\xi(k), \xi(k))_{\mathbb{C}^d}} & \text{for } k \in \mathbb{Z}^d \setminus \{0\} \end{cases},
\]
\[
\hat{G}^\mathcal{J}(k) = \begin{cases} 0 \otimes 0 & \text{for } k = 0 \\ I - \frac{(\xi(k), \xi(k))_{\mathbb{C}^d}}{(\xi(k), \xi(k))_{\mathbb{C}^d}} & \text{for } k \in \mathbb{Z}^d \setminus \{0\} \end{cases}.
\]

**Lemma 2.** The operators \( G^\mathcal{W}, G^\mathcal{E}, \text{ and } G^\mathcal{J} \) are mutually orthogonal projections with respect to the inner product on \( L^2_\#(\mathcal{Y}; \mathbb{R}^d) \), on \( \mathcal{W}, \mathcal{E}, \text{ and } \mathcal{J} \).

**Proof.** In [2] Lemma 3.2), we show in detail that \( G^\mathcal{E} \) is an orthogonal projection onto \( \mathcal{E} \). The remaining cases follow from the mutual orthogonality of \( \hat{G}^\mathcal{W}(k) : \mathbb{C}^d \to \mathbb{C}^d \) for all \( k \in \mathbb{Z}^d \) and with \( \bullet \in \{ \mathcal{W}, \mathcal{E}, \mathcal{J} \} \), cf. [39] Section 12.1]. \( \square \)
3. Homogenization, duality, and upper-lower bounds

In the present section, we define homogenized matrices via variational problems and collect several useful facts about their evaluation in the primal and the dual formulations. The connection between the matrices is established in Section 3.1 using duality arguments, which immediately provide their basic properties along with the Voigt-Reuss bounds in Section 3.2. Section 3.3 is dedicated to the determination of accurate upper-lower bounds based on conforming primal-dual minimizers, following the earlier developments by Dvorský [13, 44].

Here and in the sequel, matrix field $A : \mathcal{Y} \to \mathbb{R}^{d \times d}$ is reserved for material coefficients, which are required to be essentially bounded, symmetric, and uniformly elliptic

$$A \in L_\#^\infty(\mathcal{Y}; \mathbb{R}^{d \times d})$$

a.e. in $\mathcal{Y}$ for all $v \in \mathbb{R}^d$ with $0 < c_A \leq C_A < +\infty$; by [4] the inverse coefficients satisfy

$$A^{-1} \in L_\#^\infty(\mathcal{Y}; \mathbb{R}^{d \times d})$$

a.e. in $\mathcal{Y}$ for all $v \in \mathbb{R}^d$. We will also consider bilinear forms $a : L_\#^2(\mathcal{Y}; \mathbb{R}^d) \times L_\#^2(\mathcal{Y}; \mathbb{R}^d) \to \mathbb{R}$ and $a^{-1} : L_\#^2(\mathcal{Y}; \mathbb{R}^d) \times L_\#^2(\mathcal{Y}; \mathbb{R}^d) \to \mathbb{R}$ provided by

$$a(u, v) := (A(u, v))_{L_\#^2(\mathcal{Y}; \mathbb{R}^d)}$$

$$a^{-1}(u, v) := (A^{-1}(u, v))_{L_\#^2(\mathcal{Y}; \mathbb{R}^d)}$$

together with energetic norms

$$\|u\|_A := \sqrt{a(u, u)}$$

$$\|u\|_{A^{-1}} := \sqrt{a^{-1}(u, u)}.$$

**Definition 3** (Homogenized matrices). Let the coefficient $A$ satisfy [9]. Then the primal and dual homogenized matrices $A_H, B_H \in \mathbb{R}^{d \times d}$ are defined as

$$(A_H E, E)_{\mathbb{R}^d} = \min_{e \in \mathcal{E}} a(E + e, E + e) = a(E + e(E), E + e(E)),$$

$$(B_H J, J)_{\mathbb{R}^d} = \min_{j \in \mathcal{J}} a^{-1}(J + j, J + j) = a^{-1}(J + j(J), J + j(J)).$$

for arbitrary $E, J \in \mathbb{R}^d$.

**Remark 4.** The minimizers $e^{(E)}$ and $j^{(J)}$, thanks to the Lax-Milgram lemma, exist, are unique for any $E, J \in \mathbb{R}^d$, and satisfy the optimality conditions

$$a(e^{(E)}, v) = -a(E, v) \quad \forall v \in \mathcal{E},$$

$$a^{-1}(j^{(J)}, v) = -a^{-1}(J, v) \quad \forall v \in \mathcal{J}.$$

**Remark 5.** Notice that the primal formulation (11a) coincides with problem (2) introduced in Section 7 because the subspace $\mathcal{E}$ from (8b) admits an equivalent characterization $\mathcal{E} = \{\nabla f : f \in H_{\#,0}^1(\mathcal{Y})\}$, cf. [52, pp. 6–7].

3.1. Duality

In this section, the homogenized matrices and their formulations (11) are connected by standard duality arguments. These ideas are summarized into a proposition that is applicable to both the continuous homogenization problem (11) and also to its discrete relatives (52) and (54). In Appendix A in order to keep the exposition self-contained, we also provide its proof.
Proposition 6 (Transformation to dual formulation). Let $\mathcal{H}$ be a Hilbert space with a nontrivial orthogonal decomposition $\mathcal{H} = \mathcal{U} \oplus \mathcal{E} \oplus \mathcal{F}$, where $\mathcal{U}$ is isometrically isomorphic to $\mathbb{R}^d$. Next, let bilinear forms $\hat{a} : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ and $\hat{a}^{-1} : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ be defined as

$$\hat{a}(u, v) = (Au, v)_{\mathcal{H}}, \quad \hat{a}^{-1}(u, v) = (A^{-1}u, v)_{\mathcal{H}}$$

for symmetric, coercive, and bounded linear operator $A : \mathcal{H} \to \mathcal{H}$, so that there exist $c_A > 0$ and $C_A > 0$ such that

$$c_A\|u\|_{\mathcal{H}} \leq (A u, u)_{\mathcal{H}} \leq C_A\|u\|_{\mathcal{H}}.$$

Then matrices $\hat{A}_H, \hat{B}_H \in \mathbb{R}^{d \times d}$ defined as

$$\begin{align*}
(\hat{A}_H E, E)_{\mathbb{R}^d} &= \min_{\hat{e} \in \mathcal{E}} \hat{a}(E + \hat{e}, E + \hat{e}) = \hat{a}(E + \hat{e}(E), E + \hat{e}(E)) \\
(\hat{B}_H J, J)_{\mathbb{R}^d} &= \min_{\hat{j} \in \mathcal{F}} \hat{a}^{-1}(J + \hat{j}, J + \hat{j}) = \hat{a}^{-1}(J + \hat{j}(J), J + \hat{j}(J))
\end{align*} \tag{12}$$

for arbitrary $E, J \in \mathbb{R}^d$ satisfy

$$A_H = \hat{B}_H^{-1}. \tag{13}$$

Moreover, the minimizers $\hat{e}(E)$ and $\hat{j}(J)$ of both formulations $\text{(12)}$ are connected via

$$J + \hat{j}(J) = A[H + \hat{e}(E)] \quad \text{for } J = A_H E \text{ and } E \in \mathbb{R}^d. \tag{14}$$

Remark 7. The decomposition $\mathcal{H} = \mathcal{U} \oplus \mathcal{E} \oplus \mathcal{F}$ fits either to the standard Helmholtz framework $\text{(7)}$ or to its fully discrete variants $\text{(11)}$ and $\text{(15)}$. Note that, to be defined properly, the bilinear forms $\text{(12)}$ for $E, J \in \mathbb{R}^d$ are understood as

$$\hat{a}(E + \hat{e}, E + \hat{e}) := \hat{a}(I^{-1}[E] + \hat{e}, I^{-1}[E] + \hat{e}), \quad \hat{a}^{-1}(J + \hat{j}, J + \hat{j}) := \hat{a}^{-1}(I^{-1}[J] + \hat{j}, I^{-1}[J] + \hat{j}),$$

with the help of the isometric isomorphism $I : \mathcal{U} \to \mathbb{R}^d$, which is natural for spaces $\mathbb{R}^d$ and $\mathcal{U}$, see also Remark $\text{[3]}$ later in this paper.

Properties of primal and dual homogenization problems $\text{(11)}$ now follow as a corollary to Proposition $\text{6}$.

Corollary 8. The homogenized matrices in $\text{(11)a}$ and $\text{(11b)}$ are mutually inverse

$$A_H = B_H^{-1}. \tag{15}$$

Moreover, the minimizers are connected by

$$J + \hat{j}(J) = A(E + \hat{e}(E)) \quad \text{for } J = A_H E \text{ and } E \in \mathbb{R}^d. \tag{15}$$

Proof. The proof is a direct consequence of Proposition $\text{6}$ for

$$\mathcal{H} = \mathcal{U} \oplus \mathcal{E} \oplus \mathcal{F}, \quad L^2_{\mathbb{R}}(Y; \mathbb{R}^d) = \mathcal{U} \oplus \mathcal{E} \oplus \mathcal{F},$$

and

$$\hat{a} = a, \quad \hat{a}^{-1} = a^{-1}, \quad \hat{A}_H = A_H, \quad \hat{B}_H = B_H, \quad \hat{e}(E) = e(E), \quad \hat{j}(J) = j(J).$$
3.2. Comments on the homogenized properties and their calculation

Remark 9. The homogenized matrix $A_H \in \mathbb{R}^{d \times d}$ is symmetric positive definite and thus regular, as follows from standard arguments in homogenization theory, e.g., [7, 52, 53]. Indeed, thanks to the coercivity of coefficients [9], the quadratic form in (11) is nonnegative and equals to zero only for $e$ such that $(E + e) \equiv 0$, which is impossible because the space $\mathcal{J}$ does not contain constant fields. This implies the positive definiteness of matrix $A_H$, while its symmetry is inherited from the symmetry of coefficients [9] and consequently of the bilinear form $a$, cf. (17). In addition, the homogenized matrix satisfy Voigt [30] and Reuss [37] bounds

$$(A^{-1})^{-1} \preceq B_H^{-1} = A_H \preceq (A)$$

obtained from the equivalence [4] and the formulations in [11] tested with $e = j = 0$. The lower bound also provides another proof of the positive definiteness of homogenized matrix $A_H$.

Some additional notation is needed to analyze the homogenization problem (11) in more detail. By linearity, the solutions to (11) can be fully characterized by solutions to $d$ auxiliary problems, obtained by successively setting $E$ and $J$ equal to the basis vectors of $\mathbb{R}^d$.

Definition 10 (Auxiliary problems). The auxiliary minimizers $e^{(\alpha)} \in \mathcal{E}$ and $j^{(\alpha)} \in \mathcal{J}$ satisfy

$$a(e^{(\alpha)}, v) = -a(U^{(\alpha)}, v) \quad \forall v \in \mathcal{E},$$
$$a^{-1}(j^{(\alpha)}, v) = -a^{-1}(U^{(\alpha)}, v) \quad \forall v \in \mathcal{J}$$

with $U^{(\alpha)} = (\delta_{\alpha\beta})_\beta \in \mathbb{R}^d$.

Now, the minimizers $e^{(E)} \in \mathcal{E}$ and $j^{(J)} \in \mathcal{J}$ for $E, J \in \mathbb{R}^d$, recall Definition 3 can be obtained from the auxiliary minimizers by linear superposition

$$e^{(E)} = \sum_\alpha E_\alpha e^{(\alpha)}, \quad j^{(J)} = \sum_\alpha J_\alpha j^{(\alpha)},$$

and the components of the homogenized matrix can be expressed as

$$A_{H,\alpha\beta} = a(U^{(\beta)} + e^{(\beta)}, U^{(\alpha)} + e^{(\alpha)}), \quad B_{H,\alpha\beta} = a^{-1}(U^{(\beta)} + j^{(\beta)}, U^{(\alpha)} + j^{(\alpha)}).$$

Using (15), the dual auxiliary minimizer $j^{(\alpha)}$ can be expressed as a linear combination of primal ones $e^{(\alpha)}$, thus

$$U^{(\alpha)} + j^{(\alpha)} = A \sum_\alpha E_\alpha (U^{(\alpha)} + e^{(\alpha)}) \quad \text{where } E = A_H^{-1}U^{(\alpha)}.$$

3.3. Upper-lower bounds on the homogenized properties

Following Dvořák [33, 11], the aim of the present section is to obtain guaranteed bounds on the homogenized matrix $A_H$ by utilizing a suitable conforming approximations

$$e^{(\alpha)}_h \in \mathcal{E} \quad \text{and} \quad j^{(\alpha)}_h \in \mathcal{J},$$

as test fields in (11). Here, $h$ represents a discretization parameter related to the maximum element size for FEM or grid spacing for FFT-based methods.

Definition 11 (Upper-lower bounds on homogenized matrix, [13]). Matrices $\overline{A}_{H,h}, \overline{B}_{H,h} \in \mathbb{R}^{d \times d}$ defined as

$$\overline{A}_{H,h,\alpha\beta} = a(U^{(\beta)} + e^{(\beta)}_h, U^{(\alpha)} + e^{(\alpha)}_h), \quad \overline{B}_{H,h,\alpha\beta} = a^{-1}(U^{(\beta)} + j^{(\beta)}_h, U^{(\alpha)} + j^{(\alpha)}_h)$$

are guaranteed upper-lower bounds on the homogenized matrix $A_H$. The mean of guaranteed bounds with a guaranteed error stands for

$$\overline{A}_{H,h} = \frac{1}{2}(\overline{A}_{H,h} + \overline{B}_{H,h}^{-1}), \quad D_h = \frac{1}{2}(\overline{A}_{H,h} - \overline{B}_{H,h})^{-1}.$$
The correctness of this definition is demonstrated with the following lemma.

**Lemma 12.** The matrices from Definition 7 are symmetric positive definite and satisfy the upper-lower bounds structure

\[ A_H \preceq \overline{A}_{H,h}, \quad B_H \preceq \overline{B}_{H,h}, \quad \overline{B}_{H,h}^{-1} \preceq B_H = A_H \preceq \overline{A}_{H,h}. \] \tag{21}

Moreover, the previous bounds imply the element-wise bounds for diagonal components

\[ (\overline{B}_{H,h}^{-1})_{\alpha\alpha} \leq (B_H^{-1})_{\alpha\alpha} = (A_H)_{\alpha\alpha} \leq (\overline{A}_{H,h})_{\alpha\alpha}, \] \tag{22}

and for non-diagonal components, i.e., for \( \alpha \neq \beta \)

\[ \overline{A}_{H,h,\alpha\beta} - D_{h,\alpha\alpha} - D_{h,\beta\beta} \leq A_{H,\alpha\beta} \leq \overline{A}_{H,h,\alpha\beta} + D_{h,\alpha\alpha} + D_{h,\beta\beta}. \] \tag{23}

**Proof.** The first two inequalities in (21) are the consequence of minimality properties of primal and dual homogenized matrices \( A_H \) and \( B_H \) according to Definition 3 tested with conforming approximations (18), i.e., \( e_h^j(\cdot) \in \mathcal{E} \) and \( j = j_h^j(\cdot) \in \mathcal{J} \). The last inequality in (21) is a consequence of property (4).

The symmetry of the upper-lower bounds \( A_{H,h}, B_{H,h} \) follows from the symmetry of bilinear forms in (19), and the positive definiteness is shown by (21) once recalling that \( A_H \in \mathbb{R}^{d\times d}_{spd} \).

The estimate of the diagonal terms (22) results from the inequality (21) tested with \( U^{(\alpha)} \). For the non-diagonal terms, we have

\[ 2A_{H,\alpha\beta} = (A_H(U^{(\alpha)} + U^{(\beta)}), U^{(\alpha)} + U^{(\beta)})_{\mathbb{R}^d} - A_{H,\alpha\alpha} - A_{H,\beta\beta}. \]

The first inequality in (21) tested with \( U^{(\alpha)} + U^{(\beta)} \) provides

\[ (A_H(U^{(\alpha)} + U^{(\beta)}), U^{(\alpha)} + U^{(\beta)})_{\mathbb{R}^d} \leq (\overline{A}_{H,h}(U^{(\alpha)} + U^{(\beta)}), (U^{(\alpha)} + U^{(\beta)})_{\mathbb{R}^d}). \]

Utilizing the inequalities for diagonal components (22), we obtain the upper estimate in (23). The lower bound follows by analogous arguments.

Now, we establish the relations among auxiliary minimizers (18), homogenized matrices (19), and guaranteed error (20).

**Lemma 13 (Estimates).** The following relations hold

\[ \|e^{(\alpha)} - e_h^{(\alpha)}\|^2_A = \overline{A}_{H,h,\alpha\alpha} - A_{H,\alpha\alpha}, \quad \|j^{(\alpha)} - j_h^{(\alpha)}\|^2_{A^{-1}} = \overline{B}_{H,h,\alpha\alpha} - B_{H,\alpha\alpha} \] \tag{24}

\[ 2\text{tr} D_h \leq \sum_{\alpha} \|e^{(\alpha)} - e_h^{(\alpha)}\|^2_A + (\text{tr} A_H)^2 \|j^{(\alpha)} - j_h^{(\alpha)}\|^2_{A^{-1}} \]

\[ \leq \|A\|_{L^\infty_{\mathbb{R}^d}(\mathbb{R}^d;\mathbb{R}^d)} \sum_{\alpha} \|e^{(\alpha)} - e_h^{(\alpha)}\|^2_{L^2} + (\text{tr} A_H)^2 \|A^{-1}\|_{L^\infty_{\mathbb{R}^d}(\mathbb{R}^d;\mathbb{R}^d)} \sum_{\alpha} \|j^{(\alpha)} - j_h^{(\alpha)}\|^2_{L^2}. \] \tag{25}

**Proof.** The proof of the estimates (24) is shown only for the primal formulation, the dual case proceeds by analogy. Denoting \( e^{(\alpha)} := (U^{(\alpha)} + e^{(\alpha)}) \) and \( e_h^{(\alpha)} := (U^{(\alpha)} + e_h^{(\alpha)}) \), we obtain

\[ \|e^{(\alpha)} - e_h^{(\alpha)}\|^2 = a(e^{(\alpha)} - e_h^{(\alpha)}, e^{(\alpha)} - e_h^{(\alpha)}) = a(e^{(\alpha)}, e^{(\alpha)}) - 2a(e^{(\alpha)}, e_h^{(\alpha)}) + a(e_h^{(\alpha)}, e_h^{(\alpha)}) \]

\[ = a(e^{(\alpha)}, e^{(\alpha)}) - 2a(e^{(\alpha)}, e^{(\alpha)}) + a(e_h^{(\alpha)}, e_h^{(\alpha)}) = \overline{A}_{H,h,\alpha\alpha} - A_{H,\alpha\alpha}, \]

where we have incorporated the Galerkin orthogonality of auxiliary problem (16a) tested with \( e_h^{(\alpha)} \) and \( e^{(\alpha)} \), from which it follows

\[ a(U^{(\alpha)} + e^{(\alpha)}, U^{(\alpha)} + e_h^{(\alpha)}) = a(U^{(\alpha)} + e^{(\alpha)}, U^{(\alpha)}) = a(U^{(\alpha)} + e^{(\alpha)}, U^{(\alpha)} + e^{(\alpha)}). \]
The estimate for the guaranteed error [25] utilizes the fact that
\[
0 \leq \text{tr}(D - C) \leq \text{tr}[D(C^{-1} - D^{-1})C] \leq \text{tr} D \text{tr}(C^{-1} - D^{-1}) \text{tr} C \\
\leq (\text{tr} D)² \text{tr}(C^{-1} - D^{-1})
\]
holding for \( C, D \in \mathbb{R}^{d \times d} \) such that \( C \preceq D \). This inequality and [24] enable us to calculate
\[
2 \text{tr} D_h = \text{tr} (\mathbf{A}_H h - A_h) + \text{tr} (A_H - B_{H,h}) \leq \text{tr} (\mathbf{A}_H h - A_h) + (\text{tr} A_H)^2 \text{tr} (B_H - B_{H,h}) \\
\leq \sum_{\alpha} \| e^{(\alpha)} - e_h^{(\alpha)} \|^2_{A_h} + (\text{tr} A_H)^2 \sum_{\alpha} \| j^{(\alpha)} - j_h^{(\alpha)} \|^2_{A^{-1}},
\]
and the proof is completed with the Hölder inequality. \(\square\)

4. Trigonometric polynomials and their fully discrete counterparts

This section provides an introduction to discretization of the homogenization problem [11] using trigonometric polynomials defined on a regular grid with \( N \in \mathbb{N}^d \) points, with \( N_\alpha \) points along each Cartesian axis. Suitability of such approximations has been demonstrated in [2], following the general framework of Saranen and Vainikko [49], but only for the odd number of grid points
\[
N \in \mathbb{N}^d \text{ and } N_\alpha \text{ is odd for all } \alpha.
\] (26)

This assumption is often referred to as odd grid; non-odd or even grids are used accordingly. Obviously, [25] is restrictive from the applications point of view, so in this section we extend our earlier results from [24] to the general case. Note the difficulty in working with non-odd number of grid points was identified and partially solved in [24], Section 2.4.2] by heuristic arguments. Here, we refine this result in a way to preserve the structure of upper-lower bounds on the homogenized matrix established in Section 3.3.

This section begins with a brief notation part in Section 4.1 complemented with the basic properties of trigonometric polynomials in Section 4.2. The fully discrete representation of trigonometric polynomials is introduced in Section 4.3 and 4.4 for odd and general number of grid points, respectively.

4.1. Notation

A multi-index notation is systematically employed, in which \( X^N \) represents \( X_1^{N_1} \times \cdots \times X_d^{N_d} \) for \( N \in \mathbb{N}^d \). Then the sets \( \mathbb{R}^{d \times N} \) and \( \mathbb{R}^{d \times N}^2 \), or their complex counterparts \( \mathbb{C}^{d \times N} \) and \( \mathbb{C}^{d \times N}^2 \), represent the spaces of vectors and matrices, e.g. \( \mathbf{v} = (v_{\alpha}^{(k)})_{k \in \mathbb{Z}^d} \in \mathbb{R}^{d \times N} \) and \( \mathbf{M} = (M_{\alpha \beta}^{k,n})_{k,n \in \mathbb{Z}^d} \in \mathbb{R}^{d \times N}^2 \) with an index set \( \mathbb{Z}_d = \mathbb{Z}^d \) introduced subsequently in [28]. The objects of these discrete spaces are indicated by bold serif font, e.g. \( \mathbf{u} \) and \( \mathbf{M} \), in order to distinguish them from scalars \( u_\alpha \in \mathbb{R} \) for \( \alpha = 1, \ldots, d \), vectors \( \mathbf{u} \in \mathbb{R}^d \), scalar-valued functions \( v \in L_2^d(Y) \), or vector-valued functions \( \mathbf{w} \in L_2^d(Y; \mathbb{R}^d) \).

Sub-vectors and sub-matrices are designated by superscripts, e.g. \( \mathbf{v}^k = (v_{\alpha}^{(k)})_{\alpha \in \mathbb{R}^d} \in \mathbb{R}^{d \times N} \) or \( \mathbf{M}^{k,m} = (M_{\alpha \beta}^{k,m})_{\alpha,\beta \in \mathbb{R}^d} \in \mathbb{R}^{d \times d} \). The inner products on \( \mathbb{R}^{d \times N} \) and \( \mathbb{C}^{d \times N} \) are defined as
\[
(\mathbf{u}, \mathbf{v})_{\mathbb{R}^{d \times N}} = \frac{1}{|N|} \sum_{k \in \mathbb{Z}_d^d} (u^k, v^k)_{\mathbb{R}^d}, \quad (\mathbf{u}, \mathbf{v})_{\mathbb{C}^{d \times N}} = \sum_{k \in \mathbb{Z}_d^d} (u^k, v^k)_{\mathbb{C}^d},
\]
where \( |N| = \prod_\alpha N_\alpha \), stand for the number of grid points.

Moreover, the matrix-vector or matrix-matrix multiplications follow from
\[
(\mathbf{Mv})^k = \sum_{m \in \mathbb{Z}_d^d} M_{k,m} v^m \in \mathbb{R}^d \quad \text{or} \quad (\mathbf{ML})^{k,m} = \sum_{l \in \mathbb{Z}_d^d} M_{k,l} L_{l,m} \in \mathbb{R}^{d \times d}
\]
for \( k, m \in \mathbb{Z}_N^d \) and \( L \in \mathbb{R}^{d \times d} \). The identity operator on \( \mathbb{R}^{d \times N} \) corresponds to a matrix

\[
I = (\delta_{\alpha \beta} \delta_{km})_{\alpha, \beta, k, m} \in \mathbb{R}^{d \times d} \]

and a matrix \( A \in \mathbb{R}^{d \times N} \) is symmetric positive definite if

\[
(Au, v)_{\mathbb{R}^{d \times N}} = (u, Av)_{\mathbb{R}^{d \times N}}, \quad (Av, v)_{\mathbb{R}^{d \times N}} > 0
\]

holds for all \( u, v \in \mathbb{R}^{d \times N} \) such that \( v \neq 0 \).

### 4.2. Trigonometric polynomials

This section extends the results from [2, Section 4.1] for vector-valued trigonometric polynomials defined on grids with an odd number of points \( 26 \) to the general case. In order to facilitate the introduction of the fully discrete spaces in Sections 4.3 and 4.4, we also review the simplifications arising from the odd grid assumption \( 26 \).

**Definition 14** (Trigonometric polynomials). For \( N \in \mathbb{N}^d \), approximation and interpolation spaces of \( \mathbb{R}^d \)-valued trigonometric polynomials are defined by

\[
T_N^d = \left\{ \sum_{k \in \mathbb{Z}_N^d} \hat{v}_k \psi_k : \hat{v}_k = (\hat{v}_{-k})^T \in \mathbb{C}^d \right\} , \quad (27a)
\]

\[
\tilde{T}_N^d = \left\{ \sum_{k \in \mathbb{Z}_N^d} v_k \varphi_{N,k} : v_k \in \mathbb{R}^d \right\} , \quad (27b)
\]

where a reduced and a full index sets stand for

\[
\mathbb{Z}_N^d = \left\{ k \in \mathbb{Z}^d : -\frac{N_\alpha}{2} \leq k_\alpha < \frac{N_\alpha}{2} \right\} , \quad \mathbb{Z}^d = \left\{ k \in \mathbb{Z}^d : -\frac{N_\alpha}{2} \leq k_\alpha \leq \frac{N_\alpha}{2} \right\} , \quad (28)
\]

and the spaces \( T_N^d \) and \( \tilde{T}_N^d \) are spanned by the Fourier and fundamental trigonometric polynomials, respectively:

\[
\varphi_k(x) = \exp \left( 2\pi i \sum_{\alpha} \frac{k_\alpha x_\alpha}{Y_\alpha} \right) , \quad (29a)
\]

\[
\varphi_{N,k}(x) = \frac{1}{|N|} \sum_{m \in \mathbb{Z}_N^d} \omega_{km}^{N} \varphi_m(x) , \quad (29b)
\]

with the coefficients

\[
\omega_{km}^{N} = \exp \left( 2\pi i \sum_{\alpha} \frac{k_\alpha m_\alpha}{N_\alpha} \right) \text{ for } k, m \in \mathbb{Z}^d .
\]

The remainder of this section is devoted to clarifying the connection between the two definitions of trigonometric polynomials \( 27 \), index sets \( 28 \), and basis functions \( 29 \).

The approximation space \( T_N^d \) provides a finite-dimensional subspace to \( L^2(Y; \mathbb{R}^d) \) for the Galerkin method. Its conformity, i.e. \( T_N^d \subset L^2(Y; \mathbb{R}^d) \), is ensured once the Hermitian symmetry of the Fourier coefficients holds, compare \( 27c \) with \( 5 \). This condition is easily enforced for odd grids which are symmetric with respect to the origin, Figure 1(a). For non-odd grids the highest (Nyquist) frequencies \( k_\alpha = -N_\alpha/2 \) must be omitted, leading to the notion of the reduced index set \( \tilde{Z}_N^d \).
The interpolation space $\mathcal{H}_N^d$ will be used to perform the numerical quadrature in the Galerkin method and primarily works with data in the real instead of the Fourier domain. Its connection to the approximation space is established with the Discrete Fourier Transform (DFT) and its inverse (iDFT)

$$\hat{u}_N(k) = \frac{1}{|N|} \sum_{m \in \mathbb{Z}_N^d} \omega_N^{-km} u_N(x_N^m), \quad u_N(x_N^k) = \sum_{m \in \mathbb{Z}_N^d} \omega_N^{-km} \hat{u}_N(m) \text{ for } k \in \mathbb{Z}_N^d,$$

where we utilize an orthogonality relation

$$\sum_{n \in \mathbb{Z}_N^d} \omega_N^{-kn} \omega_N^{-nm} = |N| \delta_{km} \quad \text{for } k, m \in \mathbb{Z}_N^d,$$

and by $x_N^k$ we denote the grid points

$$x_N^k = \sum_{\alpha} \frac{Y_{\alpha}}{N} U^{(\alpha)} \quad \text{for } k \in \mathbb{Z}_N^d. \tag{31}$$

Indeed, expanding a function $u_N : \mathcal{Y} \to \mathbb{C}^d$ into Fourier series

$$u_N(x) = \sum_{k \in \mathbb{Z}_N^d} \hat{u}_N(k) \varphi_k(x) = \frac{1}{|N|} \sum_{k \in \mathbb{Z}_N^d} \sum_{m \in \mathbb{Z}_N^d} \omega_N^{-km} u_N(x_N^m) \varphi_k(x)$$

$$= \sum_{m \in \mathbb{Z}_N^d} \sum_{k \in \mathbb{Z}_N^d} \frac{1}{|N|} \omega_N^{-km} \varphi_k(x) u_N(x_N^m)$$

gives rise to the fundamental trigonometric polynomial $\varphi_{N,m}$. In addition, these basis functions possess the Dirac delta property, $\varphi_{N,k}(x_N^n) = \delta_{km}$. Figure 1(b).

For further reference, these relations can be cast in the compact form

$$u_N = \sum_{k \in \mathbb{Z}_N^d} \hat{u}_N^k \varphi_k = \sum_{k \in \mathbb{Z}_N^d} u_N^{k} \varphi_{N,k} \quad \text{with } \hat{u}_N = F_N u_N \in \mathbb{C}^{d \times N} \text{ and } u_N = F_N^{-1} \hat{u}_N \in \mathbb{C}^{d \times N}, \tag{32}$$

where $\hat{u}_N^k = \hat{u}_N(k) \in \mathbb{C}^d$ and $u_N^k = u_N(x_N^k) \in \mathbb{C}^d$, and the matrices

$$F_N = \frac{1}{|N|} (\delta_{\alpha\beta} \omega_N^{-mk})_{\alpha,\beta} \in [\mathbb{C}^{d \times N}]^2, \quad F_N^{-1} = (\delta_{\alpha\beta} \omega_N^{-mk})_{\alpha,\beta} \in [\mathbb{C}^{d \times N}]^2 \tag{33}$$
implement the vector-valued DFT and iDFT.

The relation between the two spaces of trigonometric polynomials depends on grid parity. For odd grids, \( \mathbb{Z}_N^d \backslash \hat{\mathbb{Z}}_N^d = \emptyset \), and it follows from (32) that the spaces coincide:

\[
\mathcal{S}_N^d = \hat{\mathcal{S}}_N^d, \quad \hat{\mathbb{Z}}_N^d = \mathbb{Z}_N^d \quad \text{for odd grid assumption} \ [26].
\]

This property is lost in general due to the Nyquist frequencies \( k \in \mathbb{Z}_N^d \backslash \hat{\mathbb{Z}}_N^d \), and only the following inclusions hold

\[
\mathcal{S}_N^d \subseteq \hat{\mathcal{S}}_N^d, \quad \hat{\mathbb{Z}}_N^d \subseteq \mathbb{Z}_N^d.
\]

As a result, the interpolation space is non-conforming for non-odd grids, \( \hat{\mathcal{S}}_N^d \not\subseteq \mathcal{S}_N^d \), because the fundamental trigonometric polynomials (29) become complex-valued off the grid points, despite being real-valued at the grid points due to the Dirac delta property. Thus, the interpolation space \( \hat{\mathcal{S}}_N^d \) admits an equivalent definition via Fourier coefficients

\[
\hat{\mathcal{S}}_N^d = \left\{ \sum_{k \in \hat{\mathbb{Z}}_N^d} \hat{v}_N^k \varphi_k : \hat{v}_N \in \mathcal{F}_N(\mathbb{R}^{d \times N}) \right\}.
\]

These arguments can be formalized by introducing suitable operators, which will be useful when dealing with the Galerkin approximations and their fully discrete versions later in Section 5.

**Definition 15 (Operators).** Using grid points \( x_N^k \) for \( N \in \mathbb{N}^d \) and \( k \in \mathbb{Z}_N^d \) according to (31), the interpolation operator \( \mathcal{Q}_N : C_{\#}(\mathcal{Y}; \mathbb{R}^d) \to \mathcal{L}_2^d(\mathcal{Y}; \mathbb{C}^d) \), the truncation operator \( \mathcal{P}_N : \mathcal{L}_2^d(\mathcal{Y}; \mathbb{R}^d) \to \mathcal{L}_2^d(\mathcal{Y}; \mathbb{R}^d) \), and the discretization operator \( \mathcal{I}_N : C_{\#}^0(\mathcal{Y}; \mathbb{C}^d) \to \mathbb{C}^{d \times N} \), are defined by

\[
\mathcal{Q}_N[u] = \sum_{k \in \mathbb{Z}_N^d} u(x_N^k) \varphi_N,k, \quad (34a)
\]

\[
\mathcal{P}_N[u] = \sum_{k \in \hat{\mathbb{Z}}_N^d} \hat{u}(k) \varphi_k, \quad (34b)
\]

\[
\mathcal{I}_N[u] = \left( u_{\alpha}(x_N^k) \right)_{k \in \hat{\mathbb{Z}}_N^d, \alpha = 1, \ldots, d}. \quad (34c)
\]

The following lemma summarizes the relevant properties of operators (34) and trigonometric polynomials (29). The proof generalizes the results from [49, 55, 2] obtained under the odd grid assumption [26] to the general case; it is outlined here to keep the paper self-contained.

**Lemma 16.** (i) For \( k, m \in \mathbb{Z}_N^d \) it holds

\[
\varphi_k(x_N^m) = \omega_N^{km}, \quad (35a)
\]

\[
\varphi_{N,k}(x_N^m) = \delta_{km}, \quad (35b)
\]

\[
(\varphi_{N,k}, \varphi_{N,m})_{\mathcal{L}_2^d}(\mathcal{Y}) = \delta_{km} \frac{1}{|N|}. \quad (35c)
\]

(ii) The operator \( \mathcal{I}_N \) is an one-to-one isometric map from \( \hat{\mathcal{S}}_N^d \) onto \( \mathbb{R}^{d \times N} \), i.e. for all \( u_N, v_N \in \hat{\mathcal{S}}_N^d \)

\[
(\mathcal{I}_N[u_N], \mathcal{I}_N[v_N])_{\mathbb{R}^{d \times N}} = (\mathcal{I}_N[u_N], \mathcal{I}_N[v_N])_{\mathbb{R}^{d \times N}}. \quad (36)
\]

Moreover, for all \( u \in C_{\#}^0(\mathcal{Y}; \mathbb{R}^d) \), we have

\[
\mathcal{I}_N[\mathcal{Q}_N[u]] = \mathcal{I}_N[u]. \quad (37)
\]
and their trigonometric counterparts

Proof. (i) The proof of \((35a)\) follows by direct calculations. The equalities \((35b)\) and \((35c)\) are based on the orthogonality of DFT \((30)\), the latter additionally employs the orthogonality of the Fourier trigonometric polynomials \([6]\).

(ii) From \((35b)\) we see that trigonometric polynomials, e.g. \(u_N, v_N \in \mathcal{F}_N^d\), are uniquely defined by their grid values, so that

\[
(u_N, v_N)_{L^2_{\mu}(\mathcal{Y}; \mathbb{R}^d)} = \sum_{k, m \in \mathbb{Z}^d_N} \langle u_N(x_N^k), v_N(x_N^m) \rangle \cdot \langle \varphi_N k, \varphi_N m \rangle_{L^2_{\mu}(\mathcal{Y})} = \sum_{k, m \in \mathbb{Z}^d_N} \delta_{km} = (I_N[u_N], I_N[v_N])_{\mathbb{R}^d \times \mathbb{R}^d}.
\]

(iii) follows from \((35b)\) and the definition of the space \(\mathcal{F}_N^d\).

(iv) follows from orthogonality of Fourier trigonometric polynomials \([6]\) and the definition of the space \(\mathcal{F}_N^d\).

\[\square\]

4.3. Fully discrete spaces — odd grids

The focus of this section is on the fully discrete spaces storing the values of the trigonometric polynomials at grids with the odd number of points \((26)\). As first recognized in \([2]\), the remarkable property of such discretizations is that the structure of the continuous problem is translated into the discrete case in a conforming way, cf. Figure 2.

Definition 17 (Fully discrete projections). Let \(\hat{F}^\bullet(k) \in \mathbb{R}^{d \times d}\) for \(\bullet \in \{\mathcal{U}, \mathcal{E}, \mathcal{J}\}\) and \(k \in \mathbb{Z}^d\) be the Fourier coefficients from Definition \[4\]. We define block diagonal matrices \(G_N^\mathcal{U}, \hat{G}_N^\mathcal{E}, \) and \(\hat{G}_N^\mathcal{J} \in [\mathbb{R}^{d \times N}]^2\) in the Fourier domain as

\[
(\hat{G}^\bullet_{N})_{\alpha \beta} = \hat{F}^\bullet(n \delta_{km}), \tag{38}
\]

where \(k, m \in \mathbb{Z}^d_N\) and \(\bullet \in \{\mathcal{U}, \mathcal{E}, \mathcal{J}\}\). The real domain equivalents are obtained by similarity transformations using DFT \((33)\), i.e.

\[
G_N^\mathcal{U} = F_N^{-1} \hat{G}^\mathcal{U} N F_N.
\]

Lemma 18. Matrices \(G_N^\mathcal{U}\) for \(\bullet \in \{\mathcal{U}, \mathcal{E}, \mathcal{J}\}\) constitute the identity

\[
G_N^\mathcal{U} + G_N^\mathcal{E} + G_N^\mathcal{J} = I \tag{39}
\]

and are mutually orthogonal projections on \(\mathbb{R}^{d \times N}\).

Proof. The resolution of identity \((39)\) follows from Definitions \[1\] and \[17\] and the projection properties with their orthogonality are inherited from the continuous projections, cf. Lemma \[2\] and \[30\], Section 12.1.

Definition 19 (Finite dimensional subspaces). The previously defined projections provide us with the following subspaces of \(\mathbb{R}^{d \times N}\)

\[
\mathcal{U}_N = G_N^\mathcal{U} [\mathbb{R}^{d \times N}], \quad \mathcal{E}_N = G_N^\mathcal{E} [\mathbb{R}^{d \times N}], \quad \mathcal{J}_N = G_N^\mathcal{J} [\mathbb{R}^{d \times N}],
\]

and their trigonometric counterparts

\[
\mathcal{U}_N = I_N^{-1}[\mathcal{U}_N], \quad \mathcal{E}_N = I_N^{-1}[\mathcal{E}_N], \quad \mathcal{J}_N = I_N^{-1}[\mathcal{J}_N]. \tag{40}
\]

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\[
L^2_{per}(\Omega; \mathbb{R}^d) \ni \mathcal{F}^d_N = I_N^{-1}[\mathbb{R}^d_N]
\]
\[
\mathcal{U} \ni \mathcal{Z}_N = I_N^{-1}[\mathcal{U}_N]
\]
\[
\mathcal{E} \ni \mathcal{E}_N = I_N^{-1}[\mathcal{E}_N]
\]
\[
\mathcal{J} \ni \mathcal{J}_N = I_N^{-1}[\mathcal{J}_N]
\]

Figure 2: The scheme of subspaces for odd grids

The relation of these subspaces to the Helmholtz decomposition is clarified by Figure 2 and the following lemma.

**Lemma 20.** (i) Space \( \mathbb{R}^{d \times N} \) can be decomposed into three mutually orthogonal subspaces

\[
\mathbb{R}^{d \times N} = \mathcal{U}_N \oplus \mathcal{E}_N \oplus \mathcal{J}_N.
\]

(ii) The scheme in Figure 2 is valid and

\[
\mathcal{G}^{\bullet}[\mathcal{F}^d_N] = I_N^{-1}[\mathcal{G}^{\bullet}[\mathbb{R}^{d \times N}]] \quad \text{for } \bullet \in \{\mathcal{U}, \mathcal{E}, \mathcal{J}\}.
\]

**Proof.** The Helmholtz-like decomposition of trigonometric polynomials, the second column in Figure 2, is accomplished with the same set of projections \( \mathcal{G}^{\bullet} \) for \( \bullet \in \{\mathcal{U}, \mathcal{E}, \mathcal{J}\} \) as they satisfy

\[
\mathcal{G}^{\bullet}[\mathcal{F}^d_N] \subset \mathcal{F}^d_N \quad \text{for } \bullet \in \{\mathcal{U}, \mathcal{E}, \mathcal{J}\}.
\]

The connection of continuous projections and fully discrete projections in is a consequence of isometry of the discretization operator \( I_N \) proven in Lemma 16, two representations of trigonometric polynomials, and the definition of the fully discrete projections via continuous ones. The last column in Figure 2 is then obvious.

**Remark 21.** The previous proof yields an alternative characterization of the conforming subspaces

\[
\mathcal{U}_N = \mathcal{U} \bigcap \mathcal{F}^d_N, \quad \mathcal{E}_N = \mathcal{E} \bigcap \mathcal{F}^d_N, \quad \mathcal{J}_N = \mathcal{J} \bigcap \mathcal{F}^d_N.
\]

Thus, \( \mathcal{U}_N, \mathcal{E}_N, \) and \( \mathcal{J}_N \) represent the subspaces of constant, curl-free, and divergence-free vector-valued polynomials, while \( \mathcal{U}_N = I_N[\mathcal{U}_N], \mathcal{E}_N = I_N[\mathcal{E}_N], \) and \( \mathcal{J}_N = I_N[\mathcal{J}_N] \) collect their values at the grid points.

### 4.4. Fully discrete spaces — general grids

The framework of fully discrete spaces, introduced in previous sections for odd grid assumption, is extended here to the general grids. Similarly to Section 4.2, the special attention is given to the Nyquist frequencies \( k \in \mathbb{Z}^d_N \setminus 2\mathbb{Z}^d_N \) in order to obtain the conforming approximation spaces.

**Definition 22** (Fully discrete projections). Let \( \hat{\mathcal{F}}^{\bullet}(k) \in \mathbb{R}^{d \times d} \) for \( \bullet \in \{\mathcal{U}, \mathcal{E}, \mathcal{J}\} \) and \( k \in \mathbb{Z}^d \) be the Fourier coefficients from Definition 4. We define the block diagonal matrices \( \hat{\mathcal{G}}^{\bullet}_{N,0}, \hat{\mathcal{G}}^{\bullet}_{N,1}, \hat{\mathcal{G}}^{\bullet}_{N,0}, \) and \( \hat{\mathcal{G}}^{\bullet}_{N,1} \in [\mathbb{R}^{d \times N}]^2 \) in the Fourier domain as

\[
(\hat{\mathcal{G}}^{\bullet}_{N,0})^{km}_{\alpha \beta} = (\hat{\mathcal{G}}^{\bullet}_{N,1})^{km}_{\alpha \beta} = \delta_{km},
\]

\[
(\hat{\mathcal{C}}^{\bullet}_{N,0})^{km}_{\alpha \beta} = \begin{cases} 
\hat{\mathcal{F}}^{\bullet}_{\alpha \beta}(k) \delta_{km}, & \text{for } k \in \mathbb{Z}_N, \\
0, & \text{for } k \in \mathbb{Z}_N \setminus 2\mathbb{Z}_N,
\end{cases}
\]

\[
(\hat{\mathcal{C}}^{\bullet}_{N,1})^{km}_{\alpha \beta} = \begin{cases} 
\hat{\mathcal{F}}^{\bullet}_{\alpha \beta}(k) \delta_{km}, & \text{for } k \in \mathbb{Z}_N, \\
\delta_{\alpha \beta} \delta_{km}, & \text{for } k \in \mathbb{Z}_N \setminus 2\mathbb{Z}_N,
\end{cases}
\]

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where \( k, m \in \mathbb{Z}_N^d \) and \( \bullet \in \{ \mathcal{F}, \mathcal{J} \} \). The real domain equivalents are obtained by similarity transformations using the DFT matrices \( \mathcal{F}_N \), i.e.

\[
\mathcal{G}_N = \mathcal{F}_N^{-1} \mathcal{G}_N \mathcal{F}_N,
\]

\[
\mathcal{G}_{N,0} = \mathcal{F}_N^{-1} \mathcal{G}_{N,0} \mathcal{F}_N,
\]

\[
\mathcal{G}_{N,1} = \mathcal{F}_N^{-1} \mathcal{G}_{N,1} \mathcal{F}_N
\]

for \( \bullet \in \{ \mathcal{F}, \mathcal{J} \} \).

**Lemma 23.** The two triples of matrices \( \{ \mathcal{G}_N, \mathcal{G}_{N,0}, \mathcal{G}_{N,1} \} \) and \( \{ \mathcal{G}_N, \mathcal{G}_{N,1}, \mathcal{G}_{N,0} \} \) constitute identities

\[
I = \mathcal{G}_N + \mathcal{G}_{N,0} + \mathcal{G}_{N,1},
\]

\[
I = \mathcal{G}_N + \mathcal{G}_{N,1} + \mathcal{G}_{N,0},
\]

and each triple consists of mutually orthogonal projections on \( \mathbb{R}^{d \times N} \).

**Proof.** The resolution of identity (43) follows from Definitions 1 and 22. The projection properties and their orthogonality are proven in the same way as in Lemma 18 for \( k \in \mathbb{Z}_N^d \), and are the direct consequence of Definition 22 for the Nyquist frequencies \( k \in \mathbb{Z}_N^d \setminus \mathbb{Z}_N^d \).

**Definition 24 (Finite dimensional subspaces).** With the previously defined projections, we introduce the subspaces of \( \mathbb{R}^{d \times N} \)

\[
\mathcal{U}_N = \mathcal{G}_N \mathbb{R}^{d \times N},
\]

\[
\mathcal{E}_N = \mathcal{G}_{N,0} \mathbb{R}^{d \times N},
\]

\[
\mathcal{J}_N = \mathcal{G}_{N,1} \mathbb{R}^{d \times N},
\]

and their trigonometric counterparts

\[
\mathcal{W}_N = \mathcal{I}_N^{-1}[\mathcal{U}_N],
\]

\[
\mathcal{E}_N = \mathcal{I}_N^{-1}[\mathcal{E}_N],
\]

\[
\mathcal{J}_N = \mathcal{I}_N^{-1}[\mathcal{J}_N].
\]

Compared to the previous section, the relations among these subspaces are more intricate, see Figure 3 and the following lemma.

**Lemma 25.** For the subspaces from Definition 24, the following holds:

(i) Space \( \mathbb{R}^{d \times N} \) admits two alternative orthogonal decompositions

\[
\mathbb{R}^{d \times N} = \mathcal{U}_N \oplus \mathcal{E}_N \oplus \mathcal{J}_N,
\]

\[
\mathbb{R}^{d \times N} = \mathcal{U}_N \oplus \mathcal{E}_N \oplus \mathcal{J}_N.
\]

Moreover, the subspaces \( \mathcal{E}_N \) and \( \mathcal{J}_N \) enlarge the original ones, i.e.

\[
\mathcal{E}_N \subset \mathcal{E}_N,
\]

\[
\mathcal{J}_N \subset \mathcal{J}_N.
\]

and coincide only for odd grids.

---

"Figure 3: The scheme of subspaces for general grids"
(ii) The scheme in Figure 3 is valid and
\[ G^\omega[\mathcal{T}_N^d] = \mathcal{I}_N^{-1}[U_N], \quad G^\varepsilon[\mathcal{T}_N^d] = \mathcal{I}_N^{-1}[E_N], \quad G^J[\mathcal{T}_N^d] = \mathcal{I}_N^{-1}[J_N]. \]  

Proof. Eq. (45) is a consequence of resolutions of identity [43]. The rest in (i) follows from Definition 22 of the fully discrete projections, once noticing that the pairs of matrices \( \{G^\varepsilon_{N,0}, G^\varepsilon_{N,1}\} \) and \( \{G^J_{N,0}, G^J_{N,1}\} \) coincide for odd grids [26] and differ only for the Nyquist frequencies \( k \in \mathbb{Z}_N^d \setminus 2\mathbb{Z}_N^d \).

The special case of part (ii) for odd grids [26] has already been proven in Lemma 20; in such case the spaces of trigonometric polynomials \( \mathcal{T}_N^d \) and \( \mathcal{I}_N^d \) coincide. Utilizing Lemma 16 (ii), we are left with
\[ \mathcal{U} = \mathcal{U}_N, \quad \mathcal{E} \subseteq \mathcal{E}_N, \quad \mathcal{J} \subseteq \mathcal{J}_N. \]

While the equality is evident, the inclusions follows from (46) and from a property of continuous projections
\[ G^*[\mathcal{T}_N^d] \subset \mathcal{P}_N^d \subset L^1_{\text{per}}(\mathcal{Y}; \mathbb{R}^d) \quad \text{for } \bullet \in \{\mathcal{E}, \mathcal{J}\}. \]

Finally, the proof of (46) follows from the connection of representations [12] and from the fact that the Nyquist frequencies \( k \in \mathbb{Z}_N^d \setminus 2\mathbb{Z}_N^d \) are left out in the definition of projections \( G^\varepsilon_{N,0} \) and \( G^J_{N,0} \); recall Definition 22.

Remark 26. The previous proof yields an alternative characterization of the conforming subspaces
\[ \mathcal{E}_N = \mathcal{E} \cap \mathcal{T}_N^d, \quad \mathcal{J}_N = \mathcal{J} \cap \mathcal{T}_N^d. \]

5. Galerkin approximation with numerical integration

This section deals with the discretization of (11) by the Galerkin approximation with numerical integration (GaNi), a scheme which has been introduced and analyzed in [2] Section 4.3 for the odd grids (26). Here, the method is generalized to the primal-dual setting and general grids, by utilizing the discretization strategy shown in Figure 4.

![Figure 4: Discretization strategy](image)

The discretization consists in the approximation of bilinear forms (10) using the interpolation operator (34a) and the trapezoidal integration rule (36), yielding the discretization-dependent forms \( a_N, a_N^{-1} : \mathcal{T}_N^d \times \mathcal{T}_N^d \to \mathbb{R} \) given by
\[ a_N(u_N, v_N) := (Q_N[Au_N], v_N)_{L^2_{\text{per}}(\mathcal{Y}; \mathbb{R}^d)}, \quad a_N^{-1}(u_N, v_N) := (Q_N[A^{-1}u_N], v_N)_{L^2_{\text{per}}(\mathcal{Y}; \mathbb{R}^d)}. \]

**Definition 27 (Galerkin approximation with numerical integration (GaNi)).** Let the material coefficients satisfy (3) and \( A \in C^0(\mathcal{Y}; \mathbb{R}^{d \times d}) \). Then, the approximate primal and dual homogenized matrices \( A_{H,N}, B_{H,N} \in \mathbb{R}^{d \times d} \) are defined as
\[ (A_{H,N}E, E)_{\mathbb{R}^d} = \min_{e_N \in \mathcal{E}_N} a_N(E + e_N, E + e_N) \]
\[ (B_{H,N}J, J)_{\mathbb{R}^d} = \min_{J_N \in \mathcal{J}_N} a_N^{-1}(J + J_N, J + J_N). \]

for arbitrary \( E, J \in \mathbb{R}^d \).
Remark 28. The GaNi scheme coincides with the original Moulinec-Suquet method [54, 55] as shown in [2, Section 5.3] for the variational formulation and in [26, 27] for the Lippmann-Schwinger equation. The reason for using the trapezoidal integration rule in (47) is that it can be applied to general coefficients, but the associated numerical scheme may cause a non-monotonic convergence of the approximate solutions, see Section 5.3. We will show in Section 4 that the quadrature can be avoided for a wide class of coefficients, albeit at a higher computational cost. This procedure provides the Galerkin scheme without numerical integration, proposed theoretically in [2, Section 4.2], and studied separately in [56].

Now, we proceed to the fully discrete versions of the bilinear forms (47).

Lemma 29. Under assumptions of the Definition 27, we have

\[ a_N(u_N, v_N) = a_N(u_N, v_N) \in \mathbb{R}^{d \times N}, \]

(49a)

\[ a_N^{-1}(u_N, v_N) = a_N^{-1}(u_N, v_N) \in \mathbb{R}^{d \times N}, \]

(49b)

where

\[ u_N := I_N[u_N] \in \mathbb{R}^{d \times N}, \]

\[ v_N := I_N[v_N] \in \mathbb{R}^{d \times N}, \]

and the components of the matrices \( A_N, B_N \in \mathbb{R}^{d \times N} \) are defined as

\[ A_N^{km} = A(x_N^k)\delta_{km}, \]

\[ B_N^{km} = A^{-1}(x_N^k)\delta_{km}, \]

(50)

for \( k, m \in \mathbb{Z}_N^d \). Moreover,

\[ A_N = B_N^{-1}. \]

(51)

Proof. The proof is a consequence of Lemma 16 (ii), particularly Eqs. (36) and (37), together with the definition of the operator \( I_N \) in (34c).

Remark 30. Recall that the dual formulation (48b) involves inverse coefficients \( A^{-1} \). Interestingly, this property is maintained in the fully discrete formulation (51), so that the assumptions of Proposition 6 are met, leading to the duality results in Propositions 33 and 34.

The previous lemma, particularly (10), enables us to define the homogenization problem in the fully discrete setting that represents the matrix formulation of the GaNi.

Corollary 31 (Fully discrete formulations of the GaNi). Under the assumptions of Definition 27 the primal and the dual homogenized matrices \( A_{II,N}, B_{II,N} \in \mathbb{R}^{d \times d} \) satisfy

\[ (A_{II,N}E, E)_{\mathbb{R}^d} = \min_{E,N} a_N(E + e_N, E + e_N) = a_N(E + e_N(E), E + e_N(E)), \]

(52a)

\[ (B_{II,N}J, J)_{\mathbb{R}^d} = \min_{J,N} a_N^{-1}(J + j_N, J + j_N) = a_N^{-1}(J + j_N, J + j_N), \]

(52b)

for arbitrary \( E, J \in \mathbb{R}^d \).

Moreover, the discrete minimizers \( e_N^{(E)}, j_N^{(J)} \) of both formulations (48) and (52) exist, are unique, and are connected by

\[ I_N[e_N^{(E)}] = e_N^{(E)}, \]

\[ I_N[j_N^{(J)}] = j_N^{(J)}. \]

Remark 32. The discrete bilinear forms \( a_N, a_N^{-1} \) are defined on \( \mathbb{R}^{d \times N} \times \mathbb{R}^{d \times N} \), rendering the terms \( E + e_N \) and \( J + j_N \) formally ill-defined. The sums need to be understood with the help of the isometric isomorphism \( I_N \) from (34c) that identifies \( \mathbb{R}^d \) or \( \mathbb{Z}^d \) with \( U_N \), e.g.

\[ a_N(E + e_N, E + e_N) = a_N(I_N[E] + e_N, I_N[E] + e_N) \quad \text{with} \quad (I_N[E] + e_N)^a = E_a + e_{N,a}. \]
5.1. Duality for odd grids

In this section, the perturbation duality theorem, Proposition 6, is applied to the fully discrete formulation of the GaNi [22]. For discretization with odd number of grid points [26], it leads to a surprising result: the discrete formulations are mutually dual, so that the duality of continuous formulations [11] is preserved under the discretization.

Proposition 33. Assuming odd grids [26], the following holds for the fully discrete homogenization problem (52):

(i) The primal and the dual homogenized matrices are mutually inverse

\[ A_{H,N}^{-1} = B_{H,N}^{-1}. \]

(ii) The primal and the dual discrete minimizers \( e^{(\alpha)}_N \in E_N, j^{(\alpha)}_N \in J_N \) are related via

\[ U^{(\beta)} + j^{(\beta)}_N = A_N \sum_{\alpha} E_{\alpha}(U^{(\alpha)} + e^{(\alpha)}_N), \]

where \( E = A_{H,N}^{-1}U^{(\beta)}. \)

Proof. The proof is a direct consequence of Proposition 6 for

\[ H = \mathcal{H} = \mathcal{U} \oplus \mathcal{E} \oplus \mathcal{J} \quad \mathbb{R}^d \times N = U_N \oplus E_N \oplus J_N \]

and

\[ \hat{a} = a_N, \quad \hat{a}^{-1} = a^{-1}_N, \quad \hat{A}_H = A_{H,N}, \quad \hat{B}_H = B_{H,N}, \quad \hat{e}^{(E)} = e^{(E)}_N, \quad \hat{j}^{(J)} = j^{(J)}_N. \]

5.2. Duality for general grids

For general grids, the fully discrete formulations [52] lack the mutual duality as the fully discrete subspaces may not exhaust the whole \( \mathbb{R}^d \times N \), i.e.

\[ U_N \oplus E_N \oplus J_N \subseteq \mathbb{R}^d \times N \] and the equality holds only for odd grids [26], cf. Figure 3. However, Proposition 34 below shows that the formulations for matrices \( A_{H,N} \) and \( B_{H,N} \) from [52] are in duality with

\[ (\hat{B}_{H,N}J, J)_{\mathbb{R}^d} = \min_{J_N \in J_N} a_N^{-1}(J + j_N, J + j_N) = a_N^{-1}(J + j^{(J)}_N, J + j^{(J)}_N), \]

(54a)

\[ (\hat{A}_{H,N}E, E)_{\mathbb{R}^d} = \min_{E_N \in E_N} a_N(E + e_N, E + e_N) = a_N(E + e^{(E)}_N, E + e^{(E)}_N), \]

(54b)

when using the dual spaces \( \hat{E}_N \) and \( \hat{J}_N \) from [44b].

Proposition 34. The following holds for the fully discrete homogenization problems [52] and [54]:

(i) The homogenized matrices from the fully discrete formulations [52a] and [52b] coincide with those in [54a] and [54b], respectively

\[ A_{H,N} = \hat{B}_{H,N}^{-1}, \quad B_{H,N}^{-1} = \hat{A}_{H,N}. \]

(55)
(ii) The discrete minimizers $\mathbf{e}_N^{(\beta)} \in \mathbb{E}_N$ and $\mathbf{j}_N^{(\alpha)} \in \mathbb{J}_N$ of (52a) and (52b) are related to the minimizers $\hat{\mathbf{e}}_N^{(\alpha)} \in \bar{\mathbb{E}}_N$ and $\hat{\mathbf{j}}_N^{(\alpha)} \in \bar{\mathbb{J}}_N$ of (5-1a) and (5-1b) via
\[ U^{(\beta)} + \mathbf{e}_N^{(\beta)} = A_N \sum_{\alpha} J_\alpha(U^{(\alpha)} + \hat{\mathbf{e}}_N^{(\alpha)}), \quad U^{(\beta)} + \hat{\mathbf{j}}_N^{(\beta)} = A_N \sum_{\alpha} E_\alpha(U^{(\alpha)} + \hat{\mathbf{e}}_N^{(\alpha)}), \] (56)

with $E := B_{H,N}U^{(\beta)}$ and $J := A_{H,N}U^{(\beta)}$.

(iii) The primal and the dual homogenized matrices satisfy
\[ B_{H,N}^{-1} \preceq A_{H,N}. \] (57)

Proof. The proof of parts (i) and (ii) is a consequence of Proposition 6. The equivalence between (52a) and (54a) is shown by
\[ \mathcal{H} = \mathcal{U} \oplus \bar{\mathcal{E}} \oplus \bar{\mathcal{J}} \]
\[ \mathbb{R}^{d \times N} = \mathbb{U}_N \oplus \bar{\mathbb{E}}_N \oplus \bar{\mathbb{J}}_N \]

and
\[ \hat{a} = a_N, \quad \hat{a}^{-1} = a_N^{-1}, \quad \hat{A}_H = A_{H,N}, \quad \hat{B}_H = B_{H,N}, \quad \hat{e}^{(E)} = e^{(E)}_N, \quad \hat{j}^{(J)} = j^{(J)}_N. \]

The equivalence between (52b) and (54b) follows from
\[ \mathcal{H}_d = \mathcal{U} \oplus \bar{\mathcal{E}} \oplus \bar{\mathcal{J}} \]
\[ \mathbb{R}^{d \times N} = \mathbb{U}_N \oplus \bar{\mathbb{E}}_N \oplus \bar{\mathbb{J}}_N \]

and
\[ \hat{a} = a_N, \quad \hat{a}^{-1} = a_N^{-1}, \quad \hat{A}_H = A_{H,N}, \quad \hat{B}_H = B_{H,N}, \quad \hat{e}^{(E)} = e^{(E)}_N, \quad \hat{j}^{(J)} = j^{(J)}_N. \]

The proof of the duality gap (iii) is based on the inclusion $\mathbb{E}_N \subseteq \bar{\mathbb{E}}_N$, recall Eq. (55) in Lemma 25 (i), and the following inequality
\[ (B_{H,N}^{-1}E, E)_{\mathbb{R}^d} = \min_{e_N \in \mathbb{E}_N} a_N(E + e_N, E + e_N) \]
\[ \leq \min_{e_N \in \bar{\mathbb{E}}_N} a_N(E + e_N, E + e_N) = (A_{H,N}E, E)_{\mathbb{R}^d}, \]
holding for an arbitrary $E \in \mathbb{R}^d$.  \[ \square \]

6. Evaluation of upper-lower bounds on homogenized properties

As the GaNi scheme (48), or its fully discrete relative (52), deliver conforming approximations to the minimizers of the homogenization problem (11), i.e. $e_N^{(\alpha)} \in \mathbb{E}_N < \bar{\mathbb{E}}$ and $j_N^{(\alpha)} \in \mathbb{J}_N < \bar{\mathbb{J}}$, they can be utilized within the upper-lower bounds structure of Section 3.3. Details of these developments are gathered here with the emphasis on the evaluation of the bounds in a computationally efficient way. Recall that the GaNi scheme is defined with the approximate bilinear forms $a_N$ and $a_N^{-1}$ (47), whereas the upper-lower bounds are obtained via bilinear forms of the continuous homogenization problem (11).

\[ (A_{H,N}E, E)_{\mathbb{R}^d} = a(E + e^{(E)}_N, E + e^{(E)}_N), \] (58a)
\[ (B_{H,N}J, J)_{\mathbb{R}^d} = a^{-1}(J + j^{(J)}_N, J + j^{(J)}_N). \] (58b)
and the mean of guaranteed bounds $\overline{A}_{H,N}$ with the guaranteed error $D_N$ reads as
\begin{align}
\overline{A}_{H,N} &= \frac{1}{2} \left( \overline{A}_{H,N} + \overline{B}_{H,N}^{-1} \right), \\
D_N &= \frac{1}{2} \left( \overline{A}_{H,N} - \overline{B}_{H,N}^{-1} \right).
\end{align}
(59a)  
(59b)

For an easier orientation among the matrices, we refer to their scheme in Figure 5. Notice that the effective matrices $A_{H,N}$ and $B_{H,N}$ of the GaNi (48) or (52) are generally in no relation, in the sense of the Löwner partial order, to the homogenized matrix $A_H$ and to a posteriori upper-lower bounds $\overline{A}_{H,N}$ and $\overline{B}_{H,N}$, as confirmed with numerical experiments in Section 8.

Figure 5: Relations among homogenized matrices

Computation of the bounds involves integrals of the type
\[ (Au_N, v_N)_{L^2_p(\mathcal{Y}; \mathbb{R}^d)} \text{ for } A \in L^\infty(\mathcal{Y}; \mathbb{R}^{d \times d}) \text{ and } u_N, v_N \in \mathcal{F}^d_N, \]

(60)

recall (58). Notice that, due to the definition of spaces $\mathcal{G}_N$ and $\mathcal{F}_N$ in (40), the minimizers $e^{(\alpha)}_N, j^{(\alpha)}_N$ always belong to $\mathcal{F}^d_N$ defined in (27a), so we can work with odd grids (26) without the loss of generality.

We show in Lemma 35 that the term in (60) can be evaluated in an analogous way to the GaNi, recall Corollary 31, but the resulting matrix becomes fully populated, rendering the estimates very costly. Fortunately, we recover the block diagonal structure when defining the fully discrete quadratic forms on the double grid, Lemma 37.

**Lemma 35.** For odd grids (26), the integral (60) equals to
\[ (Au_N, v_N)_{L^2_p(\mathcal{Y}; \mathbb{R}^d)} = (\mathbf{\hat{A}}_{\text{full}}u_N, v_N)_{\mathcal{C}^{d \times N}} = (\mathbf{A}_{\text{full}}u_N, v_N)_{\mathbb{R}^{d \times N}}, \]

(61)

where vectors $u_N, v_N \in \mathbb{R}^{d \times N}$ and $\mathbf{\hat{u}}_N, \mathbf{\hat{v}}_N \in \mathbb{C}^{d \times N}$ are defined via
\[ u_N = \mathcal{I}_N[u_N], \quad v_N = \mathcal{I}_N[v_N], \quad \mathbf{\hat{u}}_N = \mathbf{F}_N\mathbf{u}_N, \quad \mathbf{\hat{v}}_N = \mathbf{F}_N\mathbf{v}_N, \]

and matrices $\mathbf{A}_{\text{full}} \in \mathbb{C}^{(d \times N)^2}$ and $\mathbf{A}_{\text{full}} \in \mathbb{R}^{(d \times N)^2}$ follow from

\[ (\mathbf{\hat{A}}_{\text{full}})^k_l = \frac{1}{|\mathcal{Y}|} \int_\mathcal{Y} A(x) \varphi_k(x) \varphi_{-1}(x) \, dx \quad \text{for } k, l \in \mathbb{Z}_N^d, \quad \mathbf{A}_{\text{full}} = \mathbf{F}_N\mathbf{\hat{A}}_{\text{full}}\mathbf{F}_N^{-1}. \]

**Proof.** To obtain the first expression in (61), we represent the vectors in (60) with their Fourier series
\[ u_N = \sum_{k \in \mathbb{Z}_N^d} \mathbf{u}^k_N \varphi_k, \quad v_N = \sum_{l \in \mathbb{Z}_N^d} \mathbf{v}^l_N \varphi_l. \]
Substitution into (60) yields
\[ (Au_N, v_N)_{L^2_p(\mathcal{Y}; \mathbb{R}^d)} = \sum_{\alpha, \beta} \sum_{k \in \mathbb{Z}_N^d} \frac{\mathbf{u}^k_N, \mathbf{v}^l_N}{|\mathcal{Y}|} \int_\mathcal{Y} A_{\alpha, \beta} \varphi_k \varphi_l \, dx = (\mathbf{A}_{\text{full}}u_N, v_N)_{\mathcal{C}^{d \times N}}. \]
To obtain the last expression in (61), we map the Fourier coefficients with DFT matrix (33) to obtain $\hat{u}_N = F_N u_N$ and $\hat{v}_N = F_N v_N$, cf. (32), from which we calculate

$$\left( \hat{A}_{\text{full}} u_N, v_N \right)_{C^d \times N} = \left( \hat{A}_{\text{full}} F_N u_N, F_N v_N \right)_{C^d \times N} = \frac{1}{|N|} \left( F_N^{-1} \hat{A}_{\text{full}} F_N u_N, v_N \right)_{C^d \times N}$$

where we have utilized $F_N^* = \frac{1}{|N|} F_N$.

**Remark 36.** The sparse quadrature involves a projection to a finer grid denoted as $u_N = I_M [u_N] \in \mathbb{R}^{d \times M}$ for $M, N \in \mathbb{R}^d$ such that $M_\alpha > N_\alpha$.

Here, we decided to use the same subscript $N$ for the trigonometric polynomial $u_N$ and its discrete representation $u_N$ in order to highlight their polynomial degree and to avoid a profusion of notation. The actual dimension of $u_N$ is understood implicitly from the context, so that the terms like $(A_M u_N, u_N)_{\mathbb{R}^d \times M}$ with $A_M \in \left[ \mathbb{R}^{d \times M} \right]^2$ remain well-defined.

**Lemma 37 (Double-grid quadrature).** For odd grids (26), the integral (60) equals to

$$\left( A u_N, v_N \right)_{L_2^d} = \left( A_{2N-1} u_N, v_N \right)_{\mathbb{R}^{d \times (2N-1)}}$$

where $u_N = I_{2N-1} [u_N]$, $v_N = I_{2N-1} [v_N] \in \mathbb{R}^{d \times (2N-1)}$, and $A_{2N-1} \in \left[ \mathbb{R}^{d \times (2N-1)} \right]^2$ has the components

$$A_{2N-1}^{km} = \delta_{km} \sum_{n \in \mathbb{Z}_{2N-1}^d} \omega_{2N-1}^{kn} \hat{A}(n) \in \mathbb{R}^{d \times d}. \quad (62)$$

**Proof.** Because the product of two trigonometric polynomials $u_N v_N \in \mathbb{R}^d_{2N-1}$ has bounded frequencies, we can express it as

$$u_{N,\beta} v_{N,\alpha} = \sum_{k \in \mathbb{Z}_{2N-1}^d} u_{N,\beta}^k (x^{2N-1})^k (x^{2N-1})^k \varphi_{2N-1, k} = \sum_{k \in \mathbb{Z}_{2N-1}^d} u_{N,\beta}^k v_{N,\alpha}^k \varphi_{2N-1, k}.$$

Substitution into (60) and direct calculations reveal

$$\left( A u_N, v_N \right)_{L_2^d} = \sum_{\alpha, \beta} \sum_{k \in \mathbb{Z}_{2N-1}^d} u_{N,\beta}^k v_{N,\alpha}^k |Y| \int_{Y} A_{\alpha,\beta}(x) \varphi_{2N-1, k}(x) \, dx$$

$$= \sum_{\alpha, \beta} \sum_{k \in \mathbb{Z}_{2N-1}^d} \left( \sum_{l \in \mathbb{Z}_{2N-1}^d} \omega_{2N-1}^{-kl} |2N-1||Y| \int_{Y} A_{\alpha,\beta}(x) \varphi_l(x) \, dx \right) u_{N,\beta}^k v_{N,\alpha}^k.$$

The statement of the lemma follows by substitution of $l$ with $-n$. \qed

To evaluate the matrix in (32), we need to determine the Fourier coefficients $[\hat{A}_{\mu,\beta}(n)]_{n \in \mathbb{Z}_{2N-1}^d}$. In the present section, these are elaborated in detail for the matrix-inclusion composites, characterized by the coefficients in the form

$$A(x) = A_{(0)} + \sum_{j=1}^{J} f_j(x - x_{(j)}) A_{(j)} \quad (63)$$

where $A_{(0)} \in \mathbb{R}^{d \times d}$ represents the coefficients of the matrix phase, matrices $A_{(j)} \in \mathbb{R}^{d \times d}$ with functions $f_j \in L_2^\infty(Y)$ for $j = 0, \ldots, J$ quantify the distribution of coefficients within inclusions, centered at $x_{(j)}$, along with their geometry (in short, the functions $f_j$ will be referred to as inclusion topologies).
Lemma 38. The matrix for coefficients is given by

\[
A_{2N-1}^{km} = \delta_{km} \left[ A^{(0)} + \sum_{j=1}^{J} A^{(j)} \left( \sum_{n \in \mathbb{Z}_d^N} \omega_{2N-1}^{km} \phi_{n}(x_{(j)}) f_{(j)}(n) \right) \right] \in \mathbb{R}^{d \times d},
\]

where \( f_{(j)}(n) \) for \( j \in \{1, \ldots, J\} \) and \( n \in \mathbb{Z}_N^d \) denote the Fourier coefficients of inclusion topologies \( f_{(j)} \).

Proof. Using basic properties of the Fourier trigonometric polynomials, namely \( \int_{\mathcal{Y}} \phi_n(x) \, dx = |\mathcal{Y}| \delta_{0n} \) and \( \phi_n(x + x_{(j)}) = \phi_n(x) \phi_n(x_{(j)}) \), we deduce

\[
A_{2N-1}^{km} = \delta_{km} \sum_{n \in \mathbb{Z}_d^N} \omega_{2N-1}^{km} \phi_{n}(x_{(j)}) \right] \phi_{n}(x) \, dx
\]

\[
= \delta_{km} \left[ A^{(0)} + \sum_{j=1}^{J} A^{(j)} \left( \sum_{n \in \mathbb{Z}_d^N} \omega_{2N-1}^{km} \phi_{n}(x_{(j)}) \phi_{n}(x) \right) \right].
\]

Remark 39. An example of the inclusion topology from is provided by a rectangle/cuboid of side lengths \( 0 < h_\alpha \leq Y_\alpha \) centered at the origin, i.e.

\[
\text{rect}_h(x) = \begin{cases} 1 & \text{if } |x_\alpha| < \frac{h_\alpha}{2} \text{ for all } \alpha, \\ 0 & \text{otherwise} \end{cases}, \quad \text{rect}_h(m) = \frac{1}{|\mathcal{Y}|} \prod_{\alpha} h_\alpha \operatorname{sinc} \left( \frac{h_\alpha m_\alpha}{Y_\alpha} \right),
\]

where

\[
\operatorname{sinc}(x) = \begin{cases} 1 & \text{for } x = 0, \\ \frac{\sin(\pi x)}{\pi x} & \text{for } x \neq 0. \end{cases}
\]

This topology is utilized in numerical examples in Section 8 and corresponds to pixel or voxel-wise definition of material coefficients, which are commonly produced by imaging techniques such as tomography or microscopy. Other examples of inclusion topologies, such as spherical and bilinear, can be found in [55, pages 137–138].

Remark 40 (Types of numerical integration). The trapezoidal integration used in GaNi scheme leads to the algorithm defined by Moulinec and Suquet. In [57, Section 13.3.2], the exact integration formula leading to the fully populated matrix according to Lemma 35 was used for the Hashin-Shtrikman functional with piece-wise constant material coefficients. Later, the Fourier coefficients of individual inclusions have been incorporated as the so-called shape functions in to enhance FFT-based homogenization schemes. Our results thus explain their good performance and introduce the numerical quadrature on double grid even in a more general setting.

7. Computational aspects

Here, we discuss computational aspects related to the determination of upper-lower bounds. Section 7.1 deals with the calculation of minimizers by the Conjugate gradients algorithms, while Section 7.2 gathers remarks on algorithm development and implementation issues.
7.1. Conjugate gradients

Restricting our attention to the primal problem (52a), we are left with the minimization of a quadratic function over a subspace
\[ e_N^{(E)} = \arg \min_{e_N \in E_N} a_N(E + e_N, E + e_N). \] (65)

This problem is suitable for the Conjugate Gradients (CG) method, as it involves symmetric and positive definite forms.

According to [2, Section 5.3], the problem (65) is equivalent to the solution of a linear system. Indeed, the minimizer satisfies the stationarity condition
\[ a_N(e_N^{(E)}, v) = -a_N(E, v) \quad \forall v \in E_N. \]

Using \( G_{N,0}^\varepsilon \), an orthogonal (symmetric) projection on \( E_N \) from Definition 22, we proceed to
\[ a_N(e_N^{(E)}, g_{N,0}^\varepsilon v) = -a_N(E, g_{N,0}^\varepsilon v) \quad \forall v \in \mathbb{R}^{d \times N}, \]
\[ (g_{N,0}^\varepsilon A_N e_N^{(E)}, v)_{\mathbb{R}^{d \times N}} = -(g_{N,0}^\varepsilon A_N E, v)_{\mathbb{R}^{d \times N}} \quad \forall v \in \mathbb{R}^{d \times N}. \]

Because the space of test functions was enlarged to \( \mathbb{R}^{d \times N} \), we pass to a linear system
\[ G_{N,0}^\varepsilon A_N \begin{pmatrix} e_N^{(E)} \\ x \end{pmatrix} = -G_{N,0}^\varepsilon A_N E \]
with \( A_N \) defined in (60). Thus, the minimization of (65) can be performed by CG applied to the linear system
\[ Cx = b \quad \text{for} \ C = F_N^{-1} \hat{G}_0 \hat{F}_N A_N \]
with an initial approximation \( x(0) \in E_N \). By analogous arguments, the minimizers of the dual problem (52b) satisfy the linear systems
\[ G_{N,0}^\varepsilon A_N^{-1} j_{N}^{(J)} = -G_{N,0}^\varepsilon A_N^{-1} J \]
that are solvable by CG with an initial approximation \( x(0) \in J_N \).

7.2. Implementation issues

**Algorithm 41.** For coefficients \( A \in L^\infty_r(\mathcal{Y}; \mathbb{R}^{d \times d}) \), the evaluation of upper-lower bounds on homogenized matrix consists of the following steps.

(i) Set the number of grid points \( N \) and assemble matrices \( A_N, A_N^{-1}, \hat{G}_0, \hat{G}_0^\varepsilon \in [\mathbb{R}^{d \times N}]^2 \) according to Definition 17 and Eq. (50).
(ii) For \( \alpha = 1, \ldots, d \), find discrete primal and dual minimizers \( e_N^{(\alpha)} \in E_N, j_{N}^{(\alpha)} \in J_N \) as solutions to linear systems (66) and (67) for \( E = J = U^{(\alpha)} \).
(iii) Evaluate upper-lower bounds (68) according to Lemmas 37 and 38.

**Remark 42.** The matrices in step (i) are block diagonal leading to a substantial reduction in memory requirements. In step (ii), the solution of linear systems requires only matrix-vector multiplications involving sequential application of matrices \( A_N, F_N, \hat{G}_0 \), and \( F_N^{-1} \). The computational cost is dominated by DFT matrices \( F_N \) and \( F_N^{-1} \) that are performed only in \( \mathcal{O}(|N| \log |N|) \) operations by the FFT algorithm.
Remark 43 (Convergence criteria). Regarding step (ii), initial approximations to CG are set to the zero vector and the convergence criterion is based on the norm of residuum, i.e., \( \| \mathbf{r}_i \|_{2^{N \times N}} \leq \varepsilon \| \mathbf{E} \|_2 \) with \( \mathbf{r}_i = \mathbf{A}_N \mathbf{E} - \mathbf{A}_N \mathbf{x}_i \) and \( \mathbf{x}_i \) denoting \( i \)-th iterate. The tolerance is set to \( \varepsilon = 10^{-8} \) in order to ensure that the overall error is dominated by the discretization error instead of the algebraic one. The norm for residuum \( \| \mathbf{r}_i \|_{2^{N \times N}} \), due to Parseval’s theorem, equals to \( \| \mathbf{T}_N^{-1} \mathbf{r}_i \|_{L^2_\alpha(\mathbb{R}^d)} \), the \( L^2_\alpha \)-norm of corresponding trigonometric polynomial. The dual case is treated in an analogous way.

Remark 44 (Divergence-free convergence criterion). The most commonly used termination criterion in FFT-based algorithms is based on the divergence-free condition for the dual fields, \( \mathbf{A}_N \mathbf{e}_{(a)}^N \in \mathbb{J}_N \) with \( \mathbf{A}_N \) from \([50]\), \([54]\) \([31]\) \([59]\). Our analysis reveals that this criterion is reasonable only for the odd grids \([26]\), namely

\[
\mathbf{e}_{(a)}^N \in \mathbb{E}_N \iff \mathbf{A}_N \mathbf{e}_{(a)}^N \in \mathbb{J}_N.
\]

cf. Proposition \([27]\). Such property is lost for general grids when either minimizers or dual fields are conforming only up to the Nyquist frequencies \( \mathbf{k} \in 2^d \mathbb{Z}_N \setminus 2^d \mathbb{Z}_N \), so that

\[
\mathbf{e}_{(a)}^N \in \mathbb{E}_N \implies \mathbf{A}_N \mathbf{e}_{(a)}^N \in \overline{\mathbb{J}_N}, \quad \text{or} \quad \mathbf{e}_{(a)}^N \in \overline{\mathbb{E}_N} \implies \mathbf{A}_N \mathbf{e}_{(a)}^N \in \mathbb{J}_N.
\]

recall Proposition \([34]\). This observation is in agreement with \([54]\) Section 2.4.2, where the projection \( \mathbf{G}_{N,I}^\xi \) from Def. \([22]\) was utilized to obtain divergence-free fields.

Remark 45. The matrix \([61]\) needed in step (ii) can be assembled in an efficient way. The Fourier coefficients \([5]\) of each inclusion topology \( \tilde{f}(j)(\mathbf{m}) \in \mathbb{Z}_N^d \) for \( j = 1, \ldots, J \) are evaluated in the closed form and shifted by distance \( \mathbf{x}(j) \) to account for its position; the shift corresponds to element-wise multiplication by the matrix \( [\varphi_{-m}(\mathbf{x}(j))]_{m \in \mathbb{Z}_N^d} \). The sum over \( \mathbf{k} \in \mathbb{Z}_N^d \) can be performed with the FFT algorithm.

Remark 46 (Avoiding the solution of dual formulation). For odd grids \([26]\), the dual discrete minimizers \( \tilde{j}_{N}^{(a)} \) can be obtained from Eq. \([53]\) if the original minimizers \( \mathbf{e}_{(a)}^N \) are the exact solutions to the corresponding linear systems, see Section \([71]\). In reality, the linear systems are solved only approximately, so that \( \tilde{j}_{N}^{(a)} \notin \mathbb{J}_N \). This non-conformity can be corrected by the projection operator \( \mathbf{G}_{N,I}^\xi \) and, when \( \mathbf{A}_N \) is badly conditioned, by performing several CG iterations for the dual formulation, recall \([22]\) and \([67]\).

Remark 47 (Arbitrary accurate bounds). In \([2]\) Proposition 4.5, the convergence of discrete minimizers to exact ones

\[
\| \mathbf{e}^{(a)} - \mathbf{e}_{(a)}^{N} \|_{L^2_\alpha(\mathbb{R}^d)} \to 0 \quad \text{for} \quad \min \alpha N \to \infty
\]

was proven for odd grids \([26]\), and the same holds for the dual minimizers. By \([25]\), the two-sided bounds, can be made arbitrarily accurate for sufficiently fine discretizations.

8. Numerical experiments

This section is dedicated to numerical experiments supporting our theoretical results, especially on the primal-dual structure and convergence of homogenized matrices. The calculations in Sections 8.1 and 8.2 are performed on a two-dimensional cell with a square inclusion first, in order to demonstrate the difference between odd and non-odd discretization grids and to study the behavior of upper-lower bounds as a function of grid spacing and contrast in coefficients. Section 8.3 deals with the determination of effective thermal conductivity of an alkali-activated fly ash foam described with a high-resolution bitmap. All results in this section were obtained with an open-source Python library FFTHomPy available at https://github.com/vondrecj/FFTHomPy.
In Sections 8.1 and 8.2, we consider problems with coefficients defined on the periodic cell $Y = (-1,1) \times (-1,1) \subset \mathbb{R}^2$ via

$$A(x) = [1 + \rho f(x)]I \quad \text{for} \quad x \in Y,$$

where $I \in \mathbb{R}^{2 \times 2}$ is the identity matrix, $f : Y \to \mathbb{R}$ is the topology function introduced in Remark 39, and $\rho \in \{10, 10^3\}$ is the phase contrast. Three types of square inclusions are considered, namely

$$f(x) = \begin{cases} 1 & \text{if } |x_\alpha| < \frac{3}{5} \text{ for all } \alpha \\ 0 & \text{otherwise} \end{cases}, \quad (68a)$$

$$f(x) = \begin{cases} 1 & \text{if } |x_\alpha| < \frac{3}{4} \text{ for all } \alpha \\ 0 & \text{otherwise} \end{cases}, \quad (68b)$$

$$f(x) = \begin{cases} 1 & \text{if } |x_\alpha| \leq \frac{3}{4} \text{ for all } \alpha \\ 0 & \text{otherwise} \end{cases}. \quad (68c)$$

The square (68a) is discretized with odd number of points $N = (n,n)$ for $n \in \{5 \cdot 3^j : j = 0,1,\ldots,6\}$, see Figure 6(a), while squares (68b) and (68c) with even number of points, $n \in \{2^j : j = 2,3,\ldots,10\}$, Figure 6(b). The difference in topologies (68b) and (68c), as demonstrated in Figure 6, is that the interface is associated with the inclusion for (68b) and with the matrix phase for (68c). For even discretizations, some of the grid points (31) are located exactly at the interface; the topologies (68b) and (68c) thus highlight the effect of the interpolation operator in GaNi scheme (48).

Because the inclusions (68a), (68b), and (68c) are symmetric with respect to the origin and the material phases are isotropic, the homogenized matrices are proportional to identity $I$ and only one diagonal component is plotted in Figures 7–11.

8.1. Homogenized matrices for odd discretization

For odd grids (26), the approximate homogenized matrices $A_{H,N}, B_{H,N}$ calculated from GaNi, recall (48), are mutually inverse $A_{H,N} = B_{H,N}^{-1}$, as stated in Proposition 33. The inequality $B_{H,N}^{-1} \preceq A_{H,N}$ of upper-lower bounds, stated in Lemma 12 (i), is satisfied and the guaranteed error (59a) converges to zero according to Lemma 13. By the same arguments, the approximate homogenized matrices $A_{H,N} = B_{H,N}^{-1}$ from GaNi and the mean of guaranteed bounds $\overline{A}_{H,N}$, (59a), converge to $A_{H}$. Since the inclusion shape is sampled with the grid points accurately, matrices $A_{H,N} = B_{H,N}^{-1}$ from GaNi approximate the homogenized properties better than the mean of guaranteed bounds $\overline{A}_{H,N}$, especially for a small number of grid points.

Figure 6: Cells with odd and even number of grid points

(a) Topology (68a) and odd grids (b) Topologies (68b), (68c) and even grids

27
No. of discretization points \( n \); \( N = (n, n) \). 

1.7
1.8
1.9
2.0
2.1
2.2
2.3

Homogenized matrix (component 11) \( A_{H,N} \), \( B^{-1}_{H,N} \). 

\[ A_{H,N} = B_{H,N}^{-1} \]

Phase contrast \( \rho = 10 \)

Figure 7: Homogenized matrices for cell (68a) and odd grids

In Figure 8 we plot analogous results to Figure 7 for a refined sequence of grid points \( N = (n, n) \) with \( n \in \{5, 7, 9, \ldots, 145\} \). The results reveal that the convergence of guaranteed error \( \varepsilon_N \), Remark 47, is not monotone with an increasing number of grid points, despite the hierarchy of approximation spaces

\[ \delta_N \subseteq \delta_M \subset \delta \quad \text{and} \quad \mathcal{F}_N \subseteq \mathcal{F}_M \subset \mathcal{F} \quad \text{for} \quad N_\alpha \leq M_\alpha. \] \hspace{1cm} (69)

We attribute this behavior to the numerical integration in approximate bilinear forms \( a_N \) and \( a_M^{-1} \) in (47), so that the solutions corresponding to two discretizations \( N \) and \( M \) from (69) are determined for different sampling of material coefficients \( A \). This “variational crime” \cite{60} results in the non-monotous convergence of the approximate solutions; their convergence is nevertheless assured by \cite[Proposition 8]{2}. Moreover, no oscillations have been observed for the Galerkin method without numerical integration \cite{56}.

8.2. Homogenized matrices for even discretization

This section is dedicated to the topologies (68b) and (68c) and discretizations with even grids, see Figure 6(b), considering phase contrasts \( \rho \in \{10, 10^3\} \).

In particular, Figures 9 and 10 show that the approximate homogenized matrices \( A_{H,N} \) and \( B_{H,N}^{-1} \) from GaNi are different for even grids, nevertheless they still satisfy \( B_{H,N}^{-1} \preceq A_{H,N} \), in agreement with Theorem 34. Moreover, the duality gap decreases as the effect of the Nyquist frequencies diminishes with
an increasing number of grid points, and both matrices converge to the homogenized matrix $A_H$. The same holds for the upper-lower bounds $A_{H,N}$, $B^{-1}_{H,N}$ and their mean $\overline{A}_{H,N}$.

![Figure 9: Homogenized matrices for cells (68b) and (68c), even grids, and phase contrast $\rho = 10$](image)

For both topologies (68b) or (68c), the matrices $A_{H,N}$ and $B^{-1}_{H,N}$ from GaNi may provide inaccurate prediction of homogenized properties as they, in some cases, fall outside the upper-lower bounds $A_{H,N}$ and $B^{-1}_{H,N}$. The mean of guaranteed bounds $\overline{A}_{H,N}$, or one of the upper-lower bounds $A_{H,N}$ or $B^{-1}_{H,N}$ if the worst case scenario is needed, always provides admissible values.

![Figure 10: Homogenized matrices for cells (68b) and (68c), even grids, and phase contrast $\rho = 10^3$](image)

Finally, in Figure 11, the upper-lower bounds $\overline{A}_{H,N}$ and $\overline{B}_{H,N}$ are compared for both topologies (68b) and (68c), which differ only at the interface. A significant difference is observed especially for the upper bound and the higher phase ratio $\rho = 10^3$, which is caused by inaccurate approximation of minimizers along the interface, cf. [34].

### 8.3. Alkali-activated ash foam

We are concerned with the determination of effective thermal conductivity of an alkali-activated ash foam, characterized with the $1,200 \times 1,200$ bitmap shown in Figure 12(a). The spatial distribution of the material coefficients

$$A(x) = [0.49 f(x) + 0.029 (1 - f(x))] I \quad \text{for} \quad x \in \mathcal{Y}$$

(70)
is defined with the help of the pixel-wise constant fly ash phase characteristic function \( f : \mathcal{Y} \rightarrow \{0, 1\} \) and the thermal conductivities of fly ash \((0.49 \text{ Wm}^{-2}\text{K}^{-1})\) and air \((0.029 \text{ Wm}^{-2}\text{K}^{-1})\) [61]. The determination of all primal-dual homogenized matrices

\[
A_{H,N} = \begin{bmatrix}
0.137997 & -0.0003841 \\
-0.0003841 & 0.1287557
\end{bmatrix}, \quad
B_{H,N}^{1} = \begin{bmatrix}
0.1379880 & -0.0003840 \\
-0.0003840 & 0.1287849
\end{bmatrix},
\]

\[
\overline{A}_{H,N} = \begin{bmatrix}
0.1409678 & -0.0004043 \\
-0.0004043 & 0.1319070
\end{bmatrix}, \quad
\overline{B}_{H,N}^{1} = \begin{bmatrix}
0.1283959 & -0.0004628 \\
-0.0004628 & 0.1200422
\end{bmatrix},
\]

\[
\underline{A}_{H,N} = \begin{bmatrix}
0.1348223 & -0.0004335 \\
-0.0004335 & 0.1259746
\end{bmatrix}, \quad
D_{N} = \begin{bmatrix}
0.0062864 & 0.0000292 \\
0.0000292 & 0.0059324
\end{bmatrix},
\]

involves solutions of two linear systems with \(2.88 \times 10^{6}\) unknowns and two right hand sides and evaluation of lower-upper bounds by the double-grid quadrature, Section 7.2 which took about fifteen minutes on a conventional laptop with Intel®Core™i5-4200M CPU @ 2.5 GHz \(\times\) 2 processor and 8 GB of RAM.

As in the previous section, the homogenized matrices of the GaNi scheme [71a] slightly differ because of the algebraic error due to iterative solution of linear systems and the effect of the Nyquist frequencies, but still satisfy \(B_{H,N}^{1} \leq A_{H,N}\) in agreement with Proposition 54. The guaranteed error \(D_{N}\), however, remains rather large, which we attribute again to inaccuracy of local fields in the vicinity of interfaces [34].

We have demonstrated in [55] pp. 142–145 that the solution accuracy can be substantially improved when smoothing the coefficients. For this purpose, we replace the grid values of the fly ash characteristic function with a local average

\[
\hat{f}_{\text{smoothed}}(x_{N}^{k}) = \frac{4}{16}f(x_{N}^{k}) + \frac{2}{16}[f(x_{N}^{k+1,0}) + f(x_{N}^{k-1,0}) + f(x_{N}^{k+0,1}) + f(x_{N}^{k-0,1})] \\
+ \frac{1}{16}[f(x_{N}^{k+1,1}) + f(x_{N}^{k-1,1}) + f(x_{N}^{k+1,-1}) + f(x_{N}^{k-1,-1})],
\]

which keeps the data almost unchanged, see Figure 12(b). The corresponding homogenized properties then read as

\[
A_{H,N} = \begin{bmatrix}
0.1418904 & -0.0004085 \\
-0.0004085 & 0.1328166
\end{bmatrix}, \quad
B_{H,N}^{1} = \begin{bmatrix}
0.1418902 & -0.0004085 \\
-0.0004085 & 0.1328162
\end{bmatrix},
\]

\[
\overline{A}_{H,N} = \begin{bmatrix}
0.1422750 & -0.0004159 \\
-0.0004159 & 0.1332686
\end{bmatrix}, \quad
\overline{B}_{H,N}^{1} = \begin{bmatrix}
0.1408147 & -0.0004152 \\
-0.0004152 & 0.1318124
\end{bmatrix},
\]

\[
\underline{A}_{H,N} = \begin{bmatrix}
0.1415448 & -0.0004155 \\
-0.0004155 & 0.1325396
\end{bmatrix}, \quad
D_{N} = \begin{bmatrix}
0.0007302 & 0.0000004 \\
0.0000004 & 0.0007272
\end{bmatrix}.
\]
Notice that, as a result of smoothing, the error (72c) decreases by an order of magnitude (even more accurate results can be obtained for the Galerkin method with exact integration [54]), while the eigenvalues of the new homogenized matrices (72a) and (72b) increase. This behavior occurs because we decided to smooth the primal coefficients $A$; the extreme case would correspond to the Voigt bound where the coefficients are replaced with the mean value $\langle A \rangle$. By analogy, smoothing of the dual coefficients $A^{-1}$ decreases the homogenized properties in the direction of the Reuss bound $\langle A^{-1} \rangle^{-1}$.

9. Conclusion

We have presented a method for the reliable determination of homogenized matrices arising from the cell problem (11) discretized with the Galerkin approximation with numerical integration (GaNi), introduced recently in [2] by the authors for uniform grids with an odd number of points. The method employs trigonometric polynomials as the approximation space and delivers conforming minimizers that are used to evaluate guaranteed upper-lower bounds on the homogenized matrix. Our most important findings are summarized as follows:

- A generalization of GaNi for a non-odd number of grid points is provided as a method for delivering conforming approximations of minimizers.
- Primal and dual formulations are investigated in discretized and fully discrete forms. Interestingly, duality is completely preserved for an odd number of grid points. For non-odd discretization, the structure is violated due to Nyquist frequencies. Our advice is to use odd grids whenever possible.
- The idea of upper-lower bounds on a homogenized properties, independently proposed by Dvořák [43] and Więckowski [46] for the Finite Element Method (FEM), has been successfully applied within the framework of FFT-Galerkin methods. Moreover, thanks to convergence result in [2, Proposition 8], these bounds can be made arbitrarily accurate. Unlike the FEM, it results in primal and dual problems with the same structure. Therefore, our developments can be easily generalized beyond the scalar elliptic problems considered in this work, as done recently by Monchiet [62] for the case of linear elasticity.
- Our theoretical findings are confirmed by numerical examples in Section 8 for both odd and even discretization as well as by analysis of a real-world material system.
Appendix A. Primal-dual formulations

This appendix is dedicated to the proof of Proposition 6 summarizing duality arguments for both continuous \cite{11} and discrete homogenization problems \cite{52} and \cite{54}. Although several related results are available in the literature, e.g. \cite{63, 52, 11}, we have failed to find them in a form compatible with our homogenization setting. Our expositions combine Dvořák’s results \cite{13, 13} with Ekeland and Temam’s general duality theory \cite{64} page 46–51. In particular, the following lemma adjusts the arguments of \cite{64} Proposition 2.1 and Remark 2.3 to the current framework, connects the primal and the dual formulations, and provides a way to prove Proposition 6.

Lemma 48 (Perturbation duality theorem). Consider Hilbert spaces $\hat{\mathcal{H}}$ and $\mathcal{H}$ such that $\hat{\mathcal{H}} \subset \mathcal{H}$, and let $\Phi : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ and $\Phi^* : \hat{\mathcal{H}} \times \mathcal{H} \to \mathbb{R}$ we denote a perturbed functional with its Fenchel’s conjugate, i.e.
\[
\Phi(u, v) = F(u + v), \quad \Phi^*(u^*, v^*) = \max_{u \in \hat{\mathcal{H}}, v \in \mathcal{H}} \left[ (u^*, u)_{\hat{\mathcal{H}}} + (v^*, v)_{\mathcal{H}} - \Phi(u, v) \right]. \tag{A.1}
\]

Then, the extremal values of the primal problem
\[
\min_{\hat{e} \in \hat{\mathcal{H}}} F(\hat{e}) = \min_{\hat{e} \in \hat{\mathcal{H}}} \Phi(\hat{e}, 0)
\]
and the dual problem
\[
\max_{v^* \in \mathcal{H}} -\Phi^*(0; v^*)
\]
coincide, i.e.
\[
\min_{\hat{e} \in \hat{\mathcal{H}}} \Phi(\hat{e}, 0) = \max_{v^* \in \mathcal{H}} -\Phi^*(0; v^*).
\]

Proof of Proposition 6. In order to utilize Lemma 48 we define a functional $F : \mathcal{H} \to \mathbb{R}$ and its perturbation $\Phi : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ for a given $E \in \mathbb{R}^d$ as
\[
F(\hat{e}) = \frac{1}{2} \hat{u}(E + \hat{e}, E + \hat{e}) \quad \quad \Phi(\hat{e}, v) = \frac{1}{2} \hat{u}(E + \hat{e} + v, E + \hat{e} + v).
\]

Because the linear operator $\hat{A}$ is coercive, the perturbation functional $\Phi$ is convex and Lemma 48 can be employed. The primal formulation is then equivalent to the dual formulation
\[
\left( \hat{A}_H E, E \right)_{\hat{\mathcal{H}}} = \min_{\hat{e} \in \hat{\mathcal{H}}} 2F(\hat{e}) = 2 \min_{\hat{e} \in \hat{\mathcal{H}}} \Phi(\hat{e}, 0) = 2 \max_{v^* \in \mathbb{R}^{\mathcal{H}}} -\Phi^*(0, v^*), \tag{A.2}
\]
where $0 \in \hat{\mathcal{H}} \subset \mathcal{H}$ is the zero vector and $\Phi^* : \hat{\mathcal{H}} \times \mathcal{H} \to \mathbb{R}$ is the Fenchel conjugate function according to $\triangledown$.1.1.

Now, we investigate (A.2) to retrieve the dual formulation (12b). Using substitution $v^* = E + \hat{e} + v$ where $v^*$ covers the whole space $\mathcal{H}$, we deduce
\[
\left( \hat{A}_H E, E \right)_{\hat{\mathcal{H}}} = 2 \max_{v^* \in \mathcal{H}} -\Phi^*(0, v^*) = 2 \max_{v^* \in \mathcal{H}} \left[ -\max_{\hat{e} \in \hat{\mathcal{H}}} \left( v^*, v^* - E - \hat{e} \right)_{\mathcal{H}} - \frac{1}{2} (\hat{A}v^*, v^*)_{\mathcal{H}} \right]
\]
\[
= 2 \max_{v^* \in \mathcal{H}} \left[ (v^*, E)_{\mathcal{H}} + \min_{\hat{e} \in \hat{\mathcal{H}}} (v^*, \hat{e})_{\mathcal{H}} - \max_{v^* \in \mathcal{H}} \left( v^*, v^* \right)_{\mathcal{H}} - \frac{1}{2} (\hat{A}v^*, v^*)_{\mathcal{H}} \right].
\]

We focus on the maximizer $\hat{v}$ of the last equation, which satisfies $\hat{A}\hat{v} = v^*$. Assuming of Proposition 6 the operator $\hat{A}$ is invertible; hence, we obtain $\hat{v} = \hat{A}^{-1} v^*$, and the inner max-term simplifies to
\[
\max_{v^* \in \mathcal{H}} \left( v^*, v^* \right)_{\mathcal{H}} - \frac{1}{2} (\hat{A}v^*, v^*)_{\mathcal{H}} = \frac{1}{2} (\hat{A}^{-1} v^*, v^*)_{\mathcal{H}}.
\]
We have utilized the decomposition \( v^* = J + \hat{\mathbf{j}} \in \hat{\mathcal{U}} \oplus \hat{\mathcal{J}} \) with \( J \in \hat{\mathcal{U}} \) and \( \hat{\mathbf{j}} \in \hat{\mathcal{J}} \).

The min-term in the last equation (A.3) already matches the dual formulation (12b), namely

\[
(B_H J, J)_{\mathbb{R}^d} = \min_{\hat{\mathbf{j}} \in \mathcal{J}} (A^{-1}(J + \hat{\mathbf{j}}), J + \hat{\mathbf{j}})_{\mathcal{H}},
\]

where we have utilized the decomposition \( v^* = J + \hat{\mathbf{j}} \in \hat{\mathcal{U}} \oplus \hat{\mathcal{J}} \) with \( J \in \hat{\mathcal{U}} \) and \( \hat{\mathbf{j}} \in \hat{\mathcal{J}} \). Now, we will show that \( \tilde{A}_H = B_H^{-1} \) as claimed in (13). Notice first that the matrix \( B_H \) is invertible as it is symmetric and coercive because the linear operator \( \tilde{A}^{-1} \) is symmetric and coercive (see Remark 9 for similar arguments). Next, the dual formulation (A.3) simplifies to

\[
(A_H E, E)_{\mathbb{R}^d} = \max_{J \in \mathbb{R}^d} \left[ 2(J, E)_{\mathbb{R}^d} - (B_H J, J)_{\mathbb{R}^d} \right]
\]

and the maximum is attained for \( J = B_H^{-1} E \) that, when substituted back to (A.4), provides the desired identity (13).

The relation between minimizers in (14) using the identity between homogenized matrices (13) must still be proven. Indeed, the stationarity condition for the primal formulation (12a), i.e. \( \hat{\mathbf{u}}_t = \hat{\mathbf{A}}_t \hat{\mathbf{u}}_t + \hat{\mathbf{v}}_t \in \hat{\mathcal{U}} \oplus \hat{\mathcal{J}} \) and \( (\hat{\mathbf{A}}_H E, E)_{\mathbb{R}^d} = \hat{\mathbf{u}}_t (E + \hat{\mathbf{v}}_t(E), E) = \hat{\mathbf{u}}_t (E + \hat{\mathbf{v}}_t(E), E), \) (A.5)

holding for arbitrary \( E \in \mathbb{R}^d \). Combining both in (A.5) and setting \( \mathbf{J} = \hat{\mathbf{A}}_H E \), we obtain \( \hat{\mathbf{A}} (E + \hat{\mathbf{v}}_t(E)) = \mathbf{J} + \hat{\mathbf{j}}_t \) with \( \hat{\mathbf{j}}_t \in \hat{\mathcal{J}} \).

The relation (14) will be established once showing that \( \hat{\mathbf{j}}_t = \hat{\mathbf{j}}_t \). For \( \hat{\mathbf{J}} = \hat{\mathbf{A}}_H E \), the extremal values in (12) coincide, so that

\[
\hat{\mathbf{u}}_t^{-1}(\mathbf{J} + \hat{\mathbf{j}}_t, J + \hat{\mathbf{j}}_t) = \hat{\mathbf{u}}_t (E + \hat{\mathbf{v}}_t(E), E + \hat{\mathbf{v}}_t(E)) = \hat{\mathbf{u}}_t (E + \hat{\mathbf{v}}_t(E), E + \hat{\mathbf{v}}_t(E))_{\mathcal{H}}
\]

and hence \( \hat{\mathbf{j}}_t = \hat{\mathbf{j}}_t \) holds because \( \hat{\mathbf{v}}_t(E) \) is the unique minimizer.

\[ \square \]

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