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Estimates of the modeling error generated by homogenization of an elliptic boundary value problem

Abstract: In this paper, we derive a posteriori bounds of the difference between the exact solution of an elliptic boundary value problem with periodic coefficients and an abridged model, which follows from the homogenization theory. The difference is measured in terms of the energy norm of the basic problem and also in the combined primal–dual norm. Using the technique of functional type *a posteriori* error estimates, we obtain two-sided bounds of the modeling error, which depends only on known data and the solution of the homogenized problem. It is proved that the majorant with properly chosen arguments possesses the same convergence rate, which was established for the true error. Numerical tests confirm the efficiency of the estimates.

Keywords: periodic structures, homogenization, elliptic boundary value problems, *a posteriori* error estimates, modeling error

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1 Introduction

Boundary value problems with periodic structures arise in various applications. Homogenization theory is the major tool used to quantitatively analyze media with periodic structures. Within the framework of the theory (see, e.g., [9, 14]), the behavior of a heterogeneous media is described with the help of a certain homogenized problem, which is typically a boundary value problem with smooth coefficients, and the solution of a specially constructed problem with periodic boundary conditions. It has been proved that the functions reconstructed by this procedure converge to the exact solution as the cell size ε tends to zero. Moreover, known a priori error estimates qualify the convergence rate in terms of ε. The goal of this paper is to derive two-sided estimates of the modeling error generated by homogenization. In other words, we wish to estimate the difference between the exact solution of the original problem and its approximation obtained by the corresponding homogenized model.

Let $\Omega \subseteq \mathbb{R}^d$ be a bounded domain with Lipschitz boundary $\partial\Omega$, such that $\Omega = \bigcup_{\mathbf{i}} \Pi_{\mathbf{i}}^{\varepsilon}$, where

$$\Pi_{\mathbf{i}}^{\varepsilon} = \mathbf{x}_{\mathbf{i}} + \varepsilon\,\widehat{\Pi} = \left\{ \mathbf{x} \in \mathbb{R}^d \;\middle|\; \frac{\mathbf{x} - \mathbf{x}_{\mathbf{i}}}{\varepsilon} \in \widehat{\Pi} \right\}$$

is the basic 'cell' (repeating element of the periodic structure, see Fig. 1), which is a simply connected domain with Lipschitz boundary, $\mathbf{x}_{\mathbf{i}}$ is the reference point of $\Pi_{\mathbf{i}}^{\varepsilon}$, and ε is a small parameter (geometrical size of a cell). Here and later on, $\mathbf{x}$ denotes the global (Cartesian) coordinate system in $\mathbb{R}^d$ and $\mathbf{i} = (i_1, i_2, \dots, i_d)$ denotes the counting multi-indices for the cells. The notations $\bigcup_{\mathbf{i}}$ and $\sum_{\mathbf{i}}$ are shorthands for the union and summation over all cells. It is assumed that the overall amount of $\Pi_{\mathbf{i}}^{\varepsilon}$ in Ω is bounded from above by the

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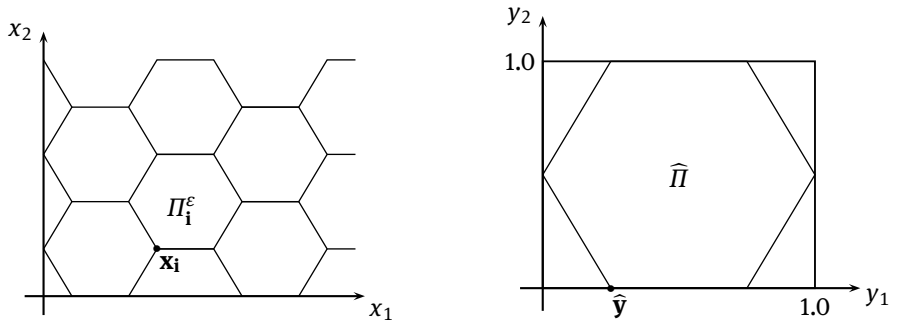

Figure 1. Periodic structure (left) and its basic cell (right).

quantity

$$c_0\,\varepsilon^{-d}, \quad c_0 = \mathcal{O}(1) \tag{1.1}$$

and the diameter of $\Pi_{\mathbf{i}}^{\varepsilon}$ satisfies the relation

$$\operatorname{diam}\Pi_{\mathbf{i}}^{\varepsilon} = \rho\,\varepsilon \tag{1.2}$$

where ρ is a parameter depending on the geometry of the cell. Usually, ρ is easy to find (e.g., for a cubic cell $\rho = \sqrt{d}$).

In the basic cell (see Fig. 1), we use local Cartesian coordinates $\mathbf{y} \in \mathbb{R}^d$. For any $\Pi_{\mathbf{i}}^{\varepsilon}$, local and global coordinates are joined by the relation

$$\mathbf{y} = \frac{\mathbf{x} - \mathbf{x_i}}{\varepsilon} \in \widehat{\Pi} \qquad \forall\,\mathbf{x} \in \Pi_{\mathbf{i}}^{\varepsilon}, \quad \forall\,\mathbf{i}.$$

On $\widehat{\Pi}$, we define a matrix function $\widehat{A} \in L^{\infty}(\widehat{\Pi}, \mathbb{R}_{\mathrm{sym}}^{d\times d})$, where $\mathbb{R}_{\mathrm{sym}}^{d\times d}$ denotes the set of symmetric $d \times d$-matrices. We assume that

$$c_1|\xi|^2 \leqslant \widehat{A}(\mathbf{y})\xi\cdot\xi \leqslant c_2|\xi|^2 \qquad \forall\,\xi \in \mathbb{R}^d, \quad \forall\,\mathbf{y} \in \widehat{\Pi} \tag{1.3}$$

where $0 < c_1 \leqslant c_2 < \infty$ and introduce the 'global' matrix

$$A_\varepsilon(\mathbf{x}) := \widehat{A}\left(\frac{\mathbf{x} - \mathbf{x_i}}{\varepsilon}\right) \qquad \forall\,\mathbf{x} \in \Pi_{\mathbf{i}}^{\varepsilon}, \quad \forall\,\mathbf{i} \tag{1.4}$$

which defines the periodic structure on Ω. In view of (1.3), A_ε (and its inverse counterpart A_ε^{-1}) satisfy similar two-sided estimates for any ε.

Consider the second-order elliptic equation

$$-\operatorname{div}(A_\varepsilon \nabla u_\varepsilon) = f \quad \text{in } \Omega, \qquad f \in L^2(\Omega) \tag{1.5}$$

with homogeneous Dirichlet boundary conditions. The corresponding generalized solution $u_\varepsilon \in H_0^1(\Omega)$ is defined by the relation

$$\int_\Omega A_\varepsilon \nabla u_\varepsilon \cdot \nabla w = \int_\Omega f w \qquad \forall\, w \in H_0^1(\Omega). \tag{1.6}$$

For any $\varepsilon > 0$, the solution u_ε exists and is unique.

For a function $\zeta \in L^1(\omega)$, where ω is a measurable subset of Ω, we define the mean value by

$$\langle\zeta\rangle_\omega := \frac{1}{|\omega|}\int_\omega \zeta. \tag{1.7}$$

If no confusion may arise, we omit in integrals the symbol of the corresponding Lebesque measure (e.g., $\mathrm{d}\mathbf{x}$). However, we write the measure explicitly if it is necessary to distinguish between integration over the global and local coordinates (as in Lemma 2.1).

If we write $\int_\omega \langle\zeta\rangle_\omega$, then the average is considered as a constant function on ω (for vector-valued functions, we apply this definition componentwise). The error caused by the averaging (1.7) is denoted by

$$\delta_\omega \zeta := \|\zeta - \langle\zeta\rangle_\omega\|_\omega$$

where $\|\cdot\|_\omega$ denotes the standard L^2–norm on ω.

For a vector $\boldsymbol{\mu} = (\mu_i)_{i=1}^d \in (\mathbb{R}_{>0})^d$ and $s \in \mathbb{R}$, $\boldsymbol{\mu}^s$ denotes the componentwise application of the power s, i.e., $\boldsymbol{\mu}^s = (\mu_i^s)_{i=1}^d$. For vector-valued functions $\boldsymbol{\zeta} = (\zeta_k)_{k=1}^d \in L^1\left(\omega, \mathbb{R}^d\right)$ and $\boldsymbol{\varphi} = (\varphi_k)_{k=1}^d \in L^1\left(\Omega, \mathbb{R}^d\right)$, we define the local and piecewise constant averages by means of the relations

$$\delta_\omega \boldsymbol{\zeta} := \left(\|\zeta_k - \langle\zeta_k\rangle_\omega\|_\omega\right)_{k=1}^d, \qquad \delta_\Omega^{\mathrm{pw}} \boldsymbol{\varphi} := \varepsilon^{d/2}\left(\sum_{\mathbf{i}} \|\varphi_k - \langle\varphi_k\rangle_{\Pi_\mathbf{i}^\varepsilon}\|_{\Pi_\mathbf{i}^\varepsilon}\right)_{k=1}^d$$

and

$$(\delta_\omega \boldsymbol{\zeta})^2 := \left(\|\zeta_k - \langle\zeta_k\rangle_\omega\|_\omega^2\right)_{k=1}^d, \qquad (\delta_\Omega^{\mathrm{pw}} \boldsymbol{\varphi})^2 := \varepsilon^d \left(\left(\sum_{\mathbf{i}} \|\varphi_k - \langle\varphi_k\rangle_{\Pi_\mathbf{i}^\varepsilon}\|_{\Pi_\mathbf{i}^\varepsilon}\right)^2\right)_{k=1}^d.$$

Within the framework of homogenization theory, an approximation of u_ε is constructed by the following procedure (see, e.g., [7, 9, 14]). First, we define (for $k = 1, 2, \ldots, d$) the solutions N_k of 'cell problems'

$$\begin{gathered} \operatorname{div}\left(\widehat{A}\,\nabla N_k\right) = \left(\operatorname{div}\widehat{A}\right)_k \quad \text{in } \widehat{\Pi} \\ N_k \text{ is periodic in } \widehat{\Pi} \\ \int_{\widehat{\Pi}} N_k = 0. \end{gathered} \tag{1.8}$$

With the help of them, the homogenized matrix

$$A_0 = \left\langle \widehat{A}\,(I - \nabla \boldsymbol{N}) \right\rangle_{\widehat{\Pi}} \tag{1.9}$$

is defined. The function $u_0 \in H_0^1(\Omega)$ such that

$$\int_\Omega A_0 \nabla u_0 \cdot \nabla w = \int_\Omega f\, w \qquad \forall\, w \in H_0^1(\Omega) \tag{1.10}$$

provides a "coarse" approximation of u_ε. It is known that (see, e.g., [7]),

$$u_\varepsilon \to u_0 \quad \text{in } L^2(\Omega), \qquad\qquad u_\varepsilon \rightharpoonup u_0 \quad \text{in } H_0^1(\Omega) \quad \text{for } \varepsilon \to 0.$$

However, it is necessary to construct a sequence of more accurate approximations, which converges in a stronger sense. For this purpose, the homogenization theory suggests to use advanced approximations

$$w_\varepsilon^1(\mathbf{x}) := u_0(\mathbf{x}) - \varepsilon \psi^\varepsilon(\mathbf{x})\, N_k\left(\frac{\mathbf{x} - \mathbf{x}_\mathbf{i}}{\varepsilon}\right) \frac{\partial u_0(\mathbf{x})}{\partial x_k} \quad \forall\, \mathbf{x} \in \Pi_\mathbf{i}^\varepsilon, \quad \forall\, \mathbf{i} \tag{1.11}$$

where $\psi^\varepsilon := \min\{1,\ \operatorname{dist}(\mathbf{x},\ \partial\Omega)/\varepsilon\}$ is a cutoff function.

To prove optimal *a priori* convergence rates for the modeling error

$$e_\varepsilon^{\mathrm{mod}} := u_\varepsilon - w_\varepsilon^1 \tag{1.12}$$

we need some extra assumptions (see [14], p.28), namely,

$$u_0 \in W^{2,\infty}(\overline{\Omega}) \tag{1.13}$$

and

$$\frac{\partial N_k}{\partial y_j} \in L^\infty(\widehat{\Pi}). \tag{1.14}$$

Then, it can be proved (see, e.g., [7], Remark 5.13; [10]; [14], p. 28) that the modeling error satisfies the asymptotic estimates:

$$\|u_\varepsilon - w_\varepsilon^1\|_{H^1(\Omega)} \leqslant \widetilde{c}\,\sqrt{\varepsilon} \tag{1.15}$$

and

$$\|A_\varepsilon \nabla u_\varepsilon - \mathbf{v_0} - \varepsilon\, \mathbf{v_1}\| \leqslant \widehat{c}\, \sqrt{\varepsilon} \tag{1.16}$$

where

$$\begin{aligned} \mathbf{v_0} &:= (I - \operatorname{curl}_{\mathbf{y}} \widetilde{N})\, \boldsymbol{\mu} \\ \boldsymbol{\mu} &:= \langle A_0^{-1}\, (I - \operatorname{curl}_{\mathbf{y}} \widetilde{N}) \rangle_{\widehat{\Pi}}^{-1}\, \nabla u_0 \\ \mathbf{v_1} &:= -\operatorname{curl}_{\mathbf{x}} (\widetilde{N}\, \boldsymbol{\mu}) \end{aligned} \tag{1.17}$$

the $d \times d$ matrix $\widetilde{N}$ with columns $\widetilde{N}_k$ is the solution of the auxiliary problem

$$\begin{gathered} \operatorname{curl} A_0^{-1} \Big(\operatorname{curl} \widetilde{N_k}(\mathbf{y}) \Big) = \operatorname{curl} \Big(A_0^{-1} \Big)_k \quad \text{in } \widehat{\Pi} \\ \operatorname{div} \widetilde{N}_k = 0 \\ \widetilde{N}_k \text{ is periodic in } \widehat{\Pi} \\ \int_{\widehat{\Pi}} \widetilde{N}_k = 0 \end{gathered} \tag{1.18}$$

and the columns of the matrix $\operatorname{curl}_{\mathbf{y}} \widetilde{N}$ are given by $\operatorname{curl}_{\mathbf{y}} \widetilde{N}_k$, $k = 1, 2, \dots, d$.

Numerical methods for homogenized problems are actively studied. Such questions as adaptivity and error indication are among the most important questions arising in quantitative analysis of periodical structures. Here, we first of all mention residual type error indicators that develop the ideas suggested in [2, 3] for finite element approximations. Since our approach is based on a different technique, we will sketch here only briefly some relevant literature on residual based estimation and refer for a detailed review, e.g., to [13]. A posteriori error estimates for the heterogeneous multiscale discretization (HMM) of elliptic problems in a periodic setting can be found in [12, 17]. In [1], an a posteriori estimate of residual type for general, possibly non-periodic, diffusion tensors with micro-scales is presented while a residual-type a posteriori error estimate for more general diffusion tensors has been developed in [13]. Also, we mention the papers [4, 5, 29, 30], which are closely related to the topic.

Our goal is to deduce estimates of $e_\varepsilon^{\mathrm{mod}}$ of a different type, which provide guaranteed and fully computable bounds of the modeling error. The corresponding error majorant uses the solution of the homogenized problem and, in addition, involves free functions and a function η defined on the cell of periodicity. This freedom can be utilized for improving the efficiency of the corresponding error bounds. Besides, the functions obtained in this way provide efficient reconstructions of the flux. In general, the estimates have the form

$$\mathcal{M}_\ominus \big(w_\varepsilon^1;\ \Theta\big) \leqslant \|\nabla (u_\varepsilon - w_\varepsilon^1)\|_{A_\varepsilon} \leqslant \mathcal{M}_\oplus \big(w_\varepsilon^1;\ \boldsymbol{\eta},\ \boldsymbol{\lambda},\ s\big) \tag{1.19}$$

where

$$\|\boldsymbol{q}\|_{A_\varepsilon} := \Big(\int_\Omega A_\varepsilon\, \boldsymbol{q} \cdot \boldsymbol{q} \Big)^{1/2}. \tag{1.20}$$

The majorant $\mathcal{M}_\oplus$ and a minorant $\mathcal{M}_\ominus$ are derived in Sections 2 and 3, respectively. Numerical tests are exposed in Section 4. They confirm the efficiency of the estimates.

2 Upper bound of the modeling error

First, we prove a subsidiary result, which states an upper bound of the L^2-product of a globally defined function and a periodic function defined on the cell.

Lemma 2.1. *For all $\mathbf{g} \in L^2(\Omega)^d$, $\boldsymbol{\eta} \in L^2(\widehat{\Pi})^d$, and all $\boldsymbol{\lambda} = (\lambda_d)_{k=1}^d \in (\mathbb{R}_{>0})^d$ it holds*

$$\sum_{\mathbf{i}} \int_{\Pi_{\mathbf{i}}^\varepsilon} \mathbf{g}(\mathbf{x}) \cdot \boldsymbol{\eta}\Big(\frac{\mathbf{x} - \mathbf{x_i}}{\varepsilon}\Big)\, \mathrm{d}\mathbf{x} \leqslant |\Omega|\, \langle \mathbf{g} \rangle_\Omega \cdot \langle \boldsymbol{\eta} \rangle_{\widehat{\Pi}} + \frac{\boldsymbol{\lambda}}{2} \cdot (\delta_\Omega^{\mathrm{pw}} \mathbf{g})^2 + \frac{\boldsymbol{\lambda}^{-1}}{2} \cdot (\delta_{\widehat{\Pi}} \boldsymbol{\eta})^2. \tag{2.1}$$

Proof. For any $\mathbf{g} \in L^2(\Omega)^d$, we have

$$\begin{aligned}\mathcal{I} &:= \sum_{\mathbf{i}} \int_{\Pi_{\mathbf{i}}^\varepsilon} \mathbf{g}(\mathbf{x}) \cdot \boldsymbol{\eta}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\,\mathrm{d}\mathbf{x} = \sum_{k=1}^{d} \sum_{\mathbf{i}} \int_{\Pi_{\mathbf{i}}^\varepsilon} g_k(\mathbf{x})\,\eta_k\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\,\mathrm{d}\mathbf{x} \\ &= \sum_{k=1}^{d} \sum_{\mathbf{i}} \int_{\Pi_{\mathbf{i}}^\varepsilon} (g_k(\mathbf{x}) - \langle g_k\rangle_{\Pi_{\mathbf{i}}^\varepsilon})\,\eta_k\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\,\mathrm{d}\mathbf{x} \;+\; \sum_{k=1}^{d} \sum_{\mathbf{i}} \int_{\Pi_{\mathbf{i}}^\varepsilon} \langle g_k\rangle_{\Pi_{\mathbf{i}}^\varepsilon}\,\eta_k\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\,\mathrm{d}\mathbf{x}.\end{aligned}$$

Since

$$\begin{aligned}\sum_{\mathbf{i}} \int_{\Pi_{\mathbf{i}}^\varepsilon} \langle g_k\rangle_{\Pi_{\mathbf{i}}^\varepsilon}\,\eta_k\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\,\mathrm{d}\mathbf{x} &= \varepsilon^d \Big(\int_{\widehat{\Pi}} \eta_k(\mathbf{y})\,\mathbf{dy}\Big) \sum_{\mathbf{i}} \frac{1}{|\Pi_{\mathbf{i}}^\varepsilon|} \int_{\Pi_{\mathbf{i}}^\varepsilon} g_k(\mathbf{x})\,\mathrm{d}\mathbf{x} \\ &= \varepsilon^d \Big(\int_{\widehat{\Pi}} \eta_k(\mathbf{y})\,\mathbf{dy}\Big) \sum_{\mathbf{i}} \frac{1}{\varepsilon^d\,|\widehat{\Pi}|} \int_{\Pi_{\mathbf{i}}^\varepsilon} g_k(\mathbf{x})\,\mathrm{d}\mathbf{x} \\ &= \int_{\widehat{\Pi}} \eta_k(\mathbf{y})\,\mathbf{dy}\,\frac{1}{|\widehat{\Pi}|} \int_{\Omega} g_k(\mathbf{x})\,\mathrm{d}\mathbf{x} \;=\; |\Omega|\,\langle g_k\rangle_{\Omega}\,\langle \eta_k\rangle_{\widehat{\Pi}}\end{aligned} \tag{2.2}$$

and for any $(c_k)_{k=1}^d \in \mathbb{R}^d$

$$\begin{aligned}\sum_{\mathbf{i}} \int_{\Pi_{\mathbf{i}}^\varepsilon} (g_k(\mathbf{x}) - \langle g_k\rangle_{\Pi_{\mathbf{i}}^\varepsilon})\,\eta_k\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\,\mathrm{d}\mathbf{x} &= \sum_{\mathbf{i}} \int_{\Pi_{\mathbf{i}}^\varepsilon} (g_k(\mathbf{x}) - \langle g_k\rangle_{\Pi_{\mathbf{i}}^\varepsilon}) \Big(\eta_k\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big) - c_k\Big)\,\mathrm{d}\mathbf{x} \\ &\leqslant \Big(\sum_{\mathbf{i}} \|g_k - \langle g_k\rangle_{\Pi_{\mathbf{i}}^\varepsilon}\|_{\Pi_{\mathbf{i}}^\varepsilon}\Big) \Big(\int_{\Pi_{\mathbf{i}}^\varepsilon} \Big(\eta_k\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big) - c_k\Big)^2\,\mathrm{d}\mathbf{x}\Big)^{1/2} \\ &= \Big(\sum_{\mathbf{i}} \|g_k - \langle g_k\rangle_{\Pi_{\mathbf{i}}^\varepsilon}\|_{\Pi_{\mathbf{i}}^\varepsilon}\Big)\;\varepsilon^{d/2}\,\|\eta_k - c_k\|_{\widehat{\Pi}}\end{aligned} \tag{2.3}$$

we find that

$$\begin{aligned}\mathcal{I} &\leqslant \sum_k \big(|\Omega|\,\langle g_k\rangle_{\Omega}\,\langle \eta_k\rangle_{\widehat{\Pi}} \;+\; (\delta_{\Omega}^{\mathrm{pw}} g)_k\,\|\eta_k - c_k\|_{\widehat{\Pi}}\big) \\ &\leqslant \sum_k \Big(|\Omega|\,\langle g_k\rangle_{\Omega}\,\langle \eta_k\rangle_{\widehat{\Pi}} \;+\; \frac{\lambda_k}{2}\,(\delta_{\Omega}^{\mathrm{pw}} g)_k^2 \;+\; \frac{1}{2\,\lambda_k}\,\|\eta_k - c_k\|_{\widehat{\Pi}}^2\Big) \\ &= |\Omega|\,\langle \mathbf{g}\rangle_{\Omega} \cdot \langle \boldsymbol{\eta}\rangle_{\widehat{\Pi}} \;+\; \frac{1}{2}\,\boldsymbol{\lambda} \cdot (\delta_{\Omega}^{\mathrm{pw}} \mathbf{g})^2 \;+\; \frac{1}{2} \int_{\widehat{\Pi}} \sum_k \frac{1}{\lambda_k} \Big(\eta_k - c_k\Big)^2\,\mathbf{dy}\end{aligned}$$

for any arbitrary vector $\boldsymbol{\lambda} \in \mathbb{R}^d_{>0}$. In particular, we set $c_k = \langle \eta_k\rangle_{\widehat{\Pi}}$, and obtain (2.1). □

In order to present the main estimate in a transparent form, we introduce the function

$$\mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x}) \;:=\; A_\varepsilon\,\nabla w_\varepsilon^1 \;-\; \boldsymbol{\tau}_0 \tag{2.4}$$

where

$$\boldsymbol{\tau}_0 \in H(\Omega,\,\mathrm{div}) := \{\boldsymbol{\vartheta} \in (L^2(\Omega))^d,\ \mathrm{div}\,\boldsymbol{\vartheta} \in L^2(\Omega)\} \tag{2.5}$$

and the quantity

$$\begin{aligned}\mathcal{F}\Big(w_\varepsilon^1;\ \boldsymbol{\tau}_0,\ \boldsymbol{\eta}, \boldsymbol{\lambda},\ s\Big) &:= \|\mathbf{g}_{\boldsymbol{\tau}_0}\|^2_{A_\varepsilon^{-1}} + 2\,\varepsilon^s\,|\Omega|\,\langle \mathbf{g}_{\boldsymbol{\tau}_0}\rangle_{\Omega} \cdot \langle \boldsymbol{\eta}\rangle_{\widehat{\Pi}} \\ &\quad + \varepsilon^s\Big(\boldsymbol{\lambda}^{-1} \cdot (\delta_{\widehat{\Pi}}\boldsymbol{\eta})^2 \;+\; \boldsymbol{\lambda} \cdot (\delta_{\Omega}^{\mathrm{pw}}(\mathbf{g}_{\boldsymbol{\tau}_0}))^2\Big) + c_0\varepsilon^{2s}\,\|\boldsymbol{\eta}\|^2_{\widehat{A}^{-1},\widehat{\Pi}}\end{aligned} \tag{2.6}$$

where $\boldsymbol{\lambda} \in \mathbb{R}^d_{>0}$, $s \in \mathbb{R}_{>0}$, and

$$\boldsymbol{\eta} \in H_0(\widehat{\Pi},\,\mathrm{div}) := \{\boldsymbol{\vartheta} \in H(\widehat{\Pi},\,\mathrm{div}),\ \langle \mathrm{div}\,\boldsymbol{\vartheta}\rangle_{\widehat{\Pi}} = 0\}. \tag{2.7}$$

Now, we can deduce the first (general) form of the majorant $\mathcal{M}_\oplus$. It is presented in Theorem 2.1 (see also [25]), which proof uses the technique developed in [19–27].

Theorem 2.1. *Let the cell of periodicity $\widehat{\Pi}$ be convex and the conditions* (1.1), (1.3), (1.9), (1.11), *and* (1.13) *be satisfied. Then, for any $\boldsymbol{\lambda} \in \mathbb{R}^d_{>0}$, $s \in \mathbb{R}_{>0}$, $\boldsymbol{\tau_0} \in H(\Omega, \operatorname{div})$ and $\boldsymbol{\eta} \in H_0(\widehat{\Pi}, \operatorname{div})$ we have the estimate*

$$\begin{aligned}\|\nabla(u_\varepsilon - w^1_\varepsilon)\|_{A_\varepsilon} \leqslant \mathcal{M}_\oplus\Big(w^1_\varepsilon, \boldsymbol{\tau_0}, \boldsymbol{\eta}, \boldsymbol{\lambda}, s\Big) := \mathcal{F}^{1/2}\Big(w^1_\varepsilon; \boldsymbol{\tau_0}, \boldsymbol{\eta}, \boldsymbol{\lambda}, s\Big) \\ + \widetilde{C}_{F_\Omega}\|\operatorname{div}\boldsymbol{\tau}_0 + f\| + \varepsilon^s \widetilde{C}\|\operatorname{div}\boldsymbol{\eta}\|_{\widehat{\Pi}}\end{aligned} \tag{2.8}$$

where $\mathcal{F}$, $\widetilde{C}_{F_\Omega}$ and $\widetilde{C}$ are defined by (2.6) *and* (2.13), *respectively.*

Proof. For any $v, w \in H^1_0(\Omega)$ and $\boldsymbol{\tau} \in H(\Omega, \operatorname{div})$, we have

$$\int_\Omega A_\varepsilon\nabla(u_\varepsilon - v)\cdot\nabla w = \int_\Omega(-A_\varepsilon\nabla v\cdot\nabla w + f\,w) = \int_\Omega(\boldsymbol{\tau} - A_\varepsilon\nabla v)\cdot\nabla w + \int_\Omega(\operatorname{div}\boldsymbol{\tau} + f)\,w. \tag{2.9}$$

We set $w = u_\varepsilon - v$ and estimate the first term in (2.9) as follows:

$$\int_\Omega(\boldsymbol{\tau} - A_\varepsilon\nabla v)\cdot\nabla(u_\varepsilon - v) \leqslant \|\nabla(u_\varepsilon - v)\|_{A_\varepsilon}\|A_\varepsilon\nabla v - \boldsymbol{\tau}\|_{A^{-1}_\varepsilon}. \tag{2.10}$$

Henceforth, we select $\boldsymbol{\tau}$ in a special form, namely,

$$\boldsymbol{\tau}(\mathbf{x}) = \boldsymbol{\tau}_0(\mathbf{x}) - \varepsilon^s\boldsymbol{\eta}\left(\frac{\mathbf{x} - \mathbf{x_i}}{\varepsilon}\right) \quad \text{on } \Pi^\varepsilon_{\mathbf{i}} \tag{2.11}$$

where

$$\boldsymbol{\eta} \in H_0(\widehat{\Pi}, \operatorname{div}).$$

Since

$$\operatorname{div}\boldsymbol{\tau}(\mathbf{x}) = \operatorname{div}\boldsymbol{\tau}_0(\mathbf{x}) - \varepsilon^s\operatorname{div}\boldsymbol{\eta}\left(\frac{\mathbf{x} - \mathbf{x_i}}{\varepsilon}\right) \quad \forall\,\mathbf{x} \in \Pi^\varepsilon_{\mathbf{i}}, \ \forall\,\mathbf{i}$$

and

$$\left\langle\operatorname{div}\boldsymbol{\eta}\left(\frac{\cdot - \mathbf{x_i}}{\varepsilon}\right)\right\rangle_{\Pi^\varepsilon_{\mathbf{i}}} = \varepsilon^{d-1}\langle\operatorname{div}\boldsymbol{\eta}\rangle_{\widehat{\Pi}} = 0$$

we obtain

$$\begin{aligned}\int_\Omega(\operatorname{div}\boldsymbol{\tau} + f)(u_\varepsilon - v)\,\mathrm{d}\mathbf{x} &= \int_\Omega(\operatorname{div}\boldsymbol{\tau}_0 + f)(u_\varepsilon - v)\,\mathrm{d}\mathbf{x} - \sum_{\mathbf{i}}\int_{\Pi^\varepsilon_{\mathbf{i}}}\varepsilon^s\operatorname{div}\boldsymbol{\eta}\left(\frac{\cdot - \mathbf{x_i}}{\varepsilon}\right)(u_\varepsilon - v)\,\mathrm{d}\mathbf{x} \\ &\leqslant C_{F_\Omega}\|\operatorname{div}\boldsymbol{\tau}_0 + f\|\,\|\nabla(u_\varepsilon - v)\| + \varepsilon^s\sum_{\mathbf{i}}\varepsilon^{d/2-1}\|\operatorname{div}\boldsymbol{\eta}\|_{\widehat{\Pi}}\,C_{\Pi^\varepsilon_{\mathbf{i}}}\|\nabla(u_\varepsilon - v)\|_{\Pi^\varepsilon_{\mathbf{i}}}\end{aligned}$$

where C_{F_Ω} is a constant in the Friedrich's inequality for Ω and $C_{\Pi^\varepsilon_{\mathbf{i}}}$ is a constant in the Poincare's inequality for $\Pi^\varepsilon_{\mathbf{i}}$. It is known (cf. [18]) that for convex $\Pi^\varepsilon_{\mathbf{i}}$

$$C_{\Pi^\varepsilon_{\mathbf{i}}} \leqslant \frac{\operatorname{diam}\Pi^\varepsilon_{\mathbf{i}}}{\pi} \qquad \forall\,d \geqslant 1.$$

We use (1.1) and (1.2) and arrive at the estimate

$$\begin{aligned}\int_\Omega(\operatorname{div}\boldsymbol{\tau} + f)(u_\varepsilon - v)\,\mathrm{d}\mathbf{x} &\leqslant C_{F_\Omega}\|\operatorname{div}\boldsymbol{\tau}_0 + f\|\,\|\nabla(u_\varepsilon - v)\| + \varepsilon^s\,\varepsilon^{d/2-1}\|\operatorname{div}\boldsymbol{\eta}\|_{\widehat{\Pi}}\sqrt{c_0}\,\varepsilon^{-d/2}\,\varepsilon\,\frac{\varrho}{\pi}\,\|\nabla(u_\varepsilon - v)\| \\ &= C_{F_\Omega}\|\operatorname{div}\boldsymbol{\tau}_0 + f\|\,\|\nabla(u_\varepsilon - v)\| + \varepsilon^s\,\frac{\varrho}{\pi}\,\sqrt{c_0}\,\|\operatorname{div}\boldsymbol{\eta}\|_{\widehat{\Pi}}\,\|\nabla(u_\varepsilon - v)\|.\end{aligned}$$

In view of (1.3), we obtain

$$\int_\Omega(\operatorname{div}\boldsymbol{\tau} + f)(u_\varepsilon - v) \leqslant \widetilde{C}_{F_\Omega}\|\operatorname{div}\boldsymbol{\tau}_0 + f\|\,\|\nabla(u_\varepsilon - v)\|_{A_\varepsilon} + \varepsilon^s\,\widetilde{C}\,\|\operatorname{div}\boldsymbol{\eta}\|_{\widehat{\Pi}}\,\|\nabla(u_\varepsilon - v)\|_{A_\varepsilon} \tag{2.12}$$

where

$$\widetilde{C}_{F_\Omega} := \frac{C_{F_\Omega}}{\sqrt{c_1}}, \qquad \widetilde{C} := \frac{\varrho}{\pi}\sqrt{\frac{c_0}{c_1}}. \tag{2.13}$$

Now (2.9), (2.10), and (2.12) imply the estimate

$$\|\nabla(u_\varepsilon - v)\|_{A_\varepsilon} \leqslant \|A_\varepsilon\nabla v - \boldsymbol{\tau}_0 + \varepsilon^s\boldsymbol{\eta}\|_{A^{-1}_\varepsilon} + \widetilde{C}_{F_\Omega}\|\operatorname{div}\boldsymbol{\tau}_0 + f\| + \varepsilon^s\,\widetilde{C}\,\|\operatorname{div}\boldsymbol{\eta}\|_{\widehat{\Pi}}. \tag{2.14}$$

Consider the first term in the right-hand side of the estimate (2.14). We have

$$\|A_\varepsilon \nabla v - \boldsymbol{\tau}_0 + \varepsilon^s \boldsymbol{\eta}\|^2_{A_\varepsilon^{-1}} = \sum_{\mathbf{i}} \int_{\Pi_\mathbf{i}^\varepsilon} \widehat{A}^{-1}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\Big(\widehat{A}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\nabla v(\mathbf{x}) - \boldsymbol{\tau}_0(\mathbf{x}) + \varepsilon^s\,\boldsymbol{\eta}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\Big)$$
$$\times\Big(\widehat{A}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\nabla v(\mathbf{x}) - \boldsymbol{\tau}_0(\mathbf{x}) + \varepsilon^s\,\boldsymbol{\eta}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\Big)\,\mathrm{d}\mathbf{x}.$$

We set $v = w_\varepsilon^1$ and obtain with the help of (2.4)

$$\|A_\varepsilon \nabla w_\varepsilon^1 - \boldsymbol{\tau}_0 + \varepsilon^s \boldsymbol{\eta}\|^2_{A_\varepsilon^{-1}} = \sum_{\mathbf{i}} \int_{\Pi_\mathbf{i}^\varepsilon} \Big(\varepsilon^{2s}\,\widehat{A}^{-1}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\boldsymbol{\eta}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\cdot\boldsymbol{\eta}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)$$
$$+\,2\,\widehat{A}^{-1}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\varepsilon^s\,\mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x})\cdot\boldsymbol{\eta}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big) + \widehat{A}^{-1}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x})\cdot\mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x})\Big)\,\mathrm{d}\mathbf{x}.$$

Now we apply Lemma 2.1 to the second term in the right-hand side of the above relation and arrive at (2.8). □

We note that the estimate (2.14) also holds in a more general setting and can be applied to any reconstruction v (including numerical one) of u_ε with the requirement that $v \in H^1(\Omega)$.

Remark 2.1. It is not difficult to show that the majorant has the same convergence rate as the *a priori* estimate (cf. (1.16)) provided that the parameters are selected as is recommended by the theory [14].

Indeed, let us choose

$$\boldsymbol{\tau_0} := \mathbf{v_0} - \varepsilon\,\mathbf{v}_1^\star \tag{2.15}$$

where $\mathbf{v_0}$ and $\mathbf{v_1}$ are defined by (1.17) and $\star$ means periodification of a function, i.e.

$$\mathbf{w}^\star(\mathbf{x}) := \mathbf{w}\Big(\mathbf{x}, \frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)$$

for any $\mathbf{x} \in \Pi_\mathbf{i}^\varepsilon$ and for any $\mathbf{i}$. Then,

$$\mathrm{div}\boldsymbol{\tau}_0 = \mathrm{div}\mathbf{v_0} - \varepsilon\ \mathrm{div}\,\mathbf{v}^\star{}_\mathbf{1} = \mathrm{div}\,\mathbf{v}_0 - \varepsilon\left((\mathrm{div}_\mathbf{x}\,\mathbf{v}_1)^\star + \varepsilon^{-1}\,(\mathrm{div}_\mathbf{y}\,\mathbf{v}_1)^\star\right).$$

Since $\mathbf{v_1} := -\mathrm{curl}_\mathbf{x}(\widetilde{N}\,\boldsymbol{\mu})$, (cf. (1.17)), the first term in the brackets vanishes and for the second one we use the fact that

$$(\mathrm{div}_\mathbf{y}\,\mathbf{v_1})^\star = f + \mathrm{div}_\mathbf{x}\,\mathbf{v_0}$$

(see, e.g., [7], p. 65). Then, we obtain

$$\mathrm{div}\,\boldsymbol{\tau}_0 = \mathrm{div}\,\mathbf{v_0} - f - \mathrm{div}\,\mathbf{v_0} = -f. \tag{2.16}$$

Therefore,

$$\|\nabla(u_\varepsilon - w_\varepsilon^1)\|_{A_\varepsilon} \leqslant \mathcal{M}_\oplus\Big(w_\varepsilon^1, \boldsymbol{\tau}_0, \boldsymbol{\eta}, \boldsymbol{\lambda}, s\Big) = \mathcal{F}^{1/2}\Big(w_\varepsilon^1;\ \boldsymbol{\tau}_0, \boldsymbol{\eta}, \boldsymbol{\lambda}, s\Big) + \varepsilon^s\,\widetilde{C}\,\|\mathrm{div}\,\boldsymbol{\eta}\|_{\widehat{\Pi}} \tag{2.17}$$

where $\mathcal{F}$ is defined by (2.6) and

$$\mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x}) = A_\varepsilon\,\nabla w_\varepsilon^1 - (\mathbf{v_0} - \varepsilon\,\mathbf{v_1}).$$

Then, with the help of (1.15), (1.16), and the triangle inequality, we find that

$$\|\mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x})\|_{A_\varepsilon^{-1}} = \|A_\varepsilon\,\nabla(w_\varepsilon^1 - u_\varepsilon + u_\varepsilon) - (\mathbf{v_0} - \varepsilon\,\mathbf{v_1})\|_{A_\varepsilon^{-1}}$$
$$\leqslant \|A_\varepsilon\,\nabla(w_\varepsilon^1 - u_\varepsilon)\|_{A_\varepsilon^{-1}} + \|A_\varepsilon\,\nabla u_\varepsilon - (\mathbf{v_0} - \varepsilon\,\mathbf{v_1})\|_{A_\varepsilon^{-1}} \leqslant c\,\sqrt{\varepsilon}.$$

We set $\boldsymbol{\eta} = \mathbf{0}$, tend all components of λ to zero and find that

$$\mathcal{M}_\oplus \leqslant c\,\varepsilon^{1/2}. \tag{2.18}$$

It is worth noting that in some special cases this asymptotic result can be proved in a simpler way. For example, if

$$A_0 = \langle\widehat{A}^{-1}\rangle_{\widehat{\Pi}}^{-1}$$

(which is always the situation in the one-dimensional case or if $\operatorname{curl}\widehat{A}^{-1} = \mathbf{0}$), then the simplest choice

$$\boldsymbol{\tau}_0 = A_0 \nabla u_0$$

implies $\operatorname{div}\boldsymbol{\tau}_0 = -f$. In this case,

$$\|\nabla(u_\varepsilon - w_\varepsilon^1)\|_{A_\varepsilon} \leqslant \mathcal{M}_\oplus\Big(w_\varepsilon^1,\, \boldsymbol{\tau}_0,\, \boldsymbol{\eta},\, \boldsymbol{\lambda},\, s\Big) := \mathcal{F}^{1/2}\Big(w_\varepsilon^1;\, \boldsymbol{\tau}_0,\, \boldsymbol{\eta}, \boldsymbol{\lambda},\, s\Big) \,+\, \varepsilon^s\, \widetilde{C}\, \|\operatorname{div}\boldsymbol{\eta}\|_{\widehat{\Pi}} \tag{2.19}$$

where $\mathcal{F}$ is defined by (2.6) and

$$\mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x}) \;=\; A_\varepsilon \nabla w_\varepsilon^1 - A_0 \nabla u_0$$

for all $\mathbf{y} \in \widehat{\Pi}$, $\mathbf{x} \in \Pi_{\mathbf{i}}^\varepsilon$. Choosing again $\eta = \mathbf{0}$ in (2.19), we obtain (2.18).

Remark 2.2. The right-hand side of the majorant (2.8) is the sum of three non-negative terms, which include a global function $\boldsymbol{\tau}_0$ and a function $\boldsymbol{\eta}$ defined on the cell of periodicity. This reflects the specifics of the considered class of problems. Hence, the computation of the majorant is based on the flux of the homogenized solution and a proper selection (cf. Section 4) of the function $\boldsymbol{\eta}$ defined on the cell of periodicity. The scalar parameters λ_i and the power s can be selected in order to minimize the overall value of the majorant. We emphasize that the computation of the majorant does not require an approximation of the flux associated with the original (global) periodic problem.

The choice

$$\tau_0 = A_0 \nabla u_0, \qquad \eta = \mathbf{0}$$

leads to the simplified error estimator

$$\begin{aligned} \|\nabla(u_\varepsilon - w_\varepsilon^1)\|_{A_\varepsilon} &\leqslant \left| \sum_{\mathbf{i}} \int_{\Pi_{\mathbf{i}}^\varepsilon} \widehat{A}^{-1}\Big(\frac{\mathbf{x}-\mathbf{x}_\mathbf{i}}{\varepsilon}\Big)\, \mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x}) \cdot \mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x})\, \mathrm{d}\mathbf{x} \right|^{1/2} \\ &= \|A_\varepsilon \nabla w_\varepsilon^1 - A_0 \nabla u_0\|_{A_\varepsilon^{-1}} =: M_\oplus(w_\varepsilon^1, u_0). \end{aligned} \tag{2.20}$$

It is easy to show that this simplified majorant is equivalent to the combined primal–dual norm

$$[u_\varepsilon - w_\varepsilon^1,\; A_\varepsilon \nabla u_\varepsilon - \tau_0] := \|\nabla(u_\varepsilon - w_\varepsilon^1)\|_{A_\varepsilon} + \|A_\varepsilon \nabla u_\varepsilon - \tau_0\|_{A_\varepsilon^{-1}} \tag{2.21}$$

Indeed, from one hand

$$\begin{aligned} [u_\varepsilon - w_\varepsilon^1,\; A_\varepsilon \nabla u_\varepsilon - \tau_0] &= \|\nabla(u_\varepsilon - w_\varepsilon^1)\|_{A_\varepsilon} + \|A_\varepsilon \nabla u_\varepsilon - A_0 \nabla u_0\|_{A_\varepsilon^{-1}} \\ &\leqslant \|\nabla(u_\varepsilon - w_\varepsilon^1)\|_{A_\varepsilon} + \|A_\varepsilon \nabla u_\varepsilon - A_\varepsilon \nabla w_\varepsilon^1\|_{A_\varepsilon^{-1}} + \|A_\varepsilon \nabla w_\varepsilon^1 - A_0 \nabla u_0\|_{A_\varepsilon^{-1}} \\ &\leqslant 3\, \|A_\varepsilon \nabla u_\varepsilon - A_0 \nabla u_0\|_{A_\varepsilon^{-1}} \,=\, 3\, M_\oplus(w_\varepsilon^1, u_0). \end{aligned} \tag{2.22}$$

From the other hand,

$$\begin{aligned} M_\oplus(w_\varepsilon^1, u_0) = \|A_\varepsilon \nabla w_\varepsilon^1 - \tau_0\|_{A_\varepsilon^{-1}} &\leqslant \|A_\varepsilon \nabla w_\varepsilon^1 - A_\varepsilon \nabla u_\varepsilon\|_{A_\varepsilon^{-1}} + \|A_\varepsilon \nabla u_\varepsilon - \tau_0\|_{A_\varepsilon^{-1}} \\ &= [u_\varepsilon - w_\varepsilon^1,\; A_\varepsilon \nabla u_\varepsilon - \tau_0]. \end{aligned} \tag{2.23}$$

Hence, we obtain

$$M_\oplus(w_\varepsilon^1, u_0) \leqslant [u_\varepsilon - w_\varepsilon^1,\; A_\varepsilon \nabla u_\varepsilon - \tau_0] \leqslant 3 M_\oplus(w_\varepsilon^1, u_0). \tag{2.24}$$

We note that this result is similar to that has been obtained in [22] for errors of mixed approximations of elliptic partial differential equations.

Remark 2.3. One can show that in the one-dimensional case, (2.20) holds as equality provided that

$$\int_\Omega \left(A_\varepsilon^{-1} \int_0^x f \right) = \int_\Omega \left(A_0^{-1} \int_0^x f \right). \tag{2.25}$$

Remark 2.4. In certain cases, we may know only numerical approximations to the solutions N_k, $\widetilde{N}_k$ and u_0 of the auxiliary cell problems (cf. (1.8), (1.18)) and of the homogenized equation (cf. (1.10)). The corresponding approximation errors can be estimated by error majorants of similar types (see [19–24] and references therein). Then, the overall error majorant will include both, approximation and modeling errors. A combined modeling-discretization strategy is suggested in [24] (where the modeling error is generated by defeaturing of a complicated structure) and in [28] (where the modeling error is generated by dimension reduction) and should be used in this case. This topic deserves a separate investigation and lies beyond the framework of this paper which is focused on the principal structure of the guaranteed error bound for homogenized problems.

3 Lower bound of the modeling error

Lower bounds of the modeling error allows us to estimate numerically the sharpness of the error majorant and to evaluate the *efficiency* of error estimation. A lower bound of the energy error norm can be derived by means of the well known relation (see, e.g., [22], pp. 85–86):

$$\|\nabla(u_\varepsilon - v)\|^2_{A_\varepsilon} \;=\; \sup_{w\in H^1_0(\Omega)} \mathcal{M}^2_\ominus(v;\; w) := \sup_{w\in H^1_0(\Omega)} \int_\Omega \Big(2\,(f\,w \;-\; A_\varepsilon\,\nabla v\cdot\nabla w) \;-\; A_\varepsilon\nabla w\cdot\nabla w \Big). \tag{3.1}$$

Clearly, for any $w \in H^1_0(\Omega)$ it holds $\|\nabla(u_\varepsilon - v)\|_{A_\varepsilon} \geqslant \mathcal{M}_\ominus(v;\; w)$. Moreover, there exists a function w such that the inequality holds as equality. We use (3.1) with $v = w^1_\varepsilon$ (cf. (1.11)) and represent w in the form $w = \rho_{\max} z$, where $z \in H^1_0(\Omega)$ is a certain specially selected function and the multiplier $\rho_{\max}$ is defined by the relation

$$\rho_{\max} \;=\; \frac{\int_\Omega (f\,z \;-\; A_\varepsilon\,\nabla w^1_\varepsilon\cdot\nabla z)}{\int_\Omega A_\varepsilon\nabla z\cdot\nabla z}.$$

In this case, $\mathcal{M}^2_\ominus(w^1_\varepsilon;\; \rho z)$ attains its maximum as a quadratic function with respect to ρ. Inserting this value into $\mathcal{M}^2_\ominus(v;\; w)$, we obtain the following lower bound of the modeling error $\|\nabla(u_\varepsilon - w^1_\varepsilon)\|_{A_\varepsilon}$:

$$\mathcal{M}_\ominus(w^1_\varepsilon;\; z) \;:=\; \frac{\left|\int_\Omega (f\,z \;-\; A_\varepsilon\,\nabla w^1_\varepsilon\cdot\nabla z)\right|}{\|\nabla z\|_{A_\varepsilon}} = \frac{\left|\int_\Omega (A_0\,\nabla u_0 \;-\; A_\varepsilon\,\nabla w^1_\varepsilon)\cdot\nabla z\right|}{\|\nabla z\|_{A_\varepsilon}}. \tag{3.2}$$

Below we consider two possible choices of the function z. Let

$$z(\mathbf{x}) := w^1_\varepsilon(\mathbf{x}) - u_0(\mathbf{x}) - \varepsilon\,\Theta\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big) \tag{3.3}$$

where $\Theta((\mathbf{x}-\mathbf{x_i})/\varepsilon)$ is a periodic function defined in $\widehat{\Pi}$, and

$$\varphi^0_\varepsilon\Big(\mathbf{x},\; \frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big) := -\psi^\varepsilon(\mathbf{x})\,\boldsymbol{N}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\cdot\nabla u_0(\mathbf{x}). \tag{3.4}$$

Then, we rewrite (1.11) in the form

$$w^1_\varepsilon = u_0 + \varepsilon\,\varphi^0_\varepsilon \tag{3.5}$$

and

$$z(\mathbf{x}) = \varepsilon\,\Big(\varphi^0_\varepsilon\Big(\mathbf{x},\; \frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big) - \Theta\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\Big) \tag{3.6}$$

we see that in this case the test function z is a periodical function. The minorant is defined by the relation

$$\mathcal{M}^2_\ominus(w^1_\varepsilon,\; \Theta) = \frac{\big(\int_\Omega [\mathbf{q}\cdot\nabla\varphi^0_\varepsilon \;-\; \mathbf{q}\cdot\nabla\Theta]\big)^2}{\int_\Omega A_\varepsilon\nabla\Big(\varphi^0_\varepsilon \;-\; \Theta\Big)\cdot\nabla\Big(\varphi^0_\varepsilon \;-\; \Theta\Big)} \tag{3.7}$$

where

$$\mathbf{q} := (A_0 - A_\varepsilon)\nabla\, u_0 \;-\; \varepsilon\, A_\varepsilon\,\nabla\varphi^0_\varepsilon. \tag{3.8}$$

For this ansatz, the best lower bound will be obtained if (3.7) is maximized with respect to the cell based function Θ and global function ψ_ε. However, in general, finding these (optimal) functions may require essential computational efforts. In the tests below, we used a much simpler choice, namely,

$$\Theta = 0, \qquad \psi_\varepsilon = \min\Big\{1,\ \frac{1}{\varepsilon}\,\mathrm{dist}(\mathbf{x}, \partial\Omega)\Big\} \tag{3.9}$$

and the minorant (3.7) is reduced to

$$\mathcal{M}_\ominus^{\mathrm{per}}(w_\varepsilon^1;\ \mathbf{0}) = \frac{\big|\int_\Omega \mathbf{q}\cdot\nabla\varphi_\varepsilon^0\,\big|}{\|\nabla\,\varphi_\varepsilon^0\|_{A_\varepsilon}}. \tag{3.10}$$

Also, we may try to find a suitable z represented aperiodically, for example in the form u_0 plus small quasi-periodical disturbances

$$z(\mathbf{x}) = \rho\,\Big(u_0\,(\mathbf{x})\ +\ \varepsilon\,\psi^\varepsilon\,\Theta\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\Big). \tag{3.11}$$

In this case,

$$\mathcal{M}_\ominus^2(w_\varepsilon^1,\ \Theta) = \frac{\Big(\int_\Omega\Big[\tilde{\mathbf{q}}\cdot\nabla u_0\ +\ \tilde{\mathbf{q}}\cdot\nabla\Big(\varepsilon\,\psi^\varepsilon\,\Theta\Big)\Big]\Big)^2}{\int_\Omega A_\varepsilon\nabla\Big(\,u_0\ +\ \varepsilon\,\psi^\varepsilon\,\Theta\Big)\cdot\nabla\Big(\,u_0\ +\ \varepsilon\,\psi^\varepsilon\,\Theta\,\Big)}, \tag{3.12}$$

where

$$\tilde{\mathbf{q}} := (A_0 - A_\varepsilon)\nabla\,u_0\ +\ \varepsilon\,A_\varepsilon\,\nabla(\psi^\varepsilon\,\boldsymbol{N}\nabla u_0). \tag{3.13}$$

In general, the minorant should be maximized with respect to Θ. However, even the simplest choice $\Theta = 0$ yields a lower bound

$$\mathcal{M}_\ominus^{\mathrm{aper}}(w_\varepsilon^1;\ \mathbf{0}) = \frac{\big|\int_\Omega \mathbf{q}\cdot\nabla u_0\big|}{\|\nabla\,u_0\|_{A_\varepsilon}}\,. \tag{3.14}$$

4 Numerical experiments

A general strategy of computing the majorant consists of minimizing $\mathcal{M}_\oplus$ with respect to parameters λ, s, vector function $\tau \in H\,(\Omega, \mathrm{div})$ and vector function $\eta \in H_0(\widehat{\Pi}, \mathrm{div})$ using finite dimensional subspaces $S_h\,(\Omega) \subset H(\Omega, \mathrm{div})$ (e.g. a finite element space) and $S_h(\widehat{\Pi}) \subset H_0(\widehat{\Pi}, \mathrm{div})$, respectively. The process can be started with

$$\boldsymbol{\tau}_0 = A_0\nabla u_0, \qquad \boldsymbol{\eta} = 0. \tag{4.1}$$

In the numerical experiments discussed below, we set $\boldsymbol{\tau}$ and $\boldsymbol{\eta}$ in accordance with (4.1) and use the simplest error estimator $M_\oplus(w_\varepsilon^1, u_0)$:

$$\|\nabla(u_\varepsilon - w_\varepsilon^1)\|_{A_\varepsilon} \leqslant \left|\sum_{\mathbf{i}}\ \int_{\Pi_\mathbf{i}^\varepsilon}\widehat{A}^{-1}\Big(\frac{\mathbf{x}-\mathbf{x_i}}{\varepsilon}\Big)\,\mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x})\cdot\mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x})\ \mathrm{d}\mathbf{x}\right|^{1/2} \tag{4.2}$$

where $\mathbf{g}_{\boldsymbol{\tau}_0}(\mathbf{x})$ is defined by (2.4). In most cases, this choice was enough in order to have sufficiently sharp estimates. This is explainable because if the periodic structure is fine and contains many cells, then the correction term is less significant and its influence can be diminished by increasing values of s. However, if a periodic structure is rather coarse (e.g., 25–50 cells) and/or the coefficients of the matrix $\widehat{A}$ have jumps, sharp oscillations, etc. then the term $\varepsilon^s\,\boldsymbol{\eta}$ may augment the homogenized flux substantially and it may be required to use the most general form of the majorant.

Below, we apply the estimates derived in Sections 2 and 3 to several one- and two-dimensional test problems. For this purpose, we select problems used in publications related to analysis of homogenized and interface problems, e.g., see [8, 13, 15, 16, 30]. Our goal is to validate the sharpness of the two-sided error bounds presented by $M_\oplus$ and two lower bounds introduced in Section 3 (i.e., $M_\ominus$ is computed by $\mathcal{M}_\ominus^{\mathrm{per}}(w_\varepsilon^1;\ \mathbf{0})$ or $\mathcal{M}_\ominus^{\mathrm{aper}}(w_\varepsilon^1;\ \mathbf{0})$; cf. (3.10) and (3.14)).

For the quantitative characterization of two-sided bounds, we use the number

$$\varkappa := \frac{M_\oplus}{M_\ominus} \tag{4.3}$$

which can be also viewed as a computable upper bound of the efficiency index

$$i_\oplus^{\mathrm{eff}} := \frac{M_\oplus}{\|\nabla(u_\varepsilon - w_\varepsilon^1)\|_{A_\varepsilon}}$$

and gives insights of the quality of the error majorant. Similarly, we define the efficiency index of the lower bound

$$i_\ominus^{\mathrm{eff}} := \frac{M_\ominus}{\|\nabla(u_\varepsilon - w_\varepsilon^1)\|_{A_\varepsilon}}.$$

In the first series of tests, we set $d = 1$ and $\Omega = (0,\ 1)$. Then, $u_\varepsilon \in H_0^1(\Omega)$ is defined by the relation

$$\int_0^1 A_\varepsilon\, u_\varepsilon'\, v' = \int_0^1 f v \quad \forall\, v \in H_0^1\,(\Omega)\,. \tag{4.4}$$

Example 4.1. Let

$$\widehat{A}\,(y) := \begin{cases} 1, & 0 < y \leqslant 1/2 \\ 2, & 1/2 < y < 1 \end{cases}$$

and A_ε is defined as in (1.4). The right-hand side is given by $f := \sin(2\,\pi x/\varepsilon)$. Here, the explicit forms of A_0, u_0', $\mathrm{d}N/\mathrm{d}y$ and N are known (they can be found from (1.9) and (1.8)):

$$\begin{aligned} A_0\,(x) &= \frac{4}{3} \\ u_0' &= \frac{3\,\varepsilon}{8\,\pi}\cos(2\,\pi\,x\,\varepsilon^{-1}) \\ \frac{\mathrm{d}N}{\mathrm{d}y}\,(y) &= \begin{cases} -\frac{1}{3}, & 0 < y \leqslant 1/2 \\ \frac{1}{3}, & 1/2 < y < 1 \end{cases} \\ N\,(y) &= \begin{cases} -\frac{y}{3} + \frac{1}{12}, & 0 < y \leqslant 1/2 \\ \frac{y}{3} - \frac{1}{4}, & 1/2 < y < 1. \end{cases} \end{aligned}$$

Example 4.2. Let $A_\varepsilon(x) = 2 + \cos\,(2\,\pi x/\varepsilon)$, $f := \mathrm{e}^{10\,x}$. Then, see (1.9) and (1.8):

$$\begin{aligned} A_0\,(x) &= \sqrt{3} \\ u_0' &= -\frac{3^{-0.5}}{10}\,\mathrm{e}^{10\,x} + \frac{3^{-0.5}}{100}\,\mathrm{e}^{10} \\ \frac{\mathrm{d}N}{\mathrm{d}y}\,(y) &= 1 - \sqrt{3}\,(2 + \cos(2\,\pi\,y))^{-1} \\ N\,(y) &= \int \left(1 - \sqrt{3}\,(2 + \cos(2\,\pi\,y))^{-1}\right) \mathrm{d}y. \end{aligned}$$

In Example 4.1, f is a periodic function. Therefore, it is natural to expect that the minorant $M_\ominus^{\mathrm{per}}$ (in which the periodicity is taken into account) will provide better results. In Example 4.2, the right-hand side is represented by a non-periodical function, and, therefore, we expect that $M_\ominus^{\mathrm{aper}}$ will be better (at least for problems with relatively small amount of cells). The corresponding numerical results are depicted in Fig. 2 and confirm the proposed choice of the lower error bound. We note that in Example 4.1 the equality (2.25) holds and (cf. Remark 2.3) the majorant (4.2) coincides with the error. This fact is confirmed numerically (see Fig. 2 a, b). Example 4.2 shows that the majorant and minorants are quite sharp if the number of cells is sufficiently large (regardless of the condition (2.25)).

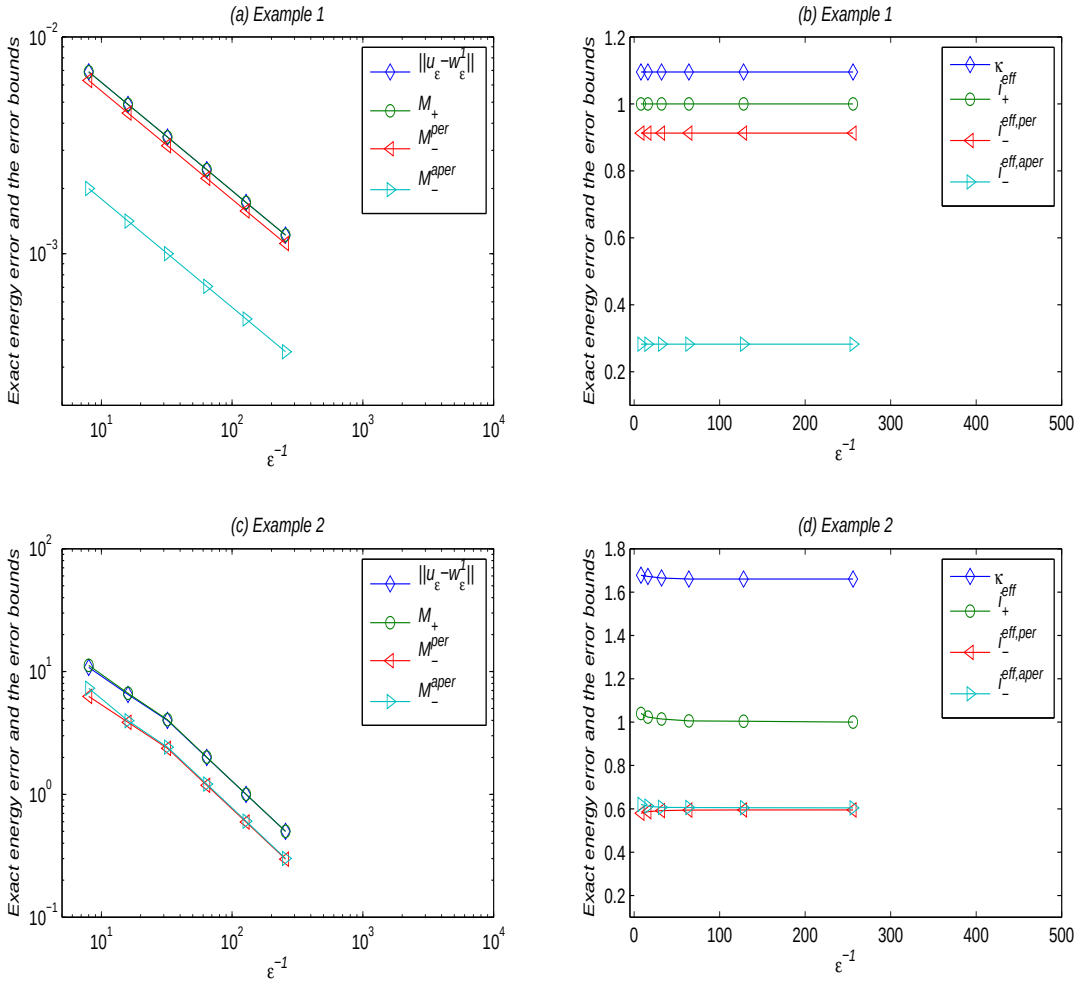

Figure 2. Error bounds (left) and efficiency indices (right) for Example 4.1 and Example 4.2.

Example 4.3. Let $d = 2$, $\Omega = (0,1)^2$, and $u_\varepsilon \in H_0^1(\Omega)$ be defined by the relation

$$\int_\Omega A_\varepsilon \nabla u_\varepsilon \cdot \nabla v = \int_\Omega f v \qquad \forall\, v \in H_0^1(\Omega)\,.$$

Here A_ε is generated by the matrix $\widehat{A} := aI$ (cf. (1.4)), where

$$a := \begin{cases} a_1 > 0 & \text{in } \left(0, \tfrac{1}{2}\right)^2 \cup \left(\tfrac{1}{2}, 1\right)^2 \\ a_2 > 0 & \text{in } (0,1)^2 \setminus \left(\left(0, \tfrac{1}{2}\right)^2 \cup \left(\tfrac{1}{2}, 1\right)^2\right). \end{cases} \qquad \widehat{\Pi}: \quad \begin{array}{|c|c|} \hline a_2 & a_1 \\ \hline a_1 & a_2 \\ \hline \end{array} \tag{4.5}$$

Then (see, e.g., [14], pp. 35–39), $A_0 = \sqrt{a_1\, a_2}$. We choose

$$f = 2\,\sqrt{a_1\, a_2}\,(x_1(1-x_1) + x_2(1-x_2))$$

such that

$$u_0(\mathbf{x}) = x_1\, x_2\, (1-x_1)(1-x_2). \tag{4.6}$$

Exact solutions of the cell problems

$$\begin{gathered} \frac{\partial}{\partial y_i}\left(\widehat{A}_{ij}(\mathbf{y})\,\frac{\partial N_k(\mathbf{y})}{\partial y_j}\right) = \frac{\partial}{\partial y_i}\,\widehat{A}_{ik}(\mathbf{y}) \quad \text{in } \widehat{\Pi} = (0,\,1)^2 \\ N_k \text{ is periodic in } \widehat{\Pi} \\ \langle N_k \rangle_{\widehat{\Pi}} = 0 \end{gathered} \tag{4.7}$$

are found in [15] in the form

$$N_k(\mathbf{y}) = v\left(\frac{\mathbf{y}+1}{2}\right) + y_k, \quad k = 1,\ 2. \tag{4.8}$$

Here $v(\mathbf{y})$ is the unique solution of the problem

$$-\operatorname{div}(a\,\nabla v) = 0 \quad \text{in } (-1,\,1)^2 \tag{4.9}$$

with homogenous Dirichlet boundary conditions and a is defined by (4.5). This solution is given in polar coordinates (r, ϑ) centered at the origin by the relation

$$v = r^\gamma\,\mu(\vartheta) \tag{4.10}$$

where

$$\mu(\vartheta) := \begin{cases} \cos(\alpha\beta)\,\cos((\vartheta - \frac{\pi}{2} + \alpha)\,\gamma), & 0 \leqslant \vartheta \leqslant \frac{\pi}{2} \\ \cos(\alpha\gamma)\,\cos((\vartheta - \pi + \beta)\,\gamma), & \frac{\pi}{2} \leqslant \vartheta \leqslant \pi \\ \cos(\alpha\beta)\,\cos((\vartheta - \pi - \alpha)\,\gamma), & \pi \leqslant \vartheta \leqslant \frac{3\pi}{2} \\ \cos((\frac{\pi}{2} - \alpha)\gamma)\,\cos((\vartheta - \frac{3\pi}{2} - \beta)\,\gamma), & \frac{3\pi}{2} \leqslant \vartheta \leqslant 2\pi \end{cases} \tag{4.11}$$

is a continuous and piecewise smooth function and the numbers α, β, and γ depend on a_1/a_2 and satisfy the relations

$$\begin{cases} \frac{a_1}{a_2} = \tan(\beta\gamma)\,\cot(\alpha\gamma) \\ \frac{a_2}{a_1} = -\tan(\alpha\gamma)\,\cot(\beta\gamma) \\ \frac{a_1}{a_2} = -\tan(\beta\gamma)\,\cot((\frac{\pi}{2} - \alpha)\gamma) \\ \frac{a_2}{a_1} = \tan((\frac{\pi}{2} - \alpha)\gamma)\,\cot(\beta\gamma) \\ \gamma > 0 \\ \max\{0,\ \pi\gamma - \pi\} < 2\alpha\gamma < \min\{\pi\gamma,\ \pi\} \\ \max\{0,\ \pi\} < -2\beta\gamma < \min\{\pi,\ 2\pi\}. \end{cases} \tag{4.12}$$

It is known that v has a restricted regularity (namely, $v \in H^{1+\gamma-\varepsilon}(\widehat{\Pi})$ for any $\varepsilon > 0$).

We use this fact in order to verify the efficiency of the error majorant in different situations, we consider two cases, in which the ratio between a_1 and a_2 (and the regularity of N_k) are quite different.

- *Case 1:* let $a_1 = 5.0$, $a_2 = 1.0$. In this case, the solution (4.9) has $\gamma = 0.53544094560$ and $\vartheta = \pi/2$ (cf. system (3.2) in [15]) so that $v \in H^{3/2}(\Omega)$.
- *Case 2:* now, we set $\gamma = 0.1$ and $\vartheta = \pi/2$. By solving (4.11) and (4.12), we find that in this case $a_1 = 161.4476387975881$ and $a_2 = 1.0$. Here, $v \in H^{1+\alpha}(\widehat{\Pi})$ with $0 < \alpha < 0.1$, i.e., it is almost an H^1 function.

To quantify the efficiency of the estimates (4.2) and (3.10), we compare them with the exact error

$$e := \|\nabla(u_\varepsilon - w^1_\varepsilon)\|_{A_\varepsilon}. \tag{4.13}$$

Since u_ε is unknown, we replace it by the 'reference' solution u_{ref} computed on a very fine mesh ($h \ll \varepsilon$). The corresponding efficiency indices are defined by the relations

$$i^{\mathrm{eff}}_{\oplus} = \frac{M_{\oplus}(w^1_\varepsilon;\ \mathbf{0},\ \mathbf{1},\ 1)}{\|\nabla(u_{\mathrm{ref}} - w^1_\varepsilon)\|_{A_\varepsilon}}, \qquad i^{\mathrm{eff,\,per}}_{\ominus} = \frac{M^{\mathrm{per}}_{\ominus}(w^1_\varepsilon;\ \mathbf{0})}{\|\nabla(u_{\mathrm{ref}} - w^1_\varepsilon)\|_{A_\varepsilon}}. \tag{4.14}$$

In Table 1 (Case 1) and 2 (Case 2), we present these quantities together with the quantity $\varkappa$ as in (4.3). We see that the estimates adequately reproduce the modeling error.

It is quite predictable that the estimates are better in the first case (related to a more regular v). For the first problem, efficiency indices of the majorant and minorant are quite close to 1. However, the estimates are also valid for the second case (minimal regularity). Indeed, the efficiency index of the majorant does not exceed 2.3 and the one of the minorant does not go below 0.7.

Table 1. Efficiency of error majorant and minorant for Example 4.3, Case 1.

ε^{-1}	$I_{\oplus}^{\mathrm{eff}}$	$I_{\ominus}^{\mathrm{eff}}$	$\varkappa$
8	1.0714	0.8824	1.2141
16	1.0874	0.8781	1.2384
32	1.0988	0.8591	1.2790
64	1.1633	0.8461	1.3749

Table 2. Efficiency of error majorant and minorant for Example 4.3, Case 2.

ε^{-1}	$I_{\oplus}^{\mathrm{eff}}$	$I_{\ominus}^{\mathrm{eff}}$	$\varkappa$
8	1.7024	0.8291	2.0533
16	1.9701	0.7961	2.4750
32	2.1848	0.7370	2.9644
64	2.2771	0.7124	3.1964

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