

A parabolic local problem with exponential decay of the resonance error for numerical homogenization

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Abstract

This paper aims at an accurate and efficient computation of effective quantities, e.g., the homogenized coefficients for approximating the solutions to partial differential equations with oscillatory coefficients. Typical multiscale methods are based on a micro-macro coupling, where the macro model describes the coarse scale behaviour, and the micro model is solved only locally to upscale the effective quantities, which are missing in the macro model. The fact that the micro problems are solved over small domains within the entire macroscopic domain, implies imposing artificial boundary conditions on the boundary of the microscopic domains. A naive treatment of these artificial boundary conditions leads to a first order error in ε/δ , where $\varepsilon < \delta$ represents the characteristic length of the small scale oscillations and δ^d is the size of micro domain. This error dominates all other errors originating from the discretization of the macro and the micro problems, and its reduction is a main issue in today's engineering multiscale computations. The objective of the present work is to analyse a parabolic approach, first announced in [A. Abdulle, D. Arjmand, E. Paganoni, C. R. Acad. Sci. Paris, Ser. I, 2019], for computing the homogenized coefficients with arbitrarily high convergence rates in ε/δ . The analysis covers the setting of periodic microstructure, and numerical simulations are provided to verify the theoretical findings for more general settings, e.g. random stationary micro structures.

Keywords: resonance error, Green's function, effective coefficients, correctors, numerical homogenization

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1 Introduction

Multiscale problems involving several spatial and temporal scales are ubiquitous in physics and engineering. We mention for example, stiff stochastic differential

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equations (SDEs) in biological and chemical systems, oscillatory physical systems, partial differential equations (PDEs) with multiscale data resonance, e.g., mechanics of composite materials, fracture dynamics of solids, PDEs with oscillating parameters, see Ref. 3,18,27,30,35 and the references therein. A common computational challenge in relation with such multiscale problems is the presence of small scales in the model which should be represented over a much larger macroscopic scale of interest. One rather classical way of overcoming this issue is to analytically derive macroscopic equations from a given microscopic model, and then solve the resulting macroscale equation at a cheaper computational cost. However, such derivations often come together with some simplifying assumptions, making the accuracy of the macroscopic model questionable once the restrictive assumptions are relaxed. In contrast, multiscale numerical methods result in models with improved accuracy and efficiency as they rely on a coupling between microscopic and macroscopic models, combining the efficiency of macroscopic models with the accuracy of microscopic ones. Inexact couplings may afflict such methods by the so-called *resonance error*, Ref. 3,28. Reducing such an error is a common problem of modern multiscale methods designed over the last two decades.

This paper concerns the numerical homogenization of elliptic partial differential equations with multiscale coefficients, whose oscillation length scale (denoted by ε) is much smaller than the size of the domain $\Omega \subset \mathbb{R}^d$, which is bounded and convex. Our model problem is the following ε -indexed family of elliptic equations on Ω

$$\begin{cases} -\nabla \cdot (a^\varepsilon(\mathbf{x})\nabla u^\varepsilon) = f & \text{in } \Omega \\ u^\varepsilon = 0 & \text{on } \partial\Omega. \end{cases} \quad (1)$$

Here $a^\varepsilon(\mathbf{x}) \in [L^\infty(\Omega)]^{d \times d}$ is symmetric, uniformly elliptic and bounded, i.e., $\exists \alpha, \beta > 0$ such that

$$\alpha |\zeta|^2 \leq \zeta \cdot a^\varepsilon(\mathbf{x})\zeta \leq \beta |\zeta|^2, \quad \forall \zeta \in \mathbb{R}^d, \text{ a.e. } \mathbf{x} \in \Omega, \quad \forall \varepsilon > 0. \quad (2)$$

The well-posedness of the original problem (1) is then well-known for any $f \in H^{-1}(\Omega)$. As $\varepsilon \rightarrow 0$, the solution of (1) can be approximated, by the solution of the so-called homogenized equation:

$$\begin{cases} -\nabla \cdot (a^0(\mathbf{x})\nabla u^0) = f & \text{in } \Omega \\ u^0 = 0 & \text{on } \partial\Omega, \end{cases} \quad (3)$$

where the coefficients a_{ij}^0 (and hence the solution u^0) no longer oscillate at the ε -scale. By using the concepts of G -convergence for the symmetric case, Ref. 41, or H -convergence for the non-symmetric case, Ref. 37, one can show that the homogenized problem (3) is the limit for $\varepsilon \rightarrow 0$ of a subsequence of problems (1). In general, we do not have explicit formulae for evaluating the homogenized tensor, unless certain structural assumptions on $a^\varepsilon(\mathbf{x})$ are made. For example,

if $a^\varepsilon(\mathbf{x}) = a(\mathbf{x}/\varepsilon)$ is periodic, then the homogenized tensor a^0 is given by

$$\mathbf{e}_i \cdot a^0 \mathbf{e}_j = \int_K \mathbf{e}_i \cdot a(\mathbf{x}) (\mathbf{e}_j + \nabla \chi^j(\mathbf{x})) \, d\mathbf{x}, \quad i, j = 1, \dots, d, \quad (4)$$

where $K := (-1/2, 1/2)^d$ is the unit cube in \mathbb{R}^d , and the functions $\{\chi^i\}_{i=1}^d$ are the solutions of the so-called *cell problems*:

$$\begin{cases} -\nabla \cdot (a(\mathbf{x}) \nabla \chi^i) = \nabla \cdot (a(\mathbf{x}) \mathbf{e}_i) & \text{in } K, \\ \chi^i & K\text{-periodic.} \end{cases} \quad (5)$$

In (4) and (5) we have used the substitution $\mathbf{y} = \frac{\mathbf{x}}{\varepsilon}$, mapping a sampling domain of size ε^d to the unit cube K . For simplicity of notation, we will again denote by \mathbf{x} (instead of \mathbf{y}) the variable on the unit cube. We refer to Ref. 14,17,31 for further technical details.

When the period of the microstructure is not known exactly or the periodicity assumption is relaxed (e.g., if a is random stationary ergodic or quasi-periodic tensor), the formula (4) breaks down. In this case, (4) may be replaced by

$$\mathbf{e}_i \cdot a_R^0 \mathbf{e}_j = \int_{K_R} \mathbf{e}_i \cdot a(\mathbf{x}) (\mathbf{e}_j + \nabla \chi_R^j(\mathbf{x})) \, d\mathbf{x}, \quad i, j = 1, \dots, d, \quad (6)$$

where $K_R := (-R/2, R/2)^d$, and¹

$$\begin{cases} -\nabla \cdot (a(\mathbf{x}) \nabla \chi_R^i) = \nabla \cdot (a(\mathbf{x}) \mathbf{e}_i) & \text{in } K_R \\ \chi_R^i(\mathbf{x}) = 0 & \text{on } \partial K_R, \end{cases} \quad (7)$$

and the homogenized coefficient a^0 is given by

$$a^0 = \lim_{R \rightarrow \infty} a_R^0.$$

Assume for a moment that the tensor a is K -periodic and that periodic BCs are imposed in (7), then the homogenized tensor a^0 will be equal to a_R^0 only when R is an integer. When R is not an integer, there will be a difference between χ_R and χ on ∂K_R , which results in a so-called resonance error, Ref. 5,19,20²,

$$e_{MOD} := \|a_R^0 - a^0\|_F \leq C \frac{1}{R}, \quad (8)$$

where $\|\cdot\|_F$ denotes the Frobenius norm for a tensor. Note that the first order rate is valid also when the problem (7) is equipped with periodic BCs. From a computational point of view, this first order decay rate of the error is the efficiency and accuracy bottleneck of numerical upscaling schemes, i.e., in order to reduce the resonance error down to practically reasonable accuracies, one

¹In (7), the choice of the boundary condition (BC) is not unique, and the homogeneous Dirichlet BCs can be safely replaced e.g., by periodic BCs without any change in (8).

²We denote the resonance error by e_{MOD} , as in Ref. 5.

needs to solve the problem (7) over large computational domains K_R , possibly on each quadrature point of a macro computational domain (see Ref. 5, 19), which becomes prohibitively expensive. Our central goal is then to design micro models which reduce the resonance error down to desired accuracies without requiring a substantial enlargement of the computational domain K_R . In what follows, we provide a review of existing strategies, some of which improve the decay rate of the resonance error.

1.1 Existing approaches for reducing the resonance error

Over the last two decades, several interesting approaches have been proposed to reduce the resonance error. These strategies can be classified in two classes: a) Methods which reduce the prefactor (but not the convergence rate) in (8), b) Methods which improve the convergence rate.

a) Methods reducing the prefactor only:

One of the very first approaches to reduce the prefactor is based on the idea of oversampling, see Ref. 28. In oversampling, the cell problem (7) is solved over K_R , while the computation of the homogenized coefficient takes place in an interior domain $K_L \subset K_R$. Another attempt is based on exploring the combined effect of oversampling and imposing different BCs (Dirichlet, Neumann and periodic) for (7), see Ref. 43. It has been found that the periodic BCs perform better than the other two. Moreover, the Dirichlet BCs tend to overestimate the effective coefficients, while Neumann BCs underestimate them. Clearly, the use of these strategies becomes questionable if one is interested in practically relevant error tolerances, since there is still a need for substantially enlarging the computational domain K_R before reaching a satisfactory accuracy.

b) Methods improving the convergence rate:

Several methods which rely on modifying the cell problem (7), while still retaining a good approximation (with higher order convergence rates in $1/R$) of the homogenized coefficient have been developed in the last few years. In Ref. 15, an approach with weight (filtering) functions in the very definition of the cell problem, as well as in the averaging formula, is proposed. While the method has arbitrarily high convergence rates in a one-dimensional setting, the convergence rate in dimensions $d > 1$ has been proved to be 2. Numerical simulations demonstrate the optimality of the second order rate in dimension $d > 1$.

Another promising strategy, proposed in Ref. 25, is to add a small zero-th order regularization term to the cell problem (7) so as to make the associated Green's function exponentially decaying. The effect of the boundary mismatch will then decay exponentially fast in the interior of $K_L \subset K_R$. However, the method will suffer from a bias (or systematic error) due to added regularization term, which limits the convergence rate to fourth order. Moreover, numerical simulations in Ref. 25 show that the method requires very large values of R to achieve the optimal fourth order asymptotic rate. In Ref. 26, Richardson extrapolation is used to increase the convergence rate to higher orders at the

expense of solving the cell problem several times with different regularization terms.

An interesting idea, proposed in Ref. 8,10, is to solve a second order wave equation on $K_R \times (0, T)$, instead of the elliptic cell problem (7), see also Ref. 9 for an analysis in locally-periodic media. Thanks to the finite speed of propagation of waves, this approach leads to an ultimate removal of the error due to inaccurate BCs if K_R is sufficiently large; i.e., the boundary values will not be seen in an interior region K_L (where the averaging takes place) if $R > L + \sqrt{\|a\|_\infty} T$. Hence, size of the computational domain should increase linearly with respect to the wave speed $\sqrt{\|a\|_\infty}$, which increases also the computational cost. Moreover, solving a wave equation is computationally more challenging than solving an elliptic PDE since an accurate discretization requires a more refined resolution per wave-length, implying a more refined stepsize for temporal discretization due to the presence of CFL condition in typical time-stepping methods for the wave equation such as the leap frog scheme.

The goal of this paper is to provide a rigorous analysis of yet another approach, announced in Ref. 4, based on parabolic cell problems which results in arbitrarily high convergence rates in $1/R$. The parabolic approach adopted here is inspired by Ref. 36 and can be classified under category b), but with significant advantages from a computational point of view in comparison to the above mentioned strategies (see the discussions in the numerical results section). Moreover, this approach can be directly used in typical upscaling based multiscale formalisms such as the Heterogeneous Multiscale Methods (HMM) Ref. 2,5,7,19, and the equation free approaches Ref. 32, as well as Multiscale Finite Elements Methods (MsFEM) Ref. 28,29, which are used to approximate either the homogenized solutions to (1) or directly approximating the oscillatory response u^ε in (1).

The paper is structured as follows: in Section 2 we collect our notations and provide some definitions that will be used to present a new approximation scheme for the homogenized tensor. The main results of the present work are reported in Section 3. Section 4 is devoted to the analysis of the modelling error, where arbitrary high order convergence rates are proved. In Section 5, numerical examples are given to verify our theoretical findings. Finally, in Section 6 the computational cost of the parabolic method is analysed theoretically and compared to the classical elliptic scheme.

2 Notations and definitions

We will use the following notations throughout the exposition:

- The Sobolev space $W^{k,p}(\Omega)$ is defined as

$$W^{k,p}(\Omega) := \{f : D^\gamma f \in L^p(\Omega) \text{ for all multi-index } \gamma \text{ with } |\gamma| \leq k\}.$$

The norm of a function $f \in W^{k,p}(\Omega)$ is given by

$$\|f\|_{W^{k,p}(\Omega)} := \begin{cases} \left(\sum_{|\gamma| \leq k} \int_{\Omega} |D^{\gamma} f(\mathbf{x})|^p d\mathbf{x} \right)^{1/p} & (1 \leq p < \infty) \\ \sum_{|\gamma| \leq k} \text{ess sup}_{\Omega} |D^{\gamma} f| & (p = \infty). \end{cases}$$

- The space $H_0^1(\Omega)$ is the closure in the $W^{1,2}$ -norm of $C_c^{\infty}(\Omega)$, the space of infinitely differentiable functions with compact support in Ω . The norm associated with $H_0^1(\Omega)$ is

$$\|f\|_{H_0^1(\Omega)}^2 := \|f\|_{L^2(\Omega)}^2 + \|\nabla f\|_{L^2(\Omega)}^2.$$

An equivalent norm, making use of the Poincaré inequality is given by

$$\|f\|_{H_0^1(\Omega)} := \|\nabla f\|_{L^2(\Omega)}.$$

We will use this second notation for the H_0^1 -norm.

- We use the notation $\langle f, g \rangle_{L^2(\Omega)} := \int_{\Omega} fg d\mathbf{x}$ to denote the L^2 inner product over Ω .
- The space H_{div} is

$$H_{\text{div}}(\Omega) := \{f : f \in [L^2(\Omega)]^d \text{ and } \nabla \cdot f \in L^2(\Omega)\}.$$

The norm associated with H_{div} is

$$\|f\|_{H_{\text{div}}(\Omega)}^2 := \|f\|_{L^2(\Omega)}^2 + \|\nabla \cdot f\|_{L^2(\Omega)}^2.$$

- The space $W_{\text{per}}^1(K)$ is defined as the closure of

$$\left\{ f \in C_{\text{per}}^{\infty}(K) : \int_K f d\mathbf{x} = 0 \right\}$$

for the H^1 -norm. Thanks to the Poincaré-Wirtinger inequality, an equivalent norm in $W_{\text{per}}^1(K)$ is

$$\|f\|_{W_{\text{per}}^1(K)} = \|\nabla f\|_{L^2(K)}.$$

- The space $L_0^2(K)$ is defined as

$$L_0^2(K) = \left\{ f \in L^2(K) : \int_K f d\mathbf{x} = 0 \right\}.$$

It is an Hilbert space with respect to the L^2 -inner product.

- Let f belong to the Bochner space $L^p(0, T; X)$, where X is a Banach space. Then the norm associated with this space is defined as

$$\|f\|_{L^p(0, T; X)} := \left(\int_0^T \|f\|_X^p dt \right)^{\frac{1}{p}}.$$

- Cubes in \mathbb{R}^d are denoted by $K_L := (-L/2, L/2)^d$. In particular, K is the unit cube $(-1/2, 1/2)^d$.
- By writing C , we mean a generic constant independent of R, L, T which may change in every subsequent occurrence.
- Boldface letters are to distinguish functions in multi-dimensions, e.g., $f(\mathbf{x})$ is to mean a function of several variable ($\mathbf{x} \in \mathbb{R}^d, d \geq 2$), while $f(x)$ will be a function of one variable ($x \in \mathbb{R}$).
- We will use the notation $f_D f(\mathbf{x}) d\mathbf{x}$ to denote the average $\frac{1}{|D|} \int_D f(\mathbf{x}) d\mathbf{x}$ over a domain D .

Definition 2.1 (Definition 3.1 in Ref. 25). *We say that a function $\mu : [-1/2, 1/2] \rightarrow \mathbb{R}^+$ belongs to the space \mathbb{K}^q with $q > 0$ if*

- i) $\mu \in C^q([-1/2, 1/2]) \cap W^{q+1, \infty}((-1/2, 1/2))$
- ii) $\int_{-1/2}^{1/2} \mu(x) dx = 1$,
- iii) $\mu^k(-1) = \mu^k(1) = 0$ for all $k \in \{0, \dots, q-1\}$.

In multi-dimensions a q -th order filter $\mu_L : K_L \rightarrow \mathbb{R}^+$ with $L > 0$ is defined by

$$\mu_L(\mathbf{x}) := L^{-d} \prod_{i=1}^d \mu\left(\frac{x_i}{L}\right),$$

where μ is a one dimensional q -th order filter and $\mathbf{x} = (x_1, x_2, \dots, x_d) \in \mathbb{R}^d$. In this case, we will say that $\mu_L \in \mathbb{K}^q(K_L)$. Note that filters μ_L are considered extended to 0 outside of K_L .

Filters have the property of approximating the average of periodic functions with arbitrary rate of accuracy, as stated in the following lemma (see Ref. 25 for a proof).

Lemma 2.1 (Lemma 3.1 in Ref. 25). *Let $\mu_L \in \mathbb{K}^q(K_L)$. Then, for any K -periodic function $f \in L^p(K)$ with $1 < p \leq 2$, we have*

$$\left| \int_{K_L} f(\mathbf{x}) \mu_L(\mathbf{x}) d\mathbf{x} - \int_K f(\mathbf{x}) d\mathbf{x} \right| \leq C \|f\|_{L^p(K)} L^{-(q+1)},$$

where C is a constant independent of L .

Remark 2.1. *The result of Lemma 2.1 was proved in Ref. 25 for K -periodic $f \in L^2(K)$ and, then, extended to the case $f \in L^p(K)$, $1 < p < 2$.*

Definition 2.2. *We say that $a \in \mathcal{M}(\alpha, \beta, \Omega)$ if $a_{ij} = a_{ji}$, $a \in [L^\infty(\Omega)]^{d \times d}$ and there are constants $0 < \alpha \leq \beta$ such that*

$$\alpha |\zeta|^2 \leq \zeta \cdot a(\mathbf{x}) \zeta \leq \beta |\zeta|^2, \quad \text{for a.e. } \mathbf{x} \in \Omega, \forall \zeta \in \mathbb{R}^d.$$

We write $a \in \mathcal{M}_{per}(\alpha, \beta, \Omega)$ if in addition a is a Ω -periodic function.

Throughout the exposition, we assume that u^i and v^i , $i = 1, \dots, d$, are the solutions of the following problems:

$$\begin{cases} \frac{\partial u^i}{\partial t} - \nabla \cdot (a(\mathbf{x})\nabla u^i) = 0 & \text{in } K_R \times (0, +\infty) \\ u^i = 0 & \text{on } \partial K_R \times (0, +\infty) \\ u^i(\mathbf{x}, 0) = \nabla \cdot (a(\mathbf{x})\mathbf{e}_i) & \text{in } K_R, \end{cases} \quad (9)$$

and

$$\begin{cases} \frac{\partial v^i}{\partial t} - \nabla \cdot (a(\mathbf{x})\nabla v^i) = 0 & \text{in } K \times (0, +\infty) \\ v^i(\cdot, t) \text{ } K\text{-periodic, } \forall t \geq 0 \\ v^i(\mathbf{x}, 0) = \nabla \cdot (a(\mathbf{x})\mathbf{e}_i) & \text{in } K. \end{cases} \quad (10)$$

The well-posedness of (9) and (10) are well-known (see, e.g., Ref. 34), and are summarized below.

Proposition 2.1. *Let $a \in \mathcal{M}(\alpha, \beta, K_R)$ and $\nabla \cdot (a(\mathbf{x})\mathbf{e}_i) \in L^2(K_R)$. Then, (9) has a unique weak solution u^i such that*

$$u^i \in L^2([0, +\infty), H_0^1(K_R)), \partial_t u^i \in L^2([0, +\infty), H^{-1}(K_R)).$$

It follows that $u^i \in C([0, +\infty), L^2(K_R))$, and there exists a constant $C > 0$ such that the following bound holds true:

$$\|u^i\|_{L^\infty([0, +\infty), L^2(K_R))} + \|u^i\|_{L^2([0, +\infty), H_0^1(K_R))} \leq C \|\nabla \cdot (a(\mathbf{x})\mathbf{e}_i)\|_{L^2(K_R)}.$$

Moreover, u^i is Hölder continuous in $K_R \times (0, T]$.

Proposition 2.2. *Let $a \in \mathcal{M}_{per}(\alpha, \beta, K)$ and $\nabla \cdot (a(\mathbf{x})\mathbf{e}_i) \in L_0^2(K)$. Then, (10) has a unique weak solution v^i such that*

$$v^i \in L^2([0, +\infty), W_{per}^1(K)), \partial_t v^i \in L^2([0, +\infty), W_{per}^1(K)').$$

It follows that $v^i \in C([0, +\infty), L^2(K))$, and there exist constants $C > 0$ such that the following bounds hold true:

$$\|v^i\|_{L^\infty([0, +\infty), L^2(K))} + \|v^i\|_{L^2([0, +\infty), W_{per}^1(K))} \leq C \|\nabla \cdot (a(\mathbf{x})\mathbf{e}_i)\|_{L^2(K)}.$$

Moreover, v^i is Hölder continuous in $K \times (0, T]$.

Here, the space $W_{per}^1(K)'$ is the dual space of $W_{per}^1(K)$ (a characterization of this space can be found in Ref. 17). With a slight abuse of notation, in the coming sections the functions v^i will indicate both the solution of (10) on the cell K and its periodic extension to the whole \mathbb{R}^d . Finally, we define the bilinear form $B : W_{per}^1(K) \times W_{per}^1(K) \mapsto \mathbb{R}$ through the formula

$$B[u, v] = \int_K \nabla u \cdot a(\mathbf{x})\nabla v \, d\mathbf{x}. \quad (11)$$

If $a \in \mathcal{M}_{\text{per}}(\alpha, \beta, K)$, the bilinear form $B[\cdot, \cdot]$ is continuous and coercive and there exists a non-decreasing sequence of strictly positive eigenvalues $\{\lambda_j\}_{j=0}^{\infty}$ and a L^2 -orthonormal set of eigenfunctions $\{\varphi_j\}_{j=0}^{\infty} \subset W_{\text{per}}^1(K)$ such that

$$B[\varphi_j, w] = \lambda_j \langle \varphi_j, w \rangle_{L^2(K)}, \quad \forall w \in W_{\text{per}}^1(K). \quad (12)$$

3 Main results

The starting point of the analysis is the following new formula for the approximation of the homogenized coefficient a^0 in (3)

$$\mathbf{e}_i \cdot a_{R,L,T}^0 \mathbf{e}_j = \int_{K_L} \mathbf{e}_i \cdot a(\mathbf{x}) \mathbf{e}_j \mu_L(\mathbf{x}) \, d\mathbf{x} - 2 \int_0^T \int_{K_L} u^i(\mathbf{x}, t) w^j(\mathbf{x}, t) \mu_L(\mathbf{x}) \, d\mathbf{x} \, dt, \quad (13)$$

where $\{u^i\}_{i=1}^d$ are the solutions of the parabolic problems (9). Note that the parabolic solutions $\{u^i\}_{i=1}^d$ are solved over K_R , from which it follows the dependency of $a_{R,L,T}^0$ on the parameter R , while the averaging is taking place over the domain $K_L \subset K_R$. The aim of this section is two-fold: first, in Subsection 3.1, we will recall a result which is proved in Ref. 4, where the equivalence between the approximate homogenized coefficient (13) (when $T = \infty$), and the approximation (6) based on elliptic cell problems (when χ_R^i is supplied with homogeneous Dirichlet BCs) is shown. Next, in Subsection 3.2, we will present our main statement in Theorem 3.2, which states that if T is chosen optimally, then we obtain arbitrarily high convergence rates for the difference between $a_{R,L,T}^0$ in (13) and the exact homogenized coefficient a^0 in (4), when $a \in \mathcal{M}_{\text{per}}(\alpha, \beta, K)$.

3.1 Equivalence between the standard and parabolic homogenized coefficients

Assume that the elliptic solutions χ_R^i in (7) are supplied either with periodic or homogeneous Dirichlet BCs. By symmetry of $a(\mathbf{x})$, we can rewrite (6) as:

$$\mathbf{e}_i \cdot a_R^0 \mathbf{e}_j = \int_{K_R} \mathbf{e}_i \cdot a(\mathbf{x}) \mathbf{e}_j \, d\mathbf{x} - \int_{K_R} \nabla \chi_R^i(\mathbf{x}) \cdot a(\mathbf{x}) \nabla \chi_R^j(\mathbf{x}) \, d\mathbf{x}.$$

Theorem 3.1 provides an alternative expression for the second integral, which will be referred to as the *correction part* of the homogenized tensor, based on the use of parabolic problems over infinite time domain. We refer to Ref. 4 for a rigorous proof.

Theorem 3.1. *Let $a(\mathbf{x}) \in \mathcal{M}(\alpha, \beta, K_R)$, $u^i \in C([0, +\infty), L^2(K_R))$ be the weak solution of (9) and $\chi_R^i \in H_0^1(K_R)$ be the weak solution of (7). Then, for $1 \leq i, j \leq d$, the following identities hold*

$$\chi_R^i = \int_0^{+\infty} u^i(\cdot, t) \, dt \quad \text{in } H_0^1(K_R), \quad (14)$$

$$\frac{1}{2} \int_{K_R} \nabla \chi_R^i(\mathbf{x}) \cdot a(\mathbf{x}) \nabla \chi_R^j(\mathbf{x}) d\mathbf{x} = \int_0^{+\infty} \int_{K_R} u^i(\mathbf{x}, t) u^j(\mathbf{x}, t) d\mathbf{x} dt. \quad (15)$$

Theorem 3.1 implies that if $T = \infty$ (and $\mu_L = L^{-d}$ in K_L with $R = L$) in (13), then the parabolic formulation does not lead to any gain in the first order convergence rate in (8) due to the equivalence relation above. It is important to notice that we do not need the periodicity assumption on the tensor a for deriving the equivalence. Moreover, the same result holds true if we substitute the homogeneous Dirichlet condition with the periodic boundary conditions, under the periodicity assumption for the tensor a . Then we have the following corollary:

Corollary 3.1. *Let $a(\mathbf{x}) \in \mathcal{M}_{per}(\alpha, \beta, K)$. Let $v^i \in C([0, +\infty), L^2_{per}(K))$ solve (10). Then*

$$\mathbf{e}_i \cdot a^0 \mathbf{e}_j = \int_K \mathbf{e}_i \cdot a(\mathbf{x}) \mathbf{e}_j d\mathbf{x} - 2 \int_0^{+\infty} \int_K v^i(\mathbf{x}, t) v^j(\mathbf{x}, t) d\mathbf{x} dt. \quad (16)$$

3.2 High order convergence rates and optimal choices for T and L

As stated in the Subsection 3.1, the consequence of the equivalence between the parabolic model and the standard elliptic model is that the first order convergence rate of the resonance error in (8) remains unchanged. In this subsection, we summarize our main result which states that we are able to achieve arbitrarily high convergence rates for the resonance error

$$e_{MOD} := \|a_{R,L,T}^0 - a^0\|_F,$$

upon choosing the parameters T and L optimally.

Theorem 3.2. *Let the coefficient matrix $a(\cdot)$ satisfy the following conditions:*

- i) $a(\cdot) \in \mathcal{M}_{per}(\alpha, \beta, K)$,
- ii) $a(\cdot) \mathbf{e}_i \in H_{div}(K_R)$, $i = 1, \dots, d$,
- iii) $a(\cdot) \in [C^{1,\gamma}(K_R)]^{d \times d}$ for some $0 < \gamma \leq 1$.

Let $K_R \subset \mathbb{R}^d$ for $d \leq 3$ and $R \geq 1$. Let $a_{R,L,T}^0$ and a^0 be defined, respectively, as in (13) and (4), with u^i satisfying (9) for any $i = 1, \dots, d$. Let $\mu_L \in \mathbb{K}^q(K_L)$, with $0 < L < R - 3/2$ and $T \leq \frac{2c}{d+1} |R - L|^2$, with $c = 1/(4\beta)$. Then, there exists constants $\lambda_0(\alpha, d)$ and $C > 0$ independent of R, L or T (but it may depend on $d, a(\cdot)$ and $\mu_L(\cdot)$) such that

$$\|a_{R,L,T}^0 - a^0\|_F \leq C \left[L^{-(q+1)} + e^{-2\lambda_0 T} + \frac{1}{T} \left(\frac{R}{\sqrt{T}} \right)^{d-1} e^{-c \frac{|R-L|^2}{T}} \right]$$

$$+ \left(\frac{T}{|R-L|^2} \right)^{3-d} e^{-2c \frac{|R-L|^2}{T}} \Big]. \quad (17)$$

Additionally, If $\nabla \cdot (a(\cdot)\mathbf{e}_i) \in W_{per}^1(K)$, then there exists a constant $C > 0$ independent of R, L or T (but it may depend on $d, a(\cdot)$ and $\mu_L(\cdot)$) such that

$$\|a_{R,L,T}^0 - a^0\|_F \leq C \left[L^{-(q+1)} + e^{-2\lambda_0 T} + \frac{1}{|R-L|} \left(\frac{R}{\sqrt{T}} + 1 \right)^{d-1} e^{-c \frac{|R-L|^2}{T}} + \frac{1}{|R-L|^2} \left(\frac{R^2}{T} \right) e^{-2c \frac{|R-L|^2}{T}} \right]. \quad (18)$$

The choice

$$L = k_o R, \quad T = k_T R,$$

with $0 < k_o < 1$ and $k_T = \sqrt{\frac{c}{2\lambda_0}}(1 - k_o)$ results in the following convergence rate in terms of R

$$\|a_{R,L,T}^0 - a^0\|_F \leq C \left[R^{-(q+1)} + e^{-\sqrt{2\lambda_0 c}(1-k_o)R} \right], \quad (19)$$

for a constant $C > 0$ independent of R, L or T .

Remark 3.1. Note that the exponent in the exponential term $\sqrt{2\lambda_0 c} \approx \sqrt{\alpha/\beta}$ depends on the contrast ratio.

Later in the analysis, it will be clear that the main idea of limiting $T \approx R$ is to exploit the mild dependence of the parabolic solutions u^i on the boundary conditions, which is the case if parabolic solutions are evolved over a sufficiently short time. Second, the use of filtering functions μ_L is to achieve high order convergence rates for the averages of oscillatory functions, which is another essential component in achieving high order rates for the resonance error. In what follows, we focus on proving Theorem 3.2.

4 Error analysis

In this section we prove the bound stated in Theorem 3.2. The proof can be outlined as follows:

Step 1: We exploit the fact that the exact homogenized coefficient a^0 in (4) is equal to (16), and we decompose the error into four terms

$$\mathbf{e}_i \cdot (a_{R,L,T}^0 - a^0) \mathbf{e}_j = \underbrace{\int_{K_{RL}} \mathbf{e}_i \cdot a(\mathbf{x}) \mathbf{e}_j \mu_L(\mathbf{x}) \, d\mathbf{x} - \int_K \mathbf{e}_i \cdot a(\mathbf{x}) \mathbf{e}_j \, d\mathbf{x}}_{I_{ij}^1}$$

$$\begin{aligned}
& \underbrace{+2 \int_0^T \int_{K_L} v^i(\mathbf{x}, t) v^j(\mathbf{x}, t) \mu_L(\mathbf{x}) d\mathbf{x} dt - 2 \int_0^T \int_{K_L} u^i(\mathbf{x}, t) u^j(\mathbf{x}, t) \mu_L(\mathbf{x}) d\mathbf{x} dt}_{I_{ij}^2} \\
& \underbrace{+2 \int_0^T \int_K v^i(\mathbf{x}, t) v^j(\mathbf{x}, t) d\mathbf{x} dt - 2 \int_0^T \int_{K_L} v^i(\mathbf{x}, t) v^j(\mathbf{x}, t) \mu_L(\mathbf{x}) d\mathbf{x} dt}_{I_{ij}^3} \\
& \underbrace{+2 \int_0^{+\infty} \int_K v^i(\mathbf{x}, t) v^j(\mathbf{x}, t) d\mathbf{x} dt - 2 \int_0^T \int_K v^i(\mathbf{x}, t) v^j(\mathbf{x}, t) d\mathbf{x} dt}_{I_{ij}^4}. \quad (20)
\end{aligned}$$

Step 2: Estimation of the *averaging* errors I_{ij}^1 and I_{ij}^3 by means of Lemma 2.1.

Step 3: Estimation of the *truncation* error I_{ij}^4 by means of the exponential decrease in time of $\|v^i(\cdot, t)\|_{L^2(Y)}$.

Step 4: Estimation of the *boundary* error I_{ij}^2 by means of upper bounds for the fundamental solution of the parabolic problem and integration over finite time intervals $[0, T]$.

The coming subsections will be devoted to the derivation of upper bounds for I_{ij}^1 , I_{ij}^2 , I_{ij}^3 and I_{ij}^4 .

4.1 Bounds for I_{ij}^1 and I_{ij}^3

The two error terms studied in this subsection originate from the fact that we are approximating the averages of periodic functions by a weighted average over a bounded domain. For such a reason, these errors will be referred to as *averaging* error for a (I_{ij}^1) and for v^i (I_{ij}^3). The Corollary 4.1 is a direct consequence of Lemma 2.1, and therefore the proof is omitted.

Corollary 4.1. *Let $a \in \mathcal{M}_{per}(\alpha, \beta, K)$ be periodically extended over K_L . Then, there exists $C_1 > 0$, independent of L , such that*

$$|I_{ij}^1| \leq C_1 L^{-(q+1)}, \quad i, j = 1, \dots, d.$$

Before providing a convergence result for I_{ij}^3 we recall the following property about product rule in Sobolev spaces (see Ref. 16 for a proof).

Lemma 4.1. *Let $u, v \in W^{1,p}(\Omega) \cap L^\infty(\Omega)$, with $1 \leq p \leq +\infty$. Then, $uv \in W^{1,p}(\Omega) \cap L^\infty(\Omega)$ and the product rule for derivation holds:*

$$\frac{\partial}{\partial x_i}(uv) = \frac{\partial u}{\partial x_i} v + u \frac{\partial v}{\partial x_i}, \quad i = 1, \dots, d.$$

Lemma 4.2. *Let $a(\cdot)$ satisfy conditions i) and ii) of Theorem 3.2, let $v^i \in L^2([0, +\infty), W_{per}^1(K))$ be the K -periodic solution of (10) and $\mu_L \in \mathbb{K}^q(K_L)$. Then, there exists $C_3 > 0$, independent of L , such that*

$$|I_{ij}^3| \leq C_3 L^{-(q+1)}.$$

Proof. By applying Lemma 2.1 to function $2v^i v^j$ we get:

$$|I_{ij}^3| \leq \int_0^T C \|v^i(\cdot, t)v^j(\cdot, t)\|_{L^p(K)} L^{-(q+1)} dt, \quad (21)$$

with $1 < p \leq 2$. Following the proof of Lemma 2.1 (see Appendix A, Ref. 25), we deduce that, for any $q \geq 2$ one can also choose $p = 1$ in the inequality above. Therefore, by the use of Cauchy-Schwarz and Hölder inequalities, I_{ij}^3 can be estimated as

$$\begin{aligned} |I_{ij}^3| &\leq \int_0^T C \|v^i(\cdot, t)v^j(\cdot, t)\|_{L^1(K)} L^{-(q+1)} dt \\ &\leq CL^{-(q+1)} \int_0^T \|v^i(\cdot, t)\|_{L^2(K)} \|v^j(\cdot, t)\|_{L^2(K)} dt \\ &\leq CL^{-(q+1)} \|v^i\|_{L^2([0, +\infty), L^2(K))} \|v^j\|_{L^2([0, +\infty), L^2(K))}. \end{aligned}$$

The result follows by choosing

$$C_3 := C \|v^i\|_{L^2([0, +\infty), L^2(K))} \|v^j\|_{L^2([0, +\infty), L^2(K))}.$$

In the case $q \in \{0, 1\}$ we cannot utilize any more the L^1 -norm of the product. In view of (21), with the choice $p = 3/2$, it follows that

$$\begin{aligned} |I_{ij}^3| &\leq \int_0^T C \|v^i(\cdot, t)v^j(\cdot, t)\|_{L^{3/2}(K)} L^{-(q+1)} dt \\ &\leq \int_0^T C \|v^i(\cdot, t)v^j(\cdot, t)\|_{W^{1,1}(K)} L^{-(q+1)} dt \\ &\leq \int_0^T C \|v^i(\cdot, t)\|_{W_{per}^1(K)} \|v^j(\cdot, t)\|_{W_{per}^1(K)} L^{-(q+1)} dt \\ &\leq CL^{-(q+1)} \|v^i\|_{L^2([0, +\infty), W_{per}^1(K))} \|v^j\|_{L^2([0, +\infty), W_{per}^1(K))}, \end{aligned}$$

where the first inequality is a direct application of Lemma 2.1, the second inequality follows from the continuous inclusion of $W^{1,1}(K)$ in $L^{3/2}(K)$, the third inequality comes from the embedding $W_{per}^1(K) \subset W^{1,1}(K)$ and the validity of Lemma 4.1 for functions v^i which implies:

$$\|v^i(\cdot, t)v^j(\cdot, t)\|_{W^{1,1}(K)} \leq C \|v^i(\cdot, t)\|_{W_{per}^1(K)} \|v^j(\cdot, t)\|_{W_{per}^1(K)}.$$

Finally, the last inequality is the Cauchy-Schwarz inequality. The result follows by choosing

$$C_3 := C \|v^i\|_{L^2([0, +\infty), W_{per}^1(K))} \|v^j\|_{L^2([0, +\infty), W_{per}^1(K))}.$$

□

4.2 Bound for I_{ij}^4

In this subsection we derive an *a-priori* estimate for the truncation error, which originates from the restriction of the time integral in (13) on the finite interval $[0, T]$. As it will be clearer from the coming analysis, the time truncation is essential for improving the convergence rate of the resonance error, as large values of T result in a pollution of the correctors. First of all, we recall the following lemma on the exponential decay in time of $\|v^i(\cdot, t)\|_{L^2(K)}$.

Lemma 4.3. *Let $v^i \in C([0, \infty), L^2(K))$ be the solution of (10) and let $\lambda_0 > 0$ be the smallest eigenvalue of the bilinear form B introduced in (11). Then*

$$\|v^i(\cdot, t)\|_{L^2(K)} \leq e^{-\lambda_0 t} \|v^i(\cdot, 0)\|_{L^2(K)}, \quad \text{a. e. } t \in [0, +\infty).$$

Proof. The weak formulation of (10) reads: Find $v^i \in L^2([0, +\infty), W_{per}^1(K))$, $\partial_t v^i \in L^2([0, +\infty), W_{per}^1(K)')$ such that

$$\begin{aligned} (\partial_t v^i, w) + B[v^i, w] &= 0, \quad \forall w \in W_{per}^1(K), \\ v^i(\cdot, 0) &= \nabla \cdot (a\mathbf{e}_i) \in L_0^2(K). \end{aligned}$$

By using $w = v^i(\cdot, t)$, the second line becomes

$$\frac{1}{2} \frac{d}{dt} \|v^i\|_{L^2(K)}^2 = -B[v^i, v^i].$$

Let $\{\lambda_j\}_{j=0}$ and $\{\varphi_j\}_{j=0}$ be, respectively, the eigenvalues and eigenfunctions of B and let us denote $\hat{v}_j^i := \langle v^i, \varphi_j \rangle_{L^2(K)}$. By orthogonality of the eigenfunctions and Parseval's identity, it holds

$$B[v^i, v^i] = \sum_{j=0}^{\infty} \lambda_j |\hat{v}_j^i|^2 \geq \lambda_0 \sum_{j=0}^{\infty} |\hat{v}_j^i|^2 = \lambda_0 \|v^i\|_{L^2(K)}^2.$$

Then, by coercivity of the bilinear form B and use of the above inequality, we get

$$\|v^i\|_{L^2(K)} \frac{d}{dt} \|v^i\|_{L^2(K)} = \frac{1}{2} \frac{d}{dt} \|v^i\|_{L^2(K)}^2 = -B[v^i, v^i] \leq -\lambda_0 \|v^i\|_{L^2(K)}^2.$$

So, the following differential inequality is derived:

$$\frac{d}{dt} \|v^i\|_{L^2(K)} \leq -\lambda_0 \|v^i\|_{L^2(K)}.$$

As proved in Ref. 21, $\|v^i(\cdot, t)\|_{L^2(K)}$ is absolutely continuous in time, and the result is obtained by Gronwall's inequality. \square

Remark 4.1. *It is easy to prove that $\lambda_0 \geq \frac{\alpha}{C_P^2}$, where the Poincaré constant for a convex domain K is $C_P = \frac{\text{diam}(K)}{\pi}$, see Ref. 39.*

Lemma 4.4 (Truncation error). *Let $v^i \in C([0, +\infty), L^2(K))$ solve (10), and let*

$$I_{ij}^4 := 2 \int_T^{+\infty} \int_K v^i(\mathbf{x}, t) v^j(\mathbf{x}, t) d\mathbf{x} dt.$$

Then, there exist $C_4 > 0$, independent of T , such that

$$|I_{ij}^4| \leq C_4 e^{-2\lambda_0 T}, \quad (22)$$

where λ_0 is the smallest eigenvalue of B .

Proof. We start by applying the Cauchy-Schwarz inequality on $L^2(K)$:

$$|I_{ij}^4| \leq \frac{2}{|K|} \int_T^\infty \|v^i(\cdot, t)\|_{L^2(K)} \|v^j(\cdot, t)\|_{L^2(K)} dt. \quad (23)$$

Then, we plug the result of Lemma 4.3 into (23):

$$\begin{aligned} |I_{ij}^4| &\leq \frac{2}{|K|} \int_T^\infty e^{-2\lambda_0 t} \|v^i(\cdot, 0)\|_{L^2(K)} \|v^j(\cdot, 0)\|_{L^2(K)} dt \\ &\leq \frac{1}{|K|} \|v^i(\cdot, 0)\|_{L^2(K)} \|v^j(\cdot, 0)\|_{L^2(K)} \frac{1}{\lambda_0} e^{-2\lambda_0 T}. \end{aligned}$$

The results follows by choosing

$$\begin{aligned} C_4 &= \frac{1}{\lambda_0 |K|} \|v^i(\cdot, 0)\|_{L^2(K)} \|v^j(\cdot, 0)\|_{L^2(K)} \\ &= \frac{1}{\lambda_0 |K|} \|\nabla \cdot (a(\cdot) \mathbf{e}_i)\|_{L^2(K)} \|\nabla \cdot (a(\cdot) \mathbf{e}_j)\|_{L^2(K)}. \end{aligned}$$

□

4.3 Bound for I_{ij}^2

From the definition,

$$I_{ij}^2 := \int_0^T \int_{K_L} (u^i u^j - v^i v^j) \mu_L d\mathbf{x} dt, \quad (24)$$

one can notice that the source of the error I_{ij}^2 is the mismatch between u^i and v^i on the boundary ∂K_R . Therefore, we refer to such an error as the *boundary error*. The boundary error converges to zero at an exponential rate, as stated in Lemma 4.5.

Lemma 4.5. *Let $a(\cdot)$ satisfy conditions i), ii) and iii) of Theorem 3.2 and let I_{ij}^2 be defined by (24). Then, there exist constants $C, c > 0$, independent of R, L and T such that*

$$|I_{ij}^2| \leq C \left[\frac{1}{T} \left(\frac{R}{\sqrt{T}} \right)^{d-1} e^{-c \frac{|R-L|^2}{T}} + \left(\frac{T}{|R-L|^2} \right)^{3-d} e^{-2c \frac{|R-L|^2}{T}} \right].$$

Additionally, If $\nabla \cdot (a(\cdot)\mathbf{e}_i) \in W_{per}^1(K)$, then there exist constants $C, c > 0$, independent of R, L and T such that

$$|I_{ij}^2| \leq C \left[\frac{1}{|R-L|} \left(\frac{R}{\sqrt{T}} + 1 \right)^{d-1} e^{-c\frac{|R-L|^2}{T}} + \frac{1}{|R-L|^2} \left(\frac{R^2}{T} \right) e^{-2c\frac{|R-L|^2}{T}} \right].$$

The proof of Lemma 4.5 directly follows from Propositions 4.1 and 4.2. We need Definitions 4.1 and 4.2 in order to define a *boundary error function* which will be used in the estimation of I_{ij}^2 .

Definition 4.1 (Boundary layer). *Let us define a sub-domain $K_{\tilde{R}} \subset K_R$, where \tilde{R} is defined to be the largest integer such that $\tilde{R} \leq R-1/2$. The boundary layer is defined as the set $\Delta := K_R \setminus K_{\tilde{R}}$. We observe that $|\Delta| = R^d - \tilde{R}^d \leq 2dR^{d-1}$.*

Definition 4.2 (Cut-off function). *A cut-off function on K_R is a function $\rho \in C^\infty(K_R, [0, 1])$ such that*

$$\rho(y) = \begin{cases} 1 & \text{in } K_{\tilde{R}} \\ 0 & \text{on } \partial K_R \end{cases} \quad \text{and} \quad |\nabla \rho(y)| \leq C \quad \text{on } \Delta,$$

where the subdomain $K_{\tilde{R}}$ and the boundary layer Δ are defined according to Definition 4.1.

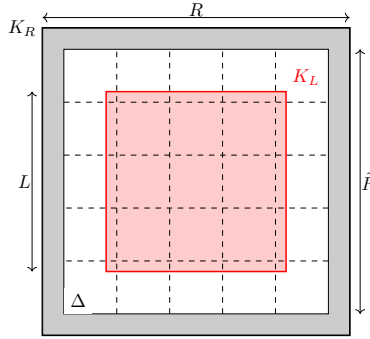


Figure 1: Scheme of the sampling domain K_R and its subsets $K_L, K_{\tilde{R}}$ and Δ .

Let us define the boundary error function $\theta^i \in L^2([0, +\infty), H_0^1(K_R))$ through the relation $\theta^i := u^i - \rho v^i$. For the analysis it is fundamental that $\rho = 1$ in $K_{\tilde{R}}$ and that $L < \tilde{R}$. By the definition of θ^i , we write

$$I_{ij}^2 = \int_0^T \int_{K_L} [v^i v^j (\rho^2 - 1) + \theta^i v^j + v^i \theta^j + \theta^i \theta^j] \mu_L \, dx \, dt.$$

One readily notice that the first term in the integral vanishes on the integration domain, since $\rho^2(\mathbf{x}) = 1$ for all $\mathbf{x} \in K_{\tilde{R}} \supset K_L$. So, we have to study the integrals

$$I_{ij}^{2,b} := \int_0^T \int_{K_L} v^i \theta^j \mu_L \, dx \, dt, \quad \text{and} \quad I_{ij}^{2,c} := \int_0^T \int_{K_L} \theta^i \theta^j \mu_L \, dx \, dt. \quad (25)$$

As both integrals depend on the values that the functions θ^i take over the averaging domain K_L , we need to provide pointwise estimates for $\theta^i(\mathbf{x}, t)$ on $K_L \times [0, T]$. This is done in subsection 4.3.1 by the use of the fundamental solution of problem (9).

4.3.1 Estimates for θ^i

Here, we derive an upper bound for θ^i on $K_L \times [0, T]$. By definition and linearity of the correctors problem, the function θ^i satisfies the problem:

$$\frac{\partial \theta^i}{\partial t} - \nabla \cdot (a(\mathbf{x}) \nabla \theta^i) = -\nabla(1 - \rho(\mathbf{x})) \cdot a(\mathbf{x}) \nabla v^i - \nabla \cdot [a(\mathbf{x}) \nabla(1 - \rho(\mathbf{x})) v^i] \quad (26)$$

in $K_R \times (0, +\infty)$, with boundary and initial conditions

$$\begin{aligned} \theta^i &= 0 && \text{on } \partial K_R \times (0, +\infty), \\ \theta^i(\mathbf{x}, 0) &= v^i(\mathbf{x}, 0)(1 - \rho(\mathbf{x})) && \text{in } K_R. \end{aligned} \quad (27)$$

As the integrals in (25) are performed over a subset K_L of the domain K_R of (26), we are not really interested in estimating the norm of θ^i over the whole K_R , but rather on K_L . Thus, thanks to the use of fundamental solution for problem (26) and (27), we will derive a-priori pointwise estimates for $\theta^i(\mathbf{x}, t)$, for $(\mathbf{x}, t) \in K_L \times (0, T)$. The legitimacy of pointwise estimates for θ^i is guaranteed by the fact that u^i and v^i are Hölder continuous functions for $t > 0$, and so is θ^i . Hence, for $t > 0$, the pointwise values of $\theta^i(\mathbf{x}, t)$ is meaningful. Moreover, since $\theta^i(\mathbf{x}, 0) = 0$ in K_L , $\theta^i(\mathbf{x}, t)$ is bounded in $K_L \times [0, +\infty)$.

Usually, the existence of a fundamental solution for equations like (26) and (27) and the derivation of its properties are done for parabolic problems in non-divergence form with Hölder continuous coefficients Ref. 23,33. In this setting it is possible to prove pointwise bounds (of the type of (61)) on the spatial (up to second order) and time (up to first order) derivatives of the fundamental solution. The existence result can be extended to the case of equations in divergence form with discontinuous coefficients, under the only assumption of uniform ellipticity, see Ref. 11. In this weaker setting it is possible to prove the well-known Nash-Aronson estimate on the fundamental solution, but there is no prove, to the best of authors' knowledge, of the existence of similar bound for the derivative. Therefore, we need to assume $C^{1,\gamma}$ -regularity for $a(\cdot)$ in order to be able to write the equation in non-divergence form and use the results of Ref. 23,33.

We will denote by $\Gamma(\mathbf{x}, t; \xi, \tau) \in C^{0,\gamma}(K_R \times (\tau, +\infty))$ the fundamental solution of the parabolic operator with homogeneous Dirichlet boundary conditions

$$\begin{aligned} L_{(\mathbf{x},t)} : L^2([\tau, +\infty), H_0^1(K_R)) &\mapsto L^2([\tau, +\infty), H^{-1}(K_R)) \\ u &\mapsto \partial_t u - \nabla_{\mathbf{x}} \cdot (a(\mathbf{x}) \nabla_{\mathbf{x}} u), \end{aligned}$$

i.e. $\Gamma(\mathbf{x}, t; \xi, \tau)$ satisfies

$$L_{(\mathbf{x},t)} \Gamma(\mathbf{x}, t; \xi, \tau) = 0, \quad (\mathbf{x}, \xi, t) \in K_R \times K_R \times (\tau, +\infty), \quad (28a)$$

$$g(\mathbf{x}) = \lim_{t \rightarrow \tau^+} \int_{K_R} \Gamma(\mathbf{x}, t; \xi, \tau) g(\xi) d\xi, \quad \forall g \in C(K_R). \quad (28b)$$

Subscript (\mathbf{x}, t) in (28a) is to indicate that the differentiation is operated with respect to the \mathbf{x} - and t -variables. Equation (28b) can be interpreted as the fact that the initial condition (given that the initial time instant is $t = \tau$) for the fundamental solution is $\Gamma(\mathbf{x}, \tau; \xi, \tau) = \delta(\mathbf{x} - \xi)$, the Dirac's delta function centred at ξ . In the same way, one can define the adjoint operator, given the symmetry of a , as

$$\begin{aligned} L_{(\mathbf{y}, s)}^* : L^2((-\infty, \tau], H_0^1(K_R)) &\mapsto L^2((-\infty, \tau], H^{-1}(K_R)) \\ u &\mapsto -\partial_s u - \nabla_{\mathbf{y}} \cdot (a(\mathbf{y}) \nabla_{\mathbf{y}} u). \end{aligned}$$

The fundamental solution of $L_{(\mathbf{y}, s)}^*$ is denoted by $\Gamma^*(\mathbf{y}, s; \mathbf{x}, t)$ and satisfies

$$\begin{aligned} L_{(\mathbf{y}, s)}^* \Gamma^*(\mathbf{y}, s; \xi, \tau) &= 0, \quad (\mathbf{y}, \xi, s) \in K_R \times K_R \times (-\infty, \tau), \\ g(\mathbf{y}) &= \lim_{s \rightarrow \tau^-} \int_{K_R} \Gamma^*(\mathbf{y}, s; \xi, \tau) g(\xi) d\xi, \quad \forall g \in C(K_R). \end{aligned}$$

A well-known result is that the differential problems

$$L_{(\mathbf{x}, t)} u = f \quad \text{and} \quad L_{(\mathbf{y}, s)}^* v = \hat{f}$$

are well-posed only for $t > \tau$ and $s < \tau$, respectively, where τ is the time of the initial (resp. final) condition. Thus, we formally define

$$\Gamma(\mathbf{x}, t; \xi, \tau) = 0, \quad \text{for } t < \tau, \quad \Gamma^*(\mathbf{y}, s; \xi, \tau) = 0, \quad \text{for } s > \tau.$$

A central property of the two fundamental solutions is

$$\Gamma(\mathbf{x}, t; \mathbf{y}, s) = \Gamma^*(\mathbf{y}, s; \mathbf{x}, t), \quad \text{for } s < t. \quad (29)$$

The identity between two fundamental solution is proved in Theorem 17, §3.7 Ref. 23 for the case of Hölder continuous coefficients, but it can be extended to the discontinuous case by following the same proof, as done in Ref. 13. Pointwise *a-priori* estimates for Γ are derived in Ref. 12, following the results obtained in Ref. 38. Such estimates can be extended to the derivatives of the fundamental solution under additional regularity assumptions, see, e.g., Ref. 23, 33. The solution of (26) can be written as

$$\begin{aligned} \theta^i(\mathbf{x}, t) &= \int_{K_R} \Gamma(\mathbf{x}, t; \mathbf{y}, 0) v^i(\mathbf{y}, 0) (1 - \rho(\mathbf{y})) d\mathbf{y} \\ &\quad - \int_{K_R} \int_0^t \Gamma(\mathbf{x}, t; \mathbf{y}, s) \nabla_{\mathbf{y}} (1 - \rho(\mathbf{y})) \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} v^i(\mathbf{y}, s) ds d\mathbf{y} \\ &\quad + \int_{K_R} \int_0^t \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s) \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} (1 - \rho(\mathbf{y})) v^i(\mathbf{y}, s) ds d\mathbf{y}, \quad (30) \end{aligned}$$

for any $t > 0$. Now, we provide a lemma for rewriting (30) in the form of boundary flux integral.

Lemma 4.6. *Let $a(\cdot)$ satisfy conditions i) and ii) of Theorem 3.2, θ^i be the weak solution of (26) and let v^i be Hölder continuous in $K_R \times (0, +\infty)$. Then, for any $(\mathbf{x}, t) \in K_L \times (0, +\infty)$,*

$$\theta^i(\mathbf{x}, t) = \int_{\partial K_R} \int_0^t \mathbf{n} \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s) v^i(\mathbf{y}, s) ds d\sigma_{\mathbf{y}}, \quad (31)$$

where \mathbf{n} denotes the unit vector orthogonal to ∂K_R pointing outward.

From now on we will distinguish two cases in the derivation of the estimates, based on the regularity of the initial condition $v^i(\cdot, 0) = \nabla \cdot (a(\cdot) \mathbf{e}_i)$, i.e. on the regularity of the tensor $a(\cdot)$.

Lemma 4.7. *Let $a(\cdot)$ satisfy conditions i), ii) and iii) of Theorem 3.2³, let $\theta^i \in C([0, +\infty), L^2(K_R))$ be the solution of (26), and let $v^i \in L^2((0, +\infty), W_{per}^1(K))$ be the solution of (10). Then, there exist a constant $\tilde{C} > 0$, independent of R and L such that*

$$\sup_{\mathbf{x} \in K_L} |\theta^i(\mathbf{x}, t)| \leq \tilde{C} \frac{R^{d-1}}{|R-L|} \|\nabla v^i\|_{L^2((0,t), L^2(K))} \left[\frac{1}{t} + \frac{1}{2c|R-L|^2} \right]^{\frac{d-1}{2}} e^{-c \frac{|R-L|^2}{t}}, \quad (32)$$

for $c = 1/4\beta$.

Otherwise, if $v^i \in C([0, +\infty) W_{per}^1(K))$, then

$$\sup_{\mathbf{x} \in K_L} |\theta^i(\mathbf{x}, t)| \leq \tilde{C} R^{d-1} \|v^i(\cdot, 0)\|_{W_{per}^1(K)} e^{-\lambda_0 t} \int_0^t \frac{1}{s^{(d+1)/2}} e^{-c \frac{|R-L|^2}{s}} e^{\lambda_0 s} ds, \quad (33)$$

where $\lambda_0 > 0$ is the smallest eigenvalue of the bilinear form B .

Lemmas 4.6 and 4.7 are proved in A.

4.3.2 Term $I^{2,b}$

Proposition 4.1. *Let the hypotheses of Lemma 4.7 be satisfied. Moreover, let $v^i \in C([0, +\infty), L^2(K))$, $\theta^i \in L^\infty(K_L \times [0, +\infty))$, let $I_{ij}^{2,b}$ be defined as in (25) and let L/R be constant. Then, there exist constants $C_{2,b}, C'_{2,b}, c > 0$ independent of R, L, T such that*

$$\left| I_{ij}^{2,b} \right| \leq \frac{C_{2,b}}{|R-L|} \|v^i\|_{L^2([0, +\infty), W_{per}^1(K))} \left(\frac{R}{\sqrt{T}} + C'_{2,b} \right)^{d-1} e^{-c \frac{|R-L|^2}{T}}, \quad (34)$$

Otherwise, if $v^i(\cdot, 0) \in W_{per}^1(K)$ and $T \leq \frac{2c}{d+1} |R-L|^2$ then there exist constants $C_{2,b}, c > 0$ independent of R, L, T such that

$$\left| I_{ij}^{2,b} \right| \leq \frac{C_{2,b}}{T} \|v^i(\cdot, 0)\|_{W_{per}^1(K)} \left(\frac{R}{\sqrt{T}} \right)^{d-1} e^{-c \frac{|R-L|^2}{T}}. \quad (35)$$

³The assumption of Hölder continuity of $\partial_k a_{ij}(\mathbf{x})$ is to ensure the correctness of (61).

Proof. Applying Hölder inequality on the space integral, we obtain:

$$\begin{aligned} \left| \int_0^T \int_{K_L} v^i(\mathbf{x}, t) \theta^j(\mathbf{x}, t) \mu_L(\mathbf{x}) dx dt \right| &\leq \int_0^T \int_{K_L} |v^i(\mathbf{x}, t) \theta^j(\mathbf{x}, t) \mu_L(\mathbf{x})| dx dt \\ &\leq \int_0^T \|v^i(\cdot, t)\|_{L^2(K_L)} \|\theta^j(\cdot, t)\|_{L^\infty(K_L)} \|\mu_L\|_{L^2(K_L)} dt. \end{aligned}$$

By assumption, $\mu_L \in L^\infty(K_L) \subset L^2(K_L)$ with continuous inclusion, and

$$\|\mu_L\|_{L^2(K_L)} \leq |K_L|^{1/2} \|\mu_L\|_{L^\infty(K_L)} \leq C_\mu L^{-d/2}.$$

Next, we estimate $\|v^i(\cdot, t)\|_{L^2(K_L)}$. Since v^i , we have for integer L

$$\|v^i(\cdot, t)\|_{L^2(K_L)} = L^{d/2} \|v^i(\cdot, t)\|_{L^2(K)},$$

while, for non-integer L

$$\|v^i(\cdot, t)\|_{L^2(K_L)} \leq \lceil L \rceil^{d/2} \|v^i(\cdot, t)\|_{L^2(K)}.$$

Finally, we recall the exponential decay of $\|v^i(\cdot, t)\|_{L^2(K)}$ and we derive the estimate:

$$\begin{aligned} \left| \int_0^T \int_{K_L} v^i(\mathbf{x}, t) \theta^j(\mathbf{x}, t) \mu_L(\mathbf{x}) dx dt \right| &\leq \\ &\leq L^{d/2} \|v^i(\cdot, 0)\|_{L^2(K)} \int_0^T e^{-\lambda_0 t} \|\theta^j(\cdot, t)\|_{L^\infty(K_L)} dt C_\mu L^{-d/2} \\ &\leq C_\mu \|v^i(\cdot, 0)\|_{L^2(K)} \int_0^T e^{-\lambda_0 t} \|\theta^j(\cdot, t)\|_{L^\infty(K_L)} dt. \quad (36) \end{aligned}$$

Case $v^i(\cdot, 0) \in L^2(K)$: We use (32) in Lemma 4.7 to bound the last integral in (36):

$$\begin{aligned} &\int_0^T e^{-\lambda_0 t} \|\theta^j(\cdot, t)\|_{L^\infty(K_L)} dt \leq \\ &\leq \tilde{C} \frac{R^{d-1}}{|R-L|} \|v^i\|_{L^2([0, +\infty), W_{per}^1(K))} \int_0^T e^{-\lambda_0 t} \left[\frac{1}{t} + \frac{1}{2c|R-L|^2} \right]^{\frac{d-1}{2}} e^{-c \frac{|R-L|^2}{t}} dt \\ &\leq \frac{\tilde{C}}{\lambda_0} \frac{R^{d-1}}{|R-L|} \|v^i\|_{L^2([0, +\infty), W_{per}^1(K))} \left[\frac{1}{T} + \frac{1}{2c|R-L|^2} \right]^{\frac{d-1}{2}} e^{-c \frac{|R-L|^2}{T}} \\ &= \frac{\tilde{C}}{\lambda_0} \|v^i\|_{L^2([0, +\infty), W_{per}^1(K))} \frac{1}{|R-L|} \left[\frac{R^2}{T} + \frac{R^2}{2c|R-L|^2} \right]^{\frac{d-1}{2}} e^{-c \frac{|R-L|^2}{T}}, \end{aligned}$$

where we bounded the integral by the $L^1 - L^\infty$ Hölder inequality. Then, by posing

$$C_{2,b} = \frac{C_\mu \tilde{C}}{\lambda_0} \|v^i(\cdot, 0)\|_{L^2(K)}, \text{ and } C'_{2,b} = \frac{1}{\sqrt{2c}(1 - L/R)}, \text{ with } 0 < L/R < 1,$$

we get (34).

Case $v^i(\cdot, 0) \in W_{per}^1(K)$: We can use the estimate (33) to bound the last integral in (36):

$$\begin{aligned} & \int_0^T e^{-\lambda_0 t} \|\theta^j(\cdot, t)\|_{L^\infty(K_L)} dt \\ & \leq \tilde{C} \|v^i(\cdot, 0)\|_{W_{per}^1(K)} R^{d-1} \int_0^T e^{-2\lambda_0 t} \int_0^t s^{-(d+1)/2} e^{-c \frac{|R-L|^2}{s}} e^{\lambda_0 s} ds dt \\ & = \tilde{C} \|v^i(\cdot, 0)\|_{W_{per}^1(K)} R^{d-1} \int_0^T \int_s^T e^{-2\lambda_0 t} dt s^{-(d+1)/2} e^{-c \frac{|R-L|^2}{s}} e^{\lambda_0 s} ds, \end{aligned} \tag{37}$$

by Fubini's theorem. We bound the double integral in time as

$$\begin{aligned} \int_0^T \int_s^T e^{-2\lambda_0 t} dt s^{-(d+1)/2} e^{-c \frac{|R-L|^2}{s}} e^{\lambda_0 s} ds & \leq \frac{1}{2\lambda_0} \int_0^T s^{-(d+1)/2} e^{-c \frac{|R-L|^2}{s}} e^{-\lambda_0 s} ds \\ & \leq \frac{1}{2\lambda_0} \left(\max_{s \in [0, T]} s^{-(d+1)/2} e^{-c \frac{|R-L|^2}{s}} \right) \int_0^T e^{-\lambda_0 s} ds \\ & \leq \frac{1}{2\lambda_0^2} T^{-(d+1)/2} e^{-c \frac{|R-L|^2}{T}}, \end{aligned}$$

under the assumption that $T \leq \frac{2c}{d+1} |R - L|^2$. Thus we get the final bound

$$\int_0^T e^{-\lambda_0 t} \|\theta^j(\cdot, t)\|_{L^\infty(K_L)} dt \leq \frac{\tilde{C}}{2\lambda_0^2} \|v^i(\cdot, 0)\|_{W_{per}^1(K)} \left(\frac{R}{\sqrt{T}} \right)^{d-1} \frac{1}{T} e^{-c \frac{|R-L|^2}{T}},$$

and the proof is complete by taking

$$C_{2,b} = \frac{C_\mu \tilde{C}}{2\lambda_0^2} \|v^i(\cdot, 0)\|_{L^2(K)}.$$

□

Remark 4.2. *The estimates provided in Proposition 4.1 for regular initial condition are subjected to the final time constraint $T \leq \frac{2c}{d+1} |R - L|^2$. If such a condition is not satisfied, then the convergence rate of the resonance error is deteriorated as the solution is polluted by the boundary error for longer times. The proof of this result is out of the scope of the present paper.*

4.3.3 Term $I^{2,c}$

Here, we provide estimates for the term $I_{ij}^{2,c}$ of (25). This term decays faster than $I_{ij}^{2,b}$ and can be considered negligible.

Proposition 4.2. *Let the hypotheses of Lemma 4.7 be satisfied. Moreover, let $v^i \in C([0, +\infty), L^2(K))$, $\theta^i \in L^\infty(K_L \times [0, +\infty))$, let $I_{ij}^{2,c}$ be defined as in (25) and let L/R be constant. Then, there exist a constants $C_{2,c}, c > 0$ independent of R, L, T such that*

$$\left| I_{ij}^{2,c} \right| \leq \frac{C_{2,c}}{|R-L|^2} \|v^i\|_{L^2([0,+\infty), W_{per}^1(K))}^2 \left(\frac{R^2}{T} \right)^{d-1} e^{-\frac{2c|R-L|^2}{T}}. \quad (38)$$

Otherwise, if $v^i \in C([0, +\infty), W_{per}^1(K))$, then, there exist constants $C_{2,c}, c > 0$ independent of R, L, T such that

$$\left| I_{ij}^{2,c} \right| \leq C_{2,c} \|v^i(\cdot, 0)\|_{W_{per}^1(K)}^2 \left(\frac{T}{c|R-L|^2} \right)^{3-d} e^{-2c\frac{|R-L|^2}{T}}. \quad (39)$$

Proof. From the positivity of μ_L and the fact that its integral is equal to one, we derive the inequality

$$\begin{aligned} \left| \int_0^T \int_{K_L} \theta^i(\mathbf{x}, t) \theta^j(\mathbf{x}, t) \mu_L(\mathbf{x}) \, d\mathbf{x} \, dt \right| &\leq \int_0^T \sup_{\mathbf{x} \in K_L} |\theta^i(\mathbf{x}, t) \theta^j(\mathbf{x}, t)| \, dt \int_{K_L} \mu_L(\mathbf{x}) \, d\mathbf{x} \\ &\leq \max_i \int_0^T \sup_{\mathbf{x} \in K_L} |\theta^i(\mathbf{x}, t)|^2 \, dt. \end{aligned}$$

Then, the task now is to estimate $\int_0^T \sup_{\mathbf{x} \in K_L} |\theta^i(\mathbf{x}, t)|^2 \, dt$.

Case $v^i(\cdot, 0) \in L^2(K)$: By (32) we derive

$$\begin{aligned} \int_0^T \sup_{\mathbf{x} \in K_L} |\theta^i(\mathbf{x}, t)|^2 \, dt &\leq \tilde{C}^2 \frac{R^{2(d-1)}}{|R-L|^2} \|v^i\|_{L^2([0,+\infty), W_{per}^1(K))}^2 \\ &\int_0^T \left[\frac{1}{t} + \frac{1}{2c|R-L|^2} \right]^{d-1} e^{-2c\frac{|R-L|^2}{t}} \, dt. \end{aligned} \quad (40)$$

By the change of variable $\sigma = 2c\frac{|R-L|^2}{t}$ we bound the integral

$$\begin{aligned} \int_0^T \left[\frac{1}{t} + \frac{1}{2c|R-L|^2} \right]^{d-1} e^{-2c\frac{|R-L|^2}{t}} \, dt \\ = \left(\frac{1}{2c|R-L|^2} \right)^{d-2} \int_{\frac{2c|R-L|^2}{T}}^{+\infty} \frac{(\sigma+1)^{d-1}}{\sigma^2} e^{-\sigma} \, d\sigma \end{aligned}$$

$$\begin{aligned}
&\leq \left(\frac{1}{2c|R-L|^2} \right)^{d-2} \left(\frac{2c|R-L|^2}{T} + 1 \right)^{d-1} \left(\frac{2c|R-L|^2}{T} \right)^{-2} \int_{\frac{2c|R-L|^2}{T}}^{+\infty} e^{-\sigma} d\sigma \\
&= \left(\frac{1}{2c|R-L|^2} \right)^{d-2} \left(1 + \frac{T}{2c|R-L|^2} \right)^{d-1} \left(\frac{T}{2c|R-L|^2} \right)^{3-d} e^{-\frac{2c|R-L|^2}{T}} \\
&\leq \frac{C}{T^{d-1}} e^{-\frac{2c|R-L|^2}{T}}, \quad (41)
\end{aligned}$$

since $\left(1 + \frac{T}{2c|R-L|^2}\right)$ and $\frac{T^2}{2c|R-L|^2}$ can be bounded from above by a constant, due to $T \leq C|R-L|$. By plugging (41) into (40) we get:

$$\begin{aligned}
&\int_0^T \sup_{\mathbf{x} \in K_L} |\theta^i(\mathbf{x}, t)|^2 dt \\
&\leq \tilde{C}^2 \|v^i\|_{L^2([0, +\infty), W_{per}^1(K))}^2 \left(\frac{R^2}{2c|R-L|^2} \right)^{d-1} \frac{1}{T^{d-1}} e^{-\frac{2c|R-L|^2}{T}} \\
&\leq \tilde{C}^2 \|v^i\|_{L^2([0, +\infty), W_{per}^1(K))}^2 \left(\frac{R^2}{T} \right)^{d-1} \frac{1}{2c|R-L|^2} e^{-\frac{2c|R-L|^2}{T}}.
\end{aligned}$$

We get (38) with $C_{2,c} = \frac{\tilde{C}^2}{2c}$.

Case $v^i(\cdot, 0) \in W_{per}^1(K)$: We recall (33) and apply Minkowski integral inequality:

$$\begin{aligned}
&\int_0^T \sup_{\mathbf{x} \in K_L} |\theta^i(\mathbf{x}, t)|^2 dt \leq \tilde{C}^2 R^{2(d-1)} \|v^i(\cdot, 0)\|_{W_{per}^1(K)}^2 \\
&\quad \int_0^T \left(e^{-\lambda_0 t} \int_0^t s^{-(d+1)/2} e^{-c\frac{|R-L|^2}{s}} e^{\lambda_0 s} ds \right)^2 dt \\
&\leq \tilde{C}^2 R^{2(d-1)} \|v^i(\cdot, 0)\|_{W_{per}^1(K)}^2 \\
&\quad \left\{ \int_0^T \left(\int_s^T e^{-2\lambda_0 t} s^{-(d+1)} e^{-2c\frac{|R-L|^2}{s}} e^{2\lambda_0 s} dt \right)^{1/2} ds \right\}^2 \\
&\leq \tilde{C}^2 R^{2(d-1)} \|v^i(\cdot, 0)\|_{W_{per}^1(K)}^2 \\
&\quad \left\{ \int_0^T \frac{1}{\sqrt{2\lambda_0}} (e^{-2\lambda_0 s} - e^{-2\lambda_0 T})^{1/2} s^{-(d+1)/2} e^{-c\frac{|R-L|^2}{s}} e^{\lambda_0 s} ds \right\}^2 \\
&\leq \frac{\tilde{C}^2}{2\lambda_0} R^{2(d-1)} \|v^i(\cdot, 0)\|_{W_{per}^1(K)}^2 \\
&\leq \frac{\tilde{C}^2}{2\lambda_0} R^{2(d-1)} \|v^i(\cdot, 0)\|_{W_{per}^1(K)}^2 \left\{ \int_0^T s^{-(d+1)/2} e^{-c\frac{|R-L|^2}{s}} ds \right\}^2,
\end{aligned}$$

by the fact that $(1 - e^{-2\lambda_0(T-s)}) \leq 1$. We estimate the integral by the change of variables $\sigma = c \frac{|R-L|^2}{s}$:

$$\begin{aligned} \int_0^T s^{-(d+1)/2} e^{-c \frac{|R-L|^2}{s}} ds &= \left(\frac{1}{c|R-L|^2} \right)^{\frac{d-1}{2}} \int_{c \frac{|R-L|^2}{T}}^{+\infty} \sigma^{(d-3)/2} e^{-\sigma} d\sigma \\ &\leq \left(\frac{1}{c|R-L|^2} \right)^{\frac{d-1}{2}} \left(\sup_{\sigma \geq c \frac{|R-L|^2}{T}} \sigma^{(d-3)/2} \right) \int_{c \frac{|R-L|^2}{T}}^{+\infty} e^{-\sigma} d\sigma \\ &\leq \frac{1}{c|R-L|^2} T^{(3-d)/2} e^{-c \frac{|R-L|^2}{T}}. \end{aligned}$$

And by plugging the bound for the integral into the bound for $\int_0^T \sup_{\mathbf{x} \in K_L} |\theta^i(\mathbf{x}, t)|^2 dt$ we get

$$\begin{aligned} \int_0^T \sup_{\mathbf{x} \in K_L} |\theta^i(\mathbf{x}, t)|^2 dt &\leq \frac{\tilde{C}^2}{2\lambda_0} R^{2(d-1)} \|v^i(\cdot, 0)\|_{W_{per}^1(K)}^2 \frac{1}{c^2 |R-L|^4} T^{3-d} e^{-2c \frac{|R-L|^2}{T}} \\ &\leq \frac{\tilde{C}^2}{2\lambda_0} \|v^i(\cdot, 0)\|_{W_{per}^1(K)}^2 \left(\frac{T}{c|R-L|^2} \right)^{3-d} \left(\frac{1}{c(1-L/R)} \right)^{2(d-1)} e^{-2c \frac{|R-L|^2}{T}}. \end{aligned}$$

since $\frac{1}{c(1-L/R)}$ is constant, we get (39) with $C_{2,c} = \frac{\tilde{C}^2}{2\lambda_0} \left(\frac{1}{c(1-L/R)} \right)^{2(d-1)}$. \square

Now, we are ready to prove Theorem 3.2.

Theorem 3.2. The decomposition (20) implies

$$\|a_{R,L,T}^0 - a^0\|_F \leq d^2 \max_{i,j} (|I_{ij}^1| + |I_{ij}^2| + |I_{ij}^3| + |I_{ij}^4|).$$

By using the upper bounds in Corollary 4.1, Lemmas 4.2 and 4.4, and Propositions 4.1 and 4.2 in the above inequality we get

$$\begin{aligned} \|a_{R,L,T}^0 - a^0\|_F &\leq C \left[L^{-(q+1)} + e^{-2\lambda_0 T} + \frac{1}{|R-L|} \left(\frac{R}{\sqrt{T}} + 1 \right)^{d-1} e^{-c \frac{|R-L|^2}{T}} \right. \\ &\quad \left. + \frac{1}{|R-L|^2} \left(\frac{R^2}{T} \right)^{d-1} e^{-2c \frac{|R-L|^2}{T}} \right], \end{aligned} \tag{42}$$

for some constant C independent of R , L and T . Using the optimal values $L = k_o R$ and $T = k_T R$, with $0 < k_o < 1$ and $k_T = \sqrt{\frac{c}{2\lambda_0}}(1 - k_o)$, we write (42) as:

$$\begin{aligned} \|a_{R,L,T}^0 - a^0\|_F &\leq C \left[R^{-(q+1)} + e^{-\sqrt{2\lambda_0 c}(1-k_o)R} + \frac{1}{R} \left(\sqrt{R} + 1 \right)^{d-1} e^{-\sqrt{2\lambda_0 c}(1-k_o)R} \right. \\ &\quad \left. + R^{d-3} e^{-2\sqrt{2\lambda_0 c}(1-k_o)R} \right], \end{aligned}$$

The last term is of higher order than the third one, so it can be omitted. Finally, we get

$$\|a_{R,L,T}^0 - a^0\|_F \leq C \left[R^{-(q+1)} + \left(1 + \frac{(\sqrt{R} + 1)^{d-1}}{R} \right) e^{-\sqrt{2\lambda_0 c}(1-k_o)R} \right]. \quad (43)$$

In the case of more regular initial conditions, $\nabla \cdot (a\mathbf{e}_i) \in W_{per}^1(Y)$, we have:

$$\|a_{R,L,T}^0 - a^0\|_F \leq C \left[L^{-(q+1)} + e^{-2\lambda_0 T} + \left(\frac{R}{\sqrt{T}} \right)^{d-1} \frac{1}{T} e^{-c \frac{|R-L|^2}{T}} + \left(\frac{T}{|R-L|^2} \right)^{3-d} e^{-2c \frac{|R-L|^2}{T}} \right].$$

Also in this case, we use $L = k_o R$ and $T = k_T R$ and omit the last term to get

$$\|a_{R,L,T}^0 - a^0\|_F \leq C \left[R^{-(q+1)} + \left(1 + R^{\frac{d-3}{2}} \right) e^{-\sqrt{2\lambda_0 c}(1-k_o)R} \right]. \quad (44)$$

Finally, using the fact that $R \geq 1$, we can bound the prefactors in front of the exponential terms in (43) and (44) by a constant independent of R and get (19). \square

5 Numerical tests

In this section we present several numerical tests which support the theoretical results of Section 4 and experimentally verify the resonance error bound of Theorem 3.2. We illustrate the expected convergence rates by varying the regularity parameter q of the filters, in a periodic, smooth setting, as rigorously proven in the previous sections. Additionally, we compare the convergence rate of the resonance error for the parabolic scheme with that of standard numerical homogenization scheme. We also test non-smooth periodic and stochastic coefficients, which violate the theoretical assumptions in the analysis. Nevertheless, we obtain results as in the smooth periodic case.

In order to numerically assess the convergence rate of the resonance error, we compute the approximations of the homogenized tensor through the described parabolic cell problems on domains of increasing size, $R \in [1, 20]$, and calculate the Frobenius norm of the difference between such approximations and the exact a^0 . In the case of periodic coefficients whose homogenized value could not be known exactly (i.e., without discretization error) the reference value is computed by solving the standard elliptic micro problem (5) with $R = 1$ and periodic boundary conditions and using formula (4). In the random setting no approximation is available without some resonance error. In this case, we take as reference value for the homogenized tensor the one computed from the

numerical approximation of the parabolic correctors over the largest domain $R_{max} = 20$.

To compute a numerical approximation of $a_{R,L,T}^0$, we use a Finite Elements (FE) discretization for the micro problems (9) in space, and a stabilised explicit Runge-Kutta method with adaptive time stepping for the time discretization. A high (fourth) order method, Ref. 1, is chosen in order to make the temporal discretization error negligible with respect to the resonance error. As we use explicit methods in time, we need a mass matrix that is cheap to invert. This is achieved by using either mass lumping (for low order FEMs) or discontinuous Galerkin methods (for arbitrary order FEMs).

As a second step, the upscaled tensor is approximated by a double integration in space and time. The spatial integral of the parabolic correctors is computed by using the FE filtered mass matrix of components

$$m_{ij} = \int_{K_L} \phi_i(\mathbf{x}) \phi_j(\mathbf{x}) \mu_L(\mathbf{x}) d\mathbf{x},$$

where $\{\phi_i\}_i$ are the FE basis functions. The integration in time is performed by the use of Newton-Cotes formulae for non-uniform discretizations.

In order to optimize the convergence rate of the error with respect to the sampling domain size R , we take the optimal values of Theorem 3.2 for the averaging domain size L ($K_L \subset K_R$) and for the final time T given by

$$L = k_o R, \text{ and } T = \frac{R - L}{\sqrt{8\beta\lambda_0}},$$

where β is the continuity constant of the tensor a and λ_0 is the smallest eigenvalue of the elliptic operator $-\nabla \cdot (a(\cdot)\nabla)$ with periodic boundary conditions. The oversampling ratio, $0 < k_o < 1$, and the order of filters, q , can be chosen freely.

5.1 Two-dimensional periodic case

We consider the upscaling of the 2×2 isotropic tensor:

$$a(\mathbf{x}) = \left(\frac{2 + 1.8 \sin(2\pi x_1)}{2 + 1.8 \cos(2\pi x_2)} + \frac{2 + \sin(2\pi x_2)}{2 + 1.8 \cos(2\pi x_1)} \right) \text{Id} \quad (45)$$

for which the homogenized tensor is

$$a^0 \approx \begin{pmatrix} 2.757 & -0.002 \\ -0.002 & 3.425 \end{pmatrix}.$$

Here, we compare the performances of the described parabolic approach (“par.” in the legends) and the standard elliptic approach (“ell.” in the legends). In comparing the two methods, we used a filtered version of (6), namely

$$\mathbf{e}_i \cdot a_{R,L}^0 \mathbf{e}_j := \int_{K_L} \mathbf{e}_i \cdot a(\mathbf{x}) \left(\mathbf{e}_j + \nabla \chi_R^j(\mathbf{x}) \right) \mu_L(\mathbf{x}) d\mathbf{x}, \quad (46)$$

that improves the error constant for the classical approach. However, we recall that the standard elliptic method provides a first order convergence rate, independently of the use of oversampling or filtering, as shown in Ref. 43. By contrast, the use of high order filters in the parabolic scheme improves the convergence rate without affecting the computational cost. The two approaches are solved using $\mathbb{P}1$ finite element discretization in space with 64 points per periodic cell. Mass lumping has been used in order to perform the time integration, which is carried out via the ROCK4 method, see Ref. 1, with $tol = 10^{-6}$. Finally Simpson’s quadrature rule is used for computing the time integral defining homogenized coefficients.

Results are depicted in Figure 2. As expected, one cannot reach a convergence rate higher than 1 for the standard elliptic approach, in contrast to the parabolic method. We notice a longer “flat” region in the convergence plot for small values of k_o and high order filters. Intuitively, for any given R , the region where the filter is “not almost zero” decreases for smaller k_o and larger q . Hence, we need larger values of R for the averaging integral to contain enough data and the error to decrease with the expected rate.

5.2 Discontinuous coefficients

In the error analysis, we made the assumption that the initial condition $\nabla \cdot (a(\cdot)\mathbf{e}_i) \in L^2(K_R)$. Nevertheless, the parabolic problem can also be solved for initial condition $\nabla \cdot (a(\cdot)\mathbf{e}_i) \in H^{-1}(K_R)$ and we are interested in verifying numerically if the provided *a-priori* estimates for the resonance error hold also for this case. For simplicity, we consider the one dimensional periodic piecewise continuous coefficient

$$a(x) = \begin{cases} 1 & \frac{1}{4} < \{x\} < \frac{3}{4}, \\ 3 & \text{elsewhere,} \end{cases} \quad (47)$$

where $\{x\}$ is the fractional part of x , i.e. $\{x\} = x - \lfloor x \rfloor$. The homogenized coefficient, which can be computed analytically, is $a^0 = \frac{3}{2}$. Convergence plots pictured in Figure 3 show that the theoretical results also apply to the case of discontinuous coefficients. The test is done with $\mathbb{P}2$ finite element discretization on a uniform grid of size $h = 1/1024$ and the ROCK4 time integration scheme with $tol = 10^{-6}$. The results are reported in Figure 3 where, for the sake of completeness, we also pictured the convergence plot for the elliptic scheme without filtering nor oversampling (this simplifying choice is motivated from the fact that filtering and oversampling have been proved to be ineffective for improving the convergence rate in the elliptic case, see subsection 5.1). Also in this case, if the filter’s order q is increased or the oversampling ratio k_o is decreased, the expected convergence rate will be reached for larger values of R .

5.3 A stochastic case

In the last numerical test, we provide an example for a stochastic tensor, which does not comply with the periodicity assumption made in Section 4. With

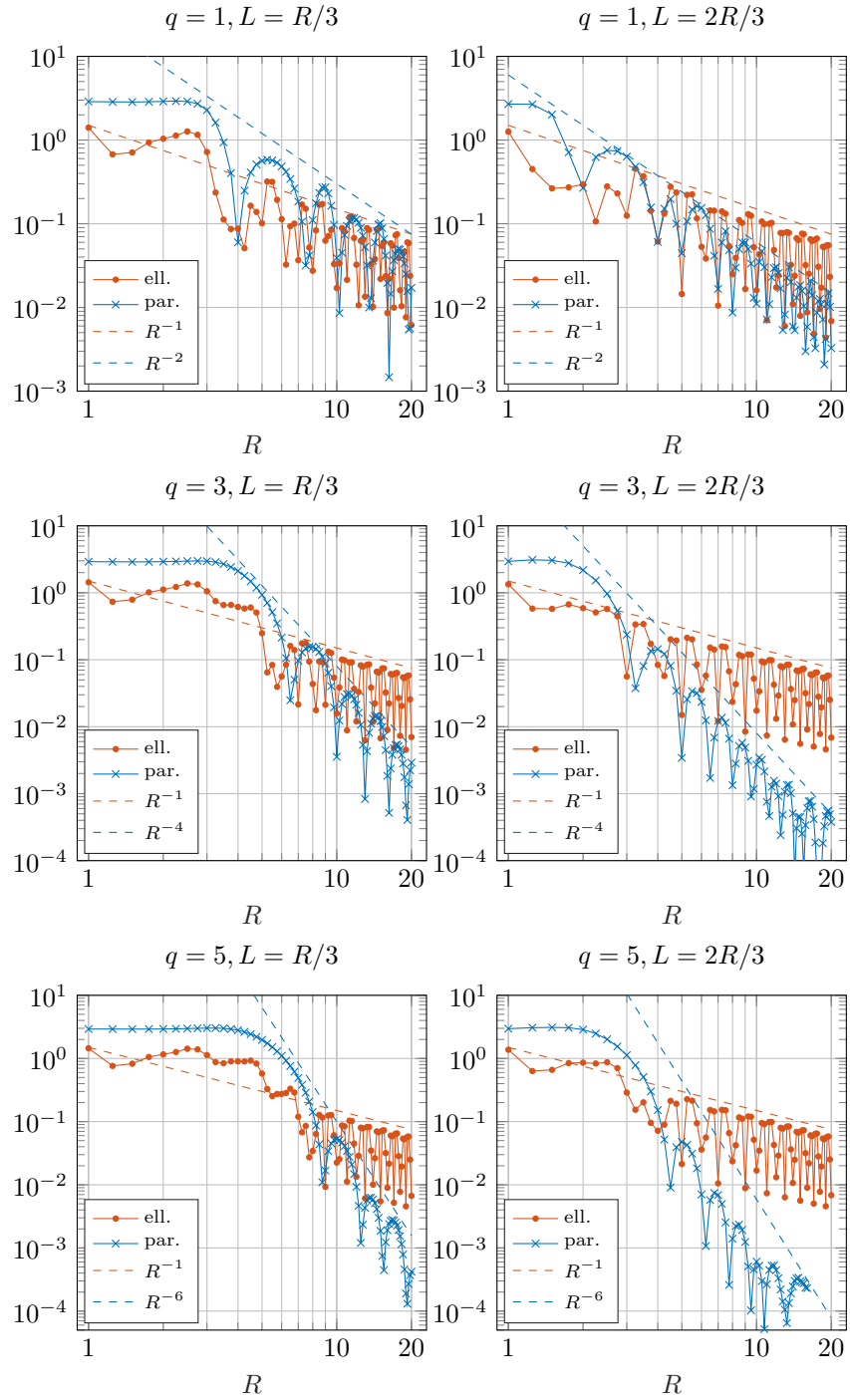


Figure 2: Comparison of the resonance error in the elliptic and parabolic models for tensor (45).

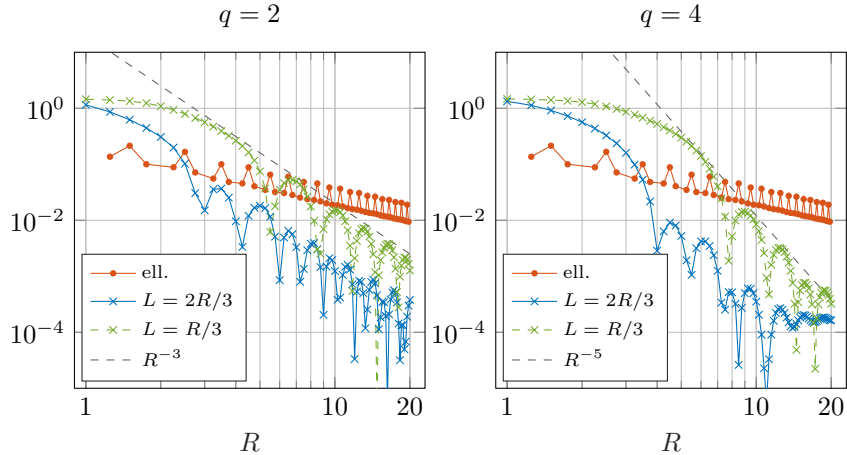


Figure 3: Resonance error in the elliptic and parabolic models for the discontinuous tensor (47). The elliptic approximation to a^0 is computed without filtering nor oversampling.

this test, we do not aim at proving any theoretical convergence rate of the error, but rather to verify numerically that the periodicity assumption is not necessary for achieving fast decaying rates of the boundary error. We consider a single realization of a stationary log-normal random field with Gaussian isotropic covariance:

$$\log a(\cdot) \sim \mathcal{N}(\mu, Cov(\mathbf{x} - \mathbf{y})), \quad Cov(\mathbf{z}) = \sigma^2 e^{-\frac{|\mathbf{z}|^2}{2\ell^2}}, \quad (48)$$

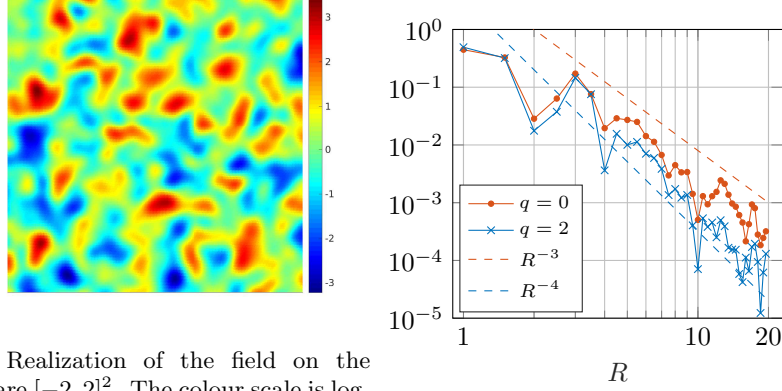
where μ and σ^2 are the mean and the variance of the field and ℓ is the correlation length. An example of such a field is depicted in Figure 4a. We are not interested in evaluating the statistical error, but only the boundary error, which is

$$\|a_{R,L,T}^0 - a_{\infty,L,T}^0\|_F.$$

In practice, we will consider $a_{R_{max},L,T}^0$ for the large value $R_{max} = 20$ in place of $a_{\infty,L,T}^0$ as a reference for evaluating the resonance error. The new reference $a_{R_{max},L,T}^0$ is computed using the numerical approximation of the parabolic corrector on $K_{R_{max}}$ with periodic BCs. The test is done with a $\mathbb{P}1$ finite element discretization on a uniform grid of size $h = 1/20$ and the ROCK4 time integration scheme with $tol = 10^{-5}$. In Figure 4b we show that the resonance error decays with a rate comprised between 3 and 4 with respect to R .

6 Computational efficiency

The goal of this section is to provide a theoretical estimate of the scaling of the computational cost with respect to the error tolerance for the proposed



(a) Realization of the field on the square $[-2, 2]^2$. The colour scale is logarithmic.

(b) Resonance error. $L = 2R/3$.

Figure 4: Log-normal random field (48) with $\mu = 0$, $\sigma^2 = 1$ and $\ell = 0.2$, and resonance error for the parabolic ell problem with filter order q and final time $T = \frac{|R-L|}{10}$.

parabolic approach and to compare it to the standard elliptic approach. Since both discretization and resonance parameters play a role in the determination of the computational cost, in our analysis we will assume that both errors are smaller than a prescribed tolerance and we derive the computational cost under these constraints. Our analysis shows that, for sufficiently high order filters, the computational cost is lower for the parabolic model than for the elliptic one, i.e. the parabolic case is asymptotically less expensive.

6.1 Standard elliptic case

Let us consider the standard elliptic homogenization scheme of (6), (7). We partition the domain K_R with uniform simplicial elements of size h and we introduce a finite elements space $S_h \subset H_0^1(K_R)$ made of piecewise polynomial functions of degree s on the simplices. The finite elements discretization of the corrector problem reads: Find $\chi_{R,h}^i \in S_h$ such that

$$\int_{K_R} a(\mathbf{x}) (\nabla \chi_{R,h}^i + \mathbf{e}_i) \cdot \nabla w_h \, d\mathbf{x} = 0, \quad \forall w_h \in S_h, \quad i = 1, \dots, d, \quad (49)$$

and the upscaled tensor is defined as

$$a_{ij}^{0,R,h} = \int_{K_R} \mathbf{e}_i \cdot a(\mathbf{x}) (\nabla \chi_{R,h}^j + \mathbf{e}_j) \, d\mathbf{x}. \quad (50)$$

Hence, the total error for the upscaled coefficients is:

$$|a_{ij}^{0,R,h} - a_{ij}^0| \leq C (h^{2s} + R^{-1}),$$

where the first term in the error estimate is the discretization error derived in Ref. 3, while the second term is the resonance error. The finite elements corrector $\chi_{R,h}^i$ is computed by solving the linear system

$$A_h \mathbf{v}_i = \mathbf{b}_i, \text{ for } i = 1, \dots, d, \quad (51)$$

where A_h is a $N \times N$ symmetric positive definite matrix and \mathbf{v}_i and \mathbf{b}_i are the coordinates of, respectively, $\chi_{R,h}^i$ and $-\nabla \cdot (a(\mathbf{x})\mathbf{e}_i)$ in the finite element space given a Lagrangian basis. Here, $N = \mathcal{O}(R^d h^{-d})$ is the dimension of the space S_h . The linear system can be solved in several ways using direct or iterative methods, whose cost depends on N . For example, for sparse LU factorization the number of operations is⁴ $\mathcal{O}(N^{3/2})$ Ref. 24, for Conjugate Gradient (CG) it is $\mathcal{O}(\sqrt{\kappa}N)$, where κ is the condition number, while for multigrid (MG) it is $\mathcal{O}(N)$, Ref. 40. In the following analysis we will assume that the latter method is used for solving the linear system. We require the total errors to scale as a given tolerance tol , so $R = \mathcal{O}(tol^{-1})$ and $h = \mathcal{O}(tol^{1/2s})$. Hence, the total cost is

$$Cost = \mathcal{O}(N) = \mathcal{O}(R^d h^{-d}) = \mathcal{O}(tol^{-d - \frac{d}{2s}}).$$

6.2 Parabolic case with explicit stabilized time integration methods

Let us consider the parabolic cell problem (9) with the upscaling formula (13). As in the elliptic case, one can discretize (9) in space and compute an approximation $u_h^i(t)$ of $u^i(\cdot, t)$ in the N -dimensional finite elements space S_h . For simplicity of notation, we will omit the superscript i . For a given basis of S_h , the function $u_h(t)$ is uniquely determined by the vectorial function $\mathbf{w}_h : [0, T] \mapsto \mathbb{R}^N$, that solve the semi-discrete problem:

$$\frac{d}{dt} \mathbf{w}_h = -M_h^{-1} A_h \mathbf{w}_h. \quad (52)$$

We assume that the mass matrix M_h is easy to invert (which hold, e.g., in the case of mass lumping or discontinuous Galerkin FEs), so that the cost of the right-hand side evaluation is negligible with respect to the solution of the ODE system. The differential equation (52) is solved by an explicit stabilised time integration scheme of order r . Examples of second order methods are RKC2 (Ref. 42) and ROCK2 (Ref. 6), while ROCK4 (Ref. 1) is a fourth order method. The fully discrete problem reads

$$\mathbf{W}_k = \Phi_h(\mathbf{W}_{k-1}), \text{ for } k = 1, \dots, N_t,$$

where the function Φ_h identifies the time integration method and N_t the number of time steps. The computed sequence $\{\mathbf{W}_k\}_{k=0}^{N_t} \subset \mathbb{R}^N$ is an approximation,

⁴The constant in this asymptotic rate depends on the sparsity pattern of the matrix, which is much worse for 3D problems than for diffusion problems in 2D.

at times $t_k = k\Delta t$, of $\mathbf{w}(t_k)$ and it determines (via the finite elements basis) a sequence $\{U_k\}_{k=0}^{N_t} \subset S_h$. The discrete approximation of the homogenized tensor is

$$a_{ij}^{0,R,h,\Delta t} = \int_{K_L} a_{ij}(y)\mu_L(\mathbf{x}) d\mathbf{x} - 2\mathcal{Q} \left(\int_{K_L} U_k U_k^j \mu_L(y) d\mathbf{x}, \Delta t \right),$$

where $\mathcal{Q}(\cdot, \Delta t)$ is a quadrature rule on the discretization $t_k = k\Delta t$ of order at least r (where r is the order of the time integration scheme). Hence, the total error for the upscaled coefficients is:

$$|a_{ij}^{0,R,h,\Delta t} - a_{ij}^0| \leq C \left(h^{s+1} + \Delta t^r + R^{-(q+1)} \right), \quad (53)$$

where we have assumed that, for sufficiently large R , the term $R^{-(q+1)}$ dominates the exponential term in the resonance error bound. This is also the convergence rate that we reported in the numerical examples of Subsections 5.1 and 5.2. Here, the constant C grows linearly with the final time T , whose optimal value scales as $R - L$. However, the ratio $(R - L)/\sqrt{8\beta\lambda_0}$ is in general $\mathcal{O}(1)$, so we can consider $T = \mathcal{O}(1)$ in the range of values used for R and L . In order for the error to scale as tol , we require that all the three summands in (53) scale as tol :

$$R = \mathcal{O}(tol^{-\frac{1}{q+1}}), \quad h = \mathcal{O}(tol^{\frac{1}{s+1}}), \quad \Delta t = \mathcal{O}(tol^{\frac{1}{r}}).$$

The global computational cost is $\mathcal{O}(N n_S N_t)$, where $N_t = T/\Delta t$ is the number of time steps, n_S is the number of function evaluations (stages) per time step for a stabilised method and $N = \mathcal{O}(R^d h^{-d})$ is the cost of each function evaluation which, in the linear case, is the cost of multiplying a sparse $N \times N$ matrix by a vector in \mathbb{R}^N . Since we are using a stabilised method we need to satisfy the weak stability condition $\rho\Delta t = cn_S^2$, where ρ is the spectral radius of the Jacobian of the ODE (52) and n_S is the number of stages for each time step. As ρ is the spectral radius of $M_h^{-1}A_h$, it scales as h^{-2} . Therefore, $n_S = \mathcal{O}(\Delta t^{1/2} h^{-1})$. From the fact that $T = \mathcal{O}(1)$ one derives that the total cost is

$$Cost = \mathcal{O}(R^d h^{-d} \Delta t^{1/2} h^{-1} \Delta t^{-1}) = \mathcal{O}(tol^{-\frac{d}{q+1} - \frac{d+1}{s+1} - \frac{1}{2r}}).$$

6.3 Comparison of the parabolic and the standard elliptic methods

Now, we are interested in evaluating under which condition the use of stabilised time integration methods is more efficient than the regularized elliptic approach. In Table 1, we summarize the dependency of computational cost and the error on resonance and discretization parameters, as well as the scaling of the cost for a given tolerance. In order for the parabolic approach to be competitive with respect to the elliptic one, the condition to satisfy is:

$$\frac{d}{q+1} + \frac{d+1}{s+1} + \frac{1}{2r} < d + \frac{d}{2s}.$$

Cell problem	Parabolic	Standard Elliptic
Error	$R^{-q-1} + h^{s+1} + \Delta t^r$	$R^{-1} + h^{2s}$
Computational cost	$R^d h^{-d-1} \Delta t^{-\frac{1}{2}}$	$R^d h^{-d}$
Computational cost (tol)	$tol^{-\frac{d}{q+1} - \frac{d+1}{s+1} - \frac{1}{2r}}$	$tol^{-d - \frac{d}{2s}}$

Table 1: Error and computational cost for two homogenization approaches.

In Figure 5 we display the theoretical increase of the computational cost for the two considered approaches. We observe that, for high order filters, the elliptic model is much more expensive than the parabolic cell problem.

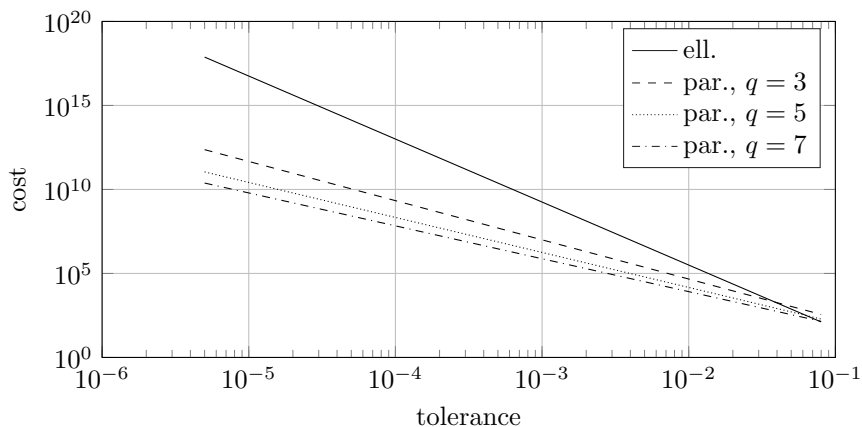


Figure 5: Theoretical computational cost for $d = 3$, $\mathbb{P}2$ -FEM, 4-th order time integration, $q = 3, 5, 7$.

7 Conclusion

In this work, we propose a novel approach for numerical homogenization, based on the solution of parabolic cell problems. We rigorously prove, by Green's function estimates, an arbitrary convergence rate for the resonance error in the smooth periodic setting, but numerical tests demonstrate the same rates also for piecewise continuous and non-periodic cases. If filters of high order are used, the computation of the parabolic solutions by means of stabilised explicit solvers is asymptotically more efficient than the inversion of the discretized elliptic operator, required by elliptic approaches.

A Proofs of Lemmas 4.6 and 4.7

In this appendix we prove the statements of Lemmas 4.6 and 4.7.

Lemma 4.6. First of all, we derive an integral equality for Γ^* . Multiplying $L_{(\mathbf{y},s)}^* \Gamma^* = 0$ by $v^i(1 - \rho)$, integrating over $K_R \times (0, t)$ and using integration by parts, one gets:

$$\begin{aligned} & \int_0^t \int_{K_R} -\partial_s \Gamma^*(\mathbf{y}, s; \mathbf{x}, t) v^i(\mathbf{y}, s) (1 - \rho(\mathbf{y})) \\ & \quad + \nabla_{\mathbf{y}} (v^i(\mathbf{y}, s) (1 - \rho(\mathbf{y}))) \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} \Gamma^*(\mathbf{y}, s; \mathbf{x}, t) \, d\mathbf{y} \, ds \\ & = \int_0^t \int_{\partial K_R} \mathbf{n} \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s) v^i(\mathbf{y}, s) (1 - \rho(\mathbf{y})) \, d\sigma_{\mathbf{y}} \, ds, \end{aligned} \quad (54)$$

since $\nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s) = \nabla_{\mathbf{y}} \Gamma^*(\mathbf{y}, s; \mathbf{x}, t)$ for any $s < t$. Then the second and third integrals in (30) are rewritten as

$$\begin{aligned} & \int_{K_R} \int_0^t -\Gamma(\mathbf{x}, t; \mathbf{y}, s) \nabla_{\mathbf{y}} (1 - \rho(\mathbf{y})) \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} v^i(\mathbf{y}, s) \, ds \, d\mathbf{y} \\ & \quad + \int_{K_R} \int_0^t \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s) \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} (1 - \rho(\mathbf{y})) v^i(\mathbf{y}, s) \, ds \, d\mathbf{y} \\ & = \int_{K_R} \int_0^t -\nabla_{\mathbf{y}} [\Gamma(\mathbf{x}, t; \mathbf{y}, s) (1 - \rho(\mathbf{y}))] \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} v^i(\mathbf{y}, s) \, ds \, d\mathbf{y} \\ & \quad + \int_{K_R} \int_0^t \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s) \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} [(1 - \rho(\mathbf{y})) v^i(\mathbf{y}, s)] \, ds \, d\mathbf{y} \\ & = \int_{K_R} \int_0^t \Gamma(\mathbf{x}, t; \mathbf{y}, s) (1 - \rho(\mathbf{y})) \partial_s v^i(\mathbf{y}, s) \, ds \, d\mathbf{y} \\ & \quad + \int_{K_R} \int_0^t \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s) \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} [(1 - \rho(\mathbf{y})) v^i(\mathbf{y}, s)] \, ds \, d\mathbf{y}, \end{aligned} \quad (55)$$

where the last equality follows from the weak form of (10). Then, we integrate the former of the two last integrals by parts, thus obtaining

$$\begin{aligned} & \int_{K_R} \int_0^t \Gamma(\mathbf{x}, t; \mathbf{y}, s) (1 - \rho(\mathbf{y})) \partial_s v^i(\mathbf{y}, s) \, ds \, d\mathbf{y} \\ & = \lim_{\epsilon \rightarrow 0^+} \int_{K_R} \Gamma(\mathbf{x}, t; \mathbf{y}, t - \epsilon) v^i(\mathbf{y}, t - \epsilon) (1 - \rho(\mathbf{y})) \, d\mathbf{y} \\ & \quad - \int_{K_R} \Gamma(\mathbf{x}, t; \mathbf{y}, 0) v^i(\mathbf{y}, 0) (1 - \rho(\mathbf{y})) \, d\mathbf{y} \\ & \quad - \int_{K_R} \int_0^t \partial_s \Gamma(\mathbf{x}, t; \mathbf{y}, s) (1 - \rho(\mathbf{y})) v^i(\mathbf{y}, s) \, ds \, d\mathbf{y}. \end{aligned} \quad (56)$$

From the fact that $\rho(\mathbf{x}) = 1$ for all $\mathbf{x} \in K_L$ and from the continuity of v^i we deduce

$$\lim_{\epsilon \rightarrow 0^+} \int_{K_R} \Gamma(\mathbf{x}, t; \mathbf{y}, t - \epsilon) v^i(\mathbf{y}, t - \epsilon) (1 - \rho(\mathbf{y})) d\mathbf{y} = v^i(\mathbf{x}, t) (1 - \rho(\mathbf{x})) = 0,$$

for any $\mathbf{x} \in K_L$. By putting (30), (55), and (56) together we get

$$\begin{aligned} \theta^i(\mathbf{x}, t) &= \int_{K_R} \int_0^t -\partial_s \Gamma(\mathbf{x}, t; \mathbf{y}, s) v^i(\mathbf{y}, s) (1 - \rho(\mathbf{y})) ds d\mathbf{y} \\ &\quad + \int_{K_R} \int_0^t \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s) \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} [v^i(\mathbf{y}, s) (1 - \rho(\mathbf{y}))] ds d\mathbf{y}. \end{aligned}$$

Finally, from (29) and (54) we conclude that

$$\theta^i(\mathbf{x}, t) = \int_{\partial K_R} \int_0^t \mathbf{n} \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s) v^i(\mathbf{y}, s) ds d\sigma_{\mathbf{y}}.$$

□

Lemma 4.7. From (31) we can write

$$|\theta^i(\mathbf{x}, t)| \leq \int_0^t \int_{\partial K_R} |\mathbf{n} \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s)| |v^i(\mathbf{y}, s)| d\sigma_{\mathbf{y}} ds.$$

By applying the Hölder inequality we get

$$|\theta^i(\mathbf{x}, t)| \leq |\partial K_R|^{1/2} \int_0^t \sup_{\mathbf{y} \in \partial K_R} |\mathbf{n} \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s)| \|v^i(\cdot, s)\|_{L^2(\partial K_R)} ds. \quad (57)$$

The value of $\|v^i(\cdot, s)\|_{L^2(\partial K_R)}$ is well defined for any time $s > 0$ (unless we have a more regular initial condition, e.g. $v^i(\cdot, 0) \in W_{per}^1(K)$, in that case the trace is defined also for $s = 0$) and we can estimate it by the following inequality

$$\|v^i(\cdot, s)\|_{L^2(\partial K_R)} = \|v^i(\cdot, s)(1 - \rho)\|_{L^2(\partial K_R)} \leq C_{tr} \|v^i(\cdot, s)(1 - \rho)\|_{H^1(\Delta)},$$

where C_{tr} is fixed, thanks to the fact that the distance between $K_{\bar{R}}$ and ∂K_R is larger or equal to $1/2$. As $\rho \in C^1(K_R)$ and $\partial_{x_k} v^i(\cdot, s) \in L^2(K_R)$ the product rule holds and we can write

$$\|\nabla(v^i(1 - \rho))\|_{L^2(\Delta)} \leq \|\nabla v^i\|_{L^2(\Delta)} + \|\nabla \rho\|_{L^\infty(\Delta)} \|v^i\|_{L^2(\Delta)}.$$

Let us now consider a covering of Δ , defined as $\Delta_K := \bigcup_{\mathbf{y} \in \partial K_{\frac{R+\bar{R}}{2}}} K + \mathbf{y}$. Then,

$|\Delta_K| = c(d) \left| \partial K_{\frac{R+\bar{R}}{2}} \right| \text{diam}(K) \leq CR^{d-1}$. By exploiting the periodic structure of v^i we have that

$$\|v^i\|_{L^2(\Delta)} \leq \|v^i\|_{L^2(\Delta_K)} \leq \left(\frac{|\Delta_K|}{|K|} \right)^{1/2} \|v^i\|_{L^2(K)},$$

$$\|\nabla v^i\|_{L^2(\Delta)} \leq \|\nabla v^i\|_{L^2(\Delta_K)} \leq \left(\frac{|\Delta_K|}{|K|}\right)^{1/2} \|\nabla v^i\|_{L^2(K)}.$$

Finally, we recall that in the space $W_{per}^1(K)$ the Poincaré-Wirtinger inequality holds:

$$\|v^i\|_{L^2(K)} \leq C_P \|\nabla v^i\|_{L^2(K)} \quad (58)$$

so that

$$\begin{aligned} \|v^i(\cdot, s)\|_{L^2(\partial K_R)} &\leq C_{tr} C_\rho C_P \left(\frac{|\Delta|}{|K|}\right)^{1/2} \|\nabla v^i(\cdot, s)\|_{L^2(K)} \\ &\leq CR^{\frac{d-1}{2}} \|\nabla v^i(\cdot, s)\|_{L^2(K)}. \end{aligned} \quad (59)$$

Now, we go back to the estimation of θ^i : putting together (57) and (59) (and recalling that $|\partial K_R| = 2dR^{d-1}$) we get

$$|\theta^i(\mathbf{x}, t)| \leq CR^{d-1} \int_0^t \sup_{\mathbf{y} \in \partial K_R} |\mathbf{n} \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s)| \|\nabla v^i(\cdot, s)\|_{L^2(K)} ds. \quad (60)$$

Now, we will derive different *a-priori* estimates for different regularity assumption on the initial condition. Both of them rely on the Nash-Aronson type estimate

$$\nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s) \leq \frac{C}{(t-s)^{\frac{d+1}{2}}} e^{-c \frac{|\mathbf{x}-\mathbf{y}|^2}{t-s}}, \quad (61)$$

with $C = (4\pi\alpha)^{-d/2}$ and $c = (4\beta)^{-1}$. The bound (61) is proved in Ref. 23,33 for parabolic equations in non-divergence form with Hölder continuous coefficients. In Ref. 22 the authors claim that (61) is valid also for parabolic equation in divergence form with Hölder continuous coefficients, but the statement remains unproved.

Case $v^i(\cdot, 0) \in L^2(K)$: We apply the Hölder inequality in time and the estimates on $\nabla_{\mathbf{y}} \Gamma$ for Hölder coefficients to get:

$$\begin{aligned} |\theta^i(\mathbf{x}, t)| &\leq CR^{d-1} \|\nabla v^i\|_{L^2((0,t), L^2(K))} \left(\int_0^t \sup_{\mathbf{y} \in \partial K_R} |\mathbf{n} \cdot a(\mathbf{y}) \nabla_{\mathbf{y}} \Gamma(\mathbf{x}, t; \mathbf{y}, s)|^2 ds \right)^{1/2} \\ &\leq CR^{d-1} \|a\|_{L^\infty(K)} \|\nabla v^i\|_{L^2((0,t), L^2(K))} \left(\int_0^t \frac{C^2}{(t-s)^{(d+1)}} e^{-2c \frac{|\mathbf{x}-\bar{\mathbf{y}}(\mathbf{x})|^2}{t-s}} ds \right)^{1/2}, \end{aligned} \quad (62)$$

where $\bar{\mathbf{y}}(\mathbf{x}) = \arg \min_{\mathbf{y} \in \partial K_R} |\mathbf{x} - \mathbf{y}|$. By the change of variables $\sigma = 2c \frac{|\mathbf{x}-\bar{\mathbf{y}}(\mathbf{x})|^2}{t-s}$ and the fact that the primitive function of $t^N e^{-t}$ (with $N \in \mathbb{N}$) is $-\sum_{k=0}^N \frac{N!}{k!} t^k e^{-t}$, the inequality (62) becomes

$$|\theta^i(\mathbf{x}, t)| \leq C \frac{\|a\|_{L^\infty(K)} \|\nabla v^i\|_{L^2((0,t), L^2(K))} R^{d-1}}{(2c |\mathbf{x} - \bar{\mathbf{y}}(\mathbf{x})|^2)^{d/2}}$$

$$\begin{aligned}
& \left[\sum_{k=0}^{d-1} \frac{(d-1)!}{k!} \left(2c \frac{|\mathbf{x} - \bar{\mathbf{y}}(\mathbf{x})|^2}{t} \right)^k \right]^{\frac{1}{2}} e^{-c \frac{|\mathbf{x} - \bar{\mathbf{y}}(\mathbf{x})|^2}{t}} \\
& \leq \frac{C}{\sqrt{2c}} \|a\|_{L^\infty(K)} \|\nabla v^i\|_{L^2((0,t), L^2(K))} \frac{R^{d-1}}{|\mathbf{x} - \bar{\mathbf{y}}(\mathbf{x})|} \\
& \quad \left[(d-1)! \sum_{k=0}^{d-1} \binom{d-1}{k} \frac{1}{t^k} \left(\frac{1}{2c |\mathbf{x} - \bar{\mathbf{y}}(\mathbf{x})|^2} \right)^{d-1-k} \right]^{\frac{1}{2}} e^{-c \frac{|\mathbf{x} - \bar{\mathbf{y}}(\mathbf{x})|^2}{t}} \\
& \leq \frac{C(d-1)!}{\sqrt{2c}} \|a\|_{L^\infty(K)} \|\nabla v^i\|_{L^2((0,t), L^2(K))} \frac{R^{d-1}}{|\mathbf{x} - \bar{\mathbf{y}}(\mathbf{x})|} \\
& \quad \left[\frac{1}{t} + \frac{1}{2c |\mathbf{x} - \bar{\mathbf{y}}(\mathbf{x})|^2} \right]^{\frac{d-1}{2}} e^{-c \frac{|\mathbf{x} - \bar{\mathbf{y}}(\mathbf{x})|^2}{t}}.
\end{aligned}$$

Including all the terms that do not depend on R , L nor t in a single constant \tilde{C} and by the lower bound $\inf_{\mathbf{x} \in K_L} |\mathbf{x} - \bar{\mathbf{y}}(\mathbf{x})| \geq |R - L|$ we deduce

$$|\theta^i(\mathbf{x}, t)| \leq \tilde{C} \frac{R^{d-1}}{|R - L|} \|\nabla v^i\|_{L^2((0,t), L^2(K))} \left[\frac{1}{t} + \frac{1}{2c |R - L|^2} \right]^{\frac{d-1}{2}} e^{-c \frac{|R - L|^2}{t}}.$$

Case $v^i(\cdot, 0) \in W_{per}^1(K)$: Again, we use the eigenvalues $\{\lambda_j\}_{j=0}^{\infty}$ and eigenvectors $\{\varphi_j\}_{j=0}^{\infty}$ of B . Let us denote $\hat{v}_j^i(t) := \langle v^i(\cdot, t), \varphi_j \rangle_{L^2(K)}$. Then,

$$\hat{v}_j^i(t) = e^{-\lambda_j t} \langle v^i(\cdot, 0), \varphi_j \rangle_{L^2(K)}.$$

From the above characterization of the components $\hat{v}_j^i(t)$ and the coercivity of B we have

$$\alpha \|\nabla v^i(\cdot, t)\|_{L^2(K)}^2 \leq B[v^i(\cdot, t), v^i(\cdot, t)] = \sum_{j=0}^{+\infty} e^{-2\lambda_j t} \lambda_j |\langle v^i(\cdot, 0), \varphi_j \rangle_{L^2(K)}|^2,$$

for any $t \geq 0$. The Parseval's identity also holds for $t = 0$, since $v^i(\cdot, 0) \in W_{per}^1(K)$, by assumption. So,

$$\begin{aligned}
\alpha \|\nabla v^i(\cdot, t)\|_{L^2(K)}^2 & \leq e^{-2\lambda_0 t} \sum_{j=0}^{+\infty} \lambda_j |\langle v^i(\cdot, 0), \varphi_j \rangle_{L^2(K)}|^2 \\
& = e^{-2\lambda_0 t} B[v^i(\cdot, 0), v^i(\cdot, 0)] \\
& \leq \beta e^{-2\lambda_0 t} \|\nabla v^i(\cdot, 0)\|_{L^2(K)}^2.
\end{aligned}$$

Thus,

$$\|\nabla v^i(\cdot, t)\|_{L^2(K)} \leq e^{-\lambda_0 t} \left(\frac{\beta}{\alpha} \right)^{1/2} \|\nabla v^i(\cdot, 0)\|_{L^2(K)}. \quad (63)$$

Then, we apply again the known inequality for $\nabla_{\mathbf{y}}\Gamma$ and the estimate in (60) becomes

$$\begin{aligned} |\theta^i(\mathbf{x}, t)| &\leq R^{d-1} \frac{\beta^{3/2}}{\alpha^{1/2}} \|v^i(\cdot, 0)\|_{W_{per}^1(K)} \int_0^t \frac{C}{(t-s)^{(d+1)/2}} e^{-c \frac{|\mathbf{x}-\bar{\mathbf{y}}(\mathbf{x})|^2}{t-s}} e^{-\lambda_0 s} ds \\ &= R^{d-1} \frac{\beta^{3/2}}{\alpha^{1/2}} e^{-\lambda_0 t} \|v^i(\cdot, 0)\|_{W_{per}^1(K)} \int_0^t \frac{C}{s^{(d+1)/2}} e^{-c \frac{|\mathbf{x}-\bar{\mathbf{y}}(\mathbf{x})|^2}{s}} e^{\lambda_0 s} ds, \end{aligned}$$

and we get the thesis by posing $\tilde{C} = \frac{C\beta^{3/2}}{\alpha^{1/2}}$ and re-using the lower bound

$$\inf_{\mathbf{x} \in K_L} |\mathbf{x} - \bar{\mathbf{y}}(\mathbf{x})| \geq |R - L|.$$

□

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References

1. Assyr Abdulle. Fourth order Chebyshev methods with recurrence relation. *SIAM J. Sci. Comput.*, 23(6):2041–2054, 2002.
2. Assyr Abdulle. On a priori error analysis of fully discrete heterogeneous multiscale FEM. *Multiscale Model. Simul.*, 4(2):447–459, 2005.
3. Assyr Abdulle. The finite element heterogeneous multiscale method: a computational strategy for multiscale PDEs. In *Multiple scales problems in biomathematics, mechanics, physics and numerics*, volume 31 of *GAKUTO Internat. Ser. Math. Sci. Appl.*, pages 133–181. Gakkōtoshō, Tokyo, 2009.
4. Assyr Abdulle, Doghonyay Arjmand, and Edoardo Paganoni. Exponential decay of the resonance error in numerical homogenization via parabolic and elliptic cell problems. *C. R. Math. Acad. Sci. Paris*, 357:545–551, 2019.
5. Assyr Abdulle, Weinan E, Björn Engquist, and Eric Vanden-Eijnden. The heterogeneous multiscale method. *Acta Numer.*, 21:1–87, 2012.
6. Assyr Abdulle and Alexei A. Medovikov. Second order Chebyshev methods based on orthogonal polynomials. *Numer. Math.*, 90(1):1–18, 2001.
7. Assyr Abdulle and Gilles Vilmart. Analysis of the finite element heterogeneous multiscale method for quasilinear elliptic homogenization problems. *Math. Comp.*, 83(286):513–536, 2014.

8. Doghony Arjmand and Olof Runborg. A time dependent approach for removing the cell boundary error in elliptic homogenization problems. *J. Comput. Phys.*, 314(Supplement C):206–227, 2016.
9. Doghony Arjmand and Olof Runborg. Estimates for the upscaling error in heterogeneous multiscale methods for wave propagation problems in locally periodic media. *Multiscale Model. Simul.*, 15(2):948–976, 2017.
10. Doghony Arjmand and Christian Stohrer. A finite element heterogeneous multiscale method with improved control over the modeling error. *Communications in Mathematical Sciences*, 14(2):463–487, 2016.
11. D. G. Aronson. On the Green’s function for second order parabolic differential equations with discontinuous coefficients. *Bull. Amer. Math. Soc.*, 69(6):841–847, 11 1963.
12. D. G. Aronson. Bounds for the fundamental solution of a parabolic equation. *Bull. Amer. Math. Soc.*, 73(6):890–896, 11 1967.
13. D. G. Aronson. Non-negative solutions of linear parabolic equations. *Ann. Sc. Norm. Super. Pisa Cl. Sci., Ser. 3*, 22(4):607–694, 1968.
14. Alain Bensoussan, Jacques-Louis Lions, and George Papanicolaou. *Asymptotic analysis for periodic structures*. North-Holland Publishing Co., Amsterdam, 1978.
15. Xavier Blanc and Claude Le Bris. Improving on computation of homogenized coefficients in the periodic and quasi-periodic settings. *Netw. Heterog. Media*, 5(1):1–29, 2010.
16. Haim Brezis. *Functional analysis, Sobolev spaces and partial differential equations*. Springer Science & Business Media, 2010.
17. Doina Cioranescu and Patrizia Donato. *An introduction to homogenization*, volume 17 of *Oxford Lecture Series in Mathematics and its Applications*. Oxford University Press, New York, 1999.
18. Weinan E. *Principles of multiscale modeling*. Cambridge University Press, Cambridge, 2011.
19. Weinan E and Björn Engquist. The heterogeneous multiscale methods. *Commun. Math. Sci.*, 1(1):87–132, 2003.
20. Weinan E, Pingbing Ming, and Pingwen Zhang. Analysis of the heterogeneous multiscale method for elliptic homogenization problems. *J. Amer. Math. Soc.*, 18(1):121–156, 2005.
21. Lawrence C. Evans. *Partial differential equations*, volume 19 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, second edition, 2010.

22. Jishan Fan, Kyoungsun Kim, Sei Nagayasu, and Gen Nakamura. A gradient estimate for solutions to parabolic equations with discontinuous coefficients. *Electronic Journal of Differential Equations*, 2013(93):1–24, 2013.
23. Avner Friedman. *Partial Differential Equations of Parabolic Type*. Englewood Cliffs, NJ, 1964.
24. A. George and E. Ng. On the complexity of sparse QR and LU factorization of finite-element matrices. *SIAM J. Sci. and Stat. Comput.*, 9(5):849–861, 1988.
25. Antoine Gloria. Reduction of the resonance error. Part 1: Approximation of homogenized coefficients. *Math. Models Methods Appl. Sci.*, 21(8):1601–1630, 2011.
26. Antoine Gloria and Zakaria Habibi. Reduction in the resonance error in numerical homogenization ii: Correctors and extrapolation. *Found. Comput. Math.*, 16(1):217–296, Feb 2016.
27. Patrick Henning and Axel Målqvist. Localized orthogonal decomposition techniques for boundary value problems. *SIAM J. Sci. Comput.*, 36(4):A1609–A1634, 2014.
28. Thomas Y. Hou and Xiao-Hui Wu. A multiscale finite element method for elliptic problems in composite materials and porous media. *J. Comput. Phys.*, 134(1):169–189, 1997.
29. Thomas Y. Hou, Xiao-Hui Wu, and Zhiqiang Cai. Convergence of a multiscale finite element method for elliptic problems with rapidly oscillating coefficients. *Math. Comp.*, 68(227):913–943, 1999.
30. Thomas J.R. Hughes, Gonzalo R. Feijóo, Luca Mazzei, and Jean-Baptiste Quinicy. The variational multiscale method – a paradigm for computational mechanics. *Comput. Methods Appl. Mech. Engrg.*, 166(1):3 – 24, 1998. *Advances in Stabilized Methods in Computational Mechanics*.
31. Vasilii V. Jikov, Sergei M. Kozlov, and Olga A. Oleinik. *Homogenization of differential operators and integral functionals*. Springer-Verlag, Berlin, Heidelberg, 1994.
32. Ioannis G. Kevrekidis, C. William Gear, James M. Hyman, Panagiotis G. Kevrekidis, Olof Runborg, and Constantinos Theodoropoulos. Equation-free, coarse-grained multiscale computation: enabling microscopic simulators to perform system-level analysis. *Commun. Math. Sci.*, 1(4):715–762, 2003.
33. Olga Aleksandrovna Ladyzhenskaya, V. A. Solonnikov, and Nina Nikolaevna Ural'tseva. *Linear and quasilinear equations of parabolic type*. Translated from the Russian by S. Smith. *Translations of Mathematical Monographs*, Vol. 23. American Mathematical Society, Providence, R.I., 1968.

34. Jacques-Louis Lions and Enrico Magenes. *Problèmes aux limites non homogènes et applications*, volume 1 of *Travaux et recherches mathématiques*. Dunod, Paris, 1968.
35. Axel Målqvist and Daniel Peterseim. Localization of elliptic multiscale problems. *Math. Comp.*, 83(290):2583–2603, 2014.
36. Jean-Christophe Mourrat. Efficient methods for the estimation of homogenized coefficients. *Found. Comput. Math.*, 19(2):435–483, Apr 2019.
37. François Murat and Luc Tartar. *H*-convergence. In *Topics in the mathematical modelling of composite materials*, volume 31 of *Progr. Nonlinear Differential Equations Appl.*, pages 21–43. Birkhäuser Boston, Boston, MA, 1997.
38. John Nash. Continuity of solutions of parabolic and elliptic equations. *Amer. J. Math.*, 80(4):931–954, 1958.
39. L. E. Payne and H. F. Weinberger. An optimal Poincaré inequality for convex domains. *Arch. Rational Mech. Anal.*, 5:286–292, 1960.
40. Yousef Saad. *Iterative methods for sparse linear systems*, volume 82. SIAM, 2003.
41. S Spagnolo. Sulla convergenza di soluzioni di equazioni paraboliche ed ellittiche. *Ann. Sc. Norm. Super. Pisa Cl. Sci.*, 22(4):571–597, 1968.
42. Pieter van der Houwen and Ben P. Sommeijer. On the internal stage Runge-Kutta methods for large m -values. *Z. Angew. Math. Mech.*, 60:479–485, 1980.
43. Xingye Yue and Weinan E. The local microscale problem in the multiscale modeling of strongly heterogeneous media: effects of boundary conditions and cell size. *J. Comput. Phys.*, 222(2):556–572, 2007.