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Research article

Hypertemperature effects in heterogeneous media and thermal flux at small-length scales

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Abstract: We propose an enriched microscopic heat conduction model that can account for size effects in heterogeneous media. Benefiting from physically relevant scaling arguments, we improve the regularity of the corrector in the classical problem of periodic homogenization of linear elliptic equations in the three-dimensional setting and, while doing so, we clarify the intimate role that correctors play in measuring the difference between the heterogeneous solution (microscopic) and the homogenized solution (macroscopic). Moreover, if the data are of form $f = \operatorname{div} \boldsymbol{F}$ with $\boldsymbol{F} \in \mathrm{L}^3(\Omega, \mathbb{R}^3)$, then we recover the classical corrector convergence theorem.

Keywords: correctors; scale-size thermal effects; generalized Fourier's law; microstructure

1. Introduction

The analysis of correctors in periodic homogenization theory for second-order elliptic equations with highly oscillatory coefficients plays a critical role in linking the microscopic and macroscopic aspects of the problem by quantifying the disparity between the heterogeneous and homogenized solutions. Moreover, it provides the key information needed to prove the convergence of multiscale approximation schemes based on, e.g., the heterogeneous multiscale method or multiscale FEM. Simultaneously, from a modeling perspective, correctors point out some of the limitations of such second-order elliptic systems due to their lack of accounting for scale-size effects e.g., micro-heterogeneous bodies. The prototypical and landmark example for the homogenization of second-order elliptic equations is Fourier's law of heat conduction. In its simplest form, Fourier's law relates the heat flux $\boldsymbol{q}$ as a linear function of the temperature gradient, that is,

$$\boldsymbol{q} = -\kappa \nabla u, \tag{1.1}$$

where u is the absolute temperature and $\kappa > 0$ is the thermal conductivity that depends on the properties of the material. In general, the proportionality coefficient κ (either scalar or tensor) may depend on temperature, space, and/or time variables, or other parameters, but it often varies so little in cases of interest that it is reasonable to neglect this variation.

The theory of periodic homogenization led to a deeper exploration of Fourier's heat conduction law as it pertains to heterogeneous periodic material with different conductivities. Effective heat fluxes were derived taking into account microstructure morphology and volume fraction. The classical problem in the periodic homogenization for stationary heat conduction states the following: Find $u_\varepsilon \in \mathrm{H}^1_0(\Omega)$ satisfying,

$$\begin{aligned} -\mathrm{div}\left(\mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon}).\nabla u_\varepsilon\right) &= f \text{ in } \Omega, \\ u_\varepsilon &= 0 \text{ on } \partial\Omega, \end{aligned} \tag{1.2}$$

where $\mathsf{K}(\boldsymbol{y}) \in \mathrm{L}^\infty(Y, \mathbb{R}^{3\times 3})$ is a uniformly elliptic, symmetric, and Y-periodic with $Y = [0,1)^3$, and explore what happens with the situation when $\varepsilon \to 0$. If $\Omega \subset \mathbb{R}^3$ is uniformly Lipschitz open set, then there exists a unique solution u_ε to Eq (1.2) such that it converges weakly to a function u in $\mathrm{H}^1_0(\Omega)$, where the function $u \in \mathrm{H}^1_0(\Omega)$ is the unique solution to

$$\begin{aligned} -\mathrm{div}\left(\mathsf{K}^{\mathrm{eff}}.\nabla u\right) &= f \text{ in } \Omega, \\ u &= 0 \text{ on } \partial\Omega, \end{aligned} \tag{1.3}$$

with $\mathsf{K}^{\mathrm{eff}}_{\ell j} := \sum_{i=1}^3 \int_Y \mathsf{K}_{\ell i}(\boldsymbol{y})(\delta_{ji} - \partial_{y_i} w_j)\, d\boldsymbol{y}$ and $w_j \in \{\mathrm{H}^1_{\mathrm{per}}(Y) \mid \int_Y w_j\, d\boldsymbol{y} = 0\}$ is a solution to

$$\begin{aligned} -\mathrm{div}_y\left(\mathsf{K}(\boldsymbol{y}).(\nabla_y w_j - \boldsymbol{e}_j)\right) &= 0 \text{ in } Y, \\ w_j &\text{ is } Y-\text{periodic}. \end{aligned} \tag{1.4}$$

The convergence of u_ε to u in $\mathrm{H}^1_0(\Omega)$ is only weak. If one seeks to improve the convergence then, usually, a corrector type term is introduced:

$$u_\varepsilon - u - \varepsilon \hat{u}(\cdot, \frac{\cdot}{\varepsilon}) \to 0 \text{ in } \mathrm{H}^1(\Omega), \tag{1.5}$$

where $\hat{u}(\boldsymbol{x}, \boldsymbol{y}) := -\sum_{k=1}^N w_k(\boldsymbol{y}) \frac{\partial u}{\partial x_k}(\boldsymbol{x})$ is the correction term. For the expression to belong in $\mathrm{H}^1(\Omega)$ it is required that $w_k \in \mathrm{W}^{1,\infty}(Y)$ and $u \in \mathrm{H}^2(\Omega)$ (see [5, pp. 33]). With the introduction of two-scale convergence in [32] (see also [2] and [28]) a rigorous justification was provided for the multiple-scale method and the corrector result (in N-dimensional space) in Eq (1.5) was made rigorous through the following theorem:

Proposition 1.1. *[2, 10, 28] Let $\tilde{u}_1 \in \mathrm{L}^s(\Omega)$ and $\hat{u}$ be given by,*

$$\hat{u}(\boldsymbol{x}, \boldsymbol{y}) = -\sum_{k=1}^N w_k(\boldsymbol{y}) \frac{\partial u}{\partial x_k}(\boldsymbol{x}) + \tilde{u}_1(\boldsymbol{x}), \tag{1.6}$$

and suppose that $\nabla_y w_k \in \mathrm{L}^r(Y, \mathbb{R}^N)$, $k = 1, \ldots, N$ and $\nabla u \in \mathrm{L}^s(\Omega, \mathbb{R}^N)$ with $1 < r, s < \infty$ and such that,

$$\frac{1}{r} + \frac{1}{s} = \frac{1}{2}. \tag{1.7}$$

Then,

$$\nabla u_\varepsilon - \nabla u - \nabla_y \hat{u}(\cdot, \frac{\cdot}{\varepsilon}) \to 0 \; in \; \mathrm{L}^2(\Omega, \mathbb{R}^N). \tag{1.8}$$

As one can immediately observe, the main unease with the above proposition is the higher integrability required on both local and homogenized solutions. However, with the introduction of periodic unfolding operators [12, 13], one can obtain a more general corrector result without requiring any regularity assumption on the cell function w_k, stating,

$$\nabla u_\varepsilon - \nabla u - \sum_{k=1}^{N} Q_\varepsilon(\frac{\partial u}{\partial x_k}) \nabla_y w_k(\frac{\cdot}{\varepsilon}) \to 0 \text{ in } \mathrm{L}^2(\Omega, \mathbb{R}^N), \tag{1.9}$$

where Q_ε is the scale-splitting operator defined in [27]; see the elegant proof in [14]. Moreover, based on the scale-splitting operator, upper bound estimates on the convergence rate in terms of ε were obtained in [27] (with some additional regularity assumptions on the homogenized solution). Furthermore, the upper bound estimates on the convergence rate can be made tighter by using boundary layer correctors (see, e.g., [3, 31, 36]). Therefore, it seems that in order to lift the (restrictive) regularity conditions in Proposition 1.1 one must have knowledge of the operator Q_ε.

The widely accepted understanding of Fourier's law of heat conduction is that it represents a limiting case approximation of a more comprehensive, potentially nonlinear, constitutive law for the heat flux, which may depend on higher-order gradients (see, e.g., [9, 15, 37]). For instance, the temperature of a rarefied gas at the slip regime, namely when $0.001 < \mathrm{Kn} < 0.3$, where Kn is the non-dimensional Knudsen number, deviates from Fourier's law of heat conduction (see, e.g., [37]). Moreover, in the same article a generalized heat conduction model, from a phenomenological point of view, was postulated under the assumption that the gas is isotropic. The authors' speculation was that the heat flux in a rarefied gas in the slip regime, depends linearly on the temperature gradient but also on higher-order temperature derivatives,

$$\boldsymbol{q} = \mathsf{K} \boldsymbol{.} \nabla u + \mathsf{L} \colon \nabla\nabla u + \mathsf{M} \vdots \nabla\nabla\nabla u, \tag{1.10}$$

where K is the classical second order heat conduction tensor*, while L and M are third and fourth order material parameter tensors, respectively (the notation $\boldsymbol{.}$, $:$, and $\vdots$ denote first, second, and third order contractions). The structure of such material parameter tensors can be determined by considering proper orthogonal transformations (compare [41]). Moreover, if we request that the material be centro-symmetric (meaning it is invariant under reflections), then the tensor $\mathsf{L} \equiv 0$ (cf. [41]). Furthermore, if the material is isotropic then reflections are not relevant since the only isotropic third order tensor is the Levi-Civita tensor which is anti-symmetric and, hence, $\mathsf{L} \colon \nabla\nabla u \equiv 0$ since it would be the product

*Interestingly, unlike the case of Fickian diffusion, a rigorous microscopic interpretation of the classical linear Fourier law (and of its variations) done at the level of stochastically interacting particles is still lacking in spite of sustained efforts in both probability and statistical physics communities (cf. e.g. [7]). It would be interesting to see, for instance, whether the simplified mechanistic approach from [38] unveiling connections between Hamiltonian chains of coupled mechanical systems and the linear Fourier law can be eventually extended to capture at least some of the second gradient effects postulated in Eq (1.10).

of a symmetric and an antisymmetric matrix which is zero. Additionally, the tensor M has a physical meaning–it is often referred to as the *spatial retardation* (see the context of [9]).

Henceforth, we assume isotropy of the medium. Thus, the higher-gradient heat flux can reduce further,

$$\boldsymbol{q} = \mathsf{K}\boldsymbol{.}\nabla u + \mathsf{M}\vdots\nabla\nabla\nabla u, \tag{1.11}$$

where $\mathsf{K}_{ij}{:=}\eta\delta_{ij}$ and $\mathsf{M}_{ijkl}{:=}\ell_1\delta_{ik}\delta_{jl}+\ell_2\delta_{il}\delta_{jk}+\ell_3\delta_{ij}\delta_{kl}$ for scalars η and ℓ_i, $i = 1, 2, 3$ that will be assumed to be constant or piece-wise constant with the heat conduction inequality asserting,

$$\boldsymbol{q}\boldsymbol{.}\nabla u \leq 0, \tag{1.12}$$

for all temperature fields.

Non-classical laws of Fourier's heat conduction have, for many years now, attracted considerable attention from the theoretical mechanics community (see, e.g., [1, 6, 21, 22]). In recent years, the motivation for deriving non-classical heat conduction models in the mechanics field stemmed from trying to understand the presence of thermal fluctuation fields in heterogeneous materials with a microstructure. Specifically, the authors in [22] postulate the existence of a free energy function that has an added dependence on the gradient of the entropy density variable. Based on this enhanced free energy, an enhanced heat equation was derived containing a term with a characteristic length related to material parameters that *can account for scale-size thermal effects in micro-heterogeneous bodies*. Finally, all of the above theoretical or computational non-classical approaches seem to have found some validation in recent experimental work where evidence of size-dependent thermal effects were reported in heterogeneous materials (see, e.g., [18, 19]).

In this work, we commence with a higher-gradient heat equation model. By introducing physically relevant scaling arguments related to the absolute size of the constituents, we point out a new length scale parameter that models scale-dependent thermal effects (see, e.g., [18, 19]). Hence, by arguing as in the work of [34], the solution of the enriched microscopic problem can be seen as a vanishing-viscosity solution that coincides with the classical homogenized solution of (1.3). However, unlike in the classical case, the local solutions w_k satisfy a higher-gradient local problem and, hence, possess better regularity properties than classical local solutions. What is remarkable is, that this aforementioned higher regularity of the local solution compensated by the mild assumption that the data are of the form $f := \operatorname{div} \boldsymbol{F}$, $\boldsymbol{F} \in \mathrm{L}^3(\Omega, \mathbb{R}^3)$ allows us to prove Proposition 1.1 under the minimal assumptions of a uniformly Lipschitz open set Ω and non-smooth material coefficients.

We have organized the paper as follows: In Section 2 we explain in detail the scaling argument we employ, present the enriched microscopic model, provide some motivation for its use, and prove some general qualitative results as they pertain to existence and uniqueness of solution as well as the variational nature of the problem. In Section 3 we state the main results, we discuss their consequences, and demonstrate symmetry relations for the higher-gradient effective coefficients as well as explore their variational structure. Section 4 is dedicated to proving the main results in Section 3. Finally, we reserve Section 5 for some discussion and remarks.

2. Problem set-up

2.1. Scale-dependent thermal effects

In this paragraph, we postulate the modified heat flux in (1.11) and derive an additional length scale parameter that encapsulates the size-dependent thermal effects in the context of an idealized periodic microstructure. The approach is motivated from generalized continuum mechanic theories (see, e.g., [20]) since it is well understood that the effective properties of heterogeneous materials can depend not only on the volume fraction of the phases or their geometrical distribution but also on the absolute size of the constituents (see, e.g., [23]).

We assume that our working domain Ω has a periodic microstructure with period ℓ and overall characteristic length L. This introduces a natural periodicity of the tensors K and M. We scale all the parameters in the model, including the material parameters, the following way:

$$\boldsymbol{x}^*=\frac{\boldsymbol{x}}{\mathrm{L}}, \quad u^*(\boldsymbol{x}^*)=\frac{u(\boldsymbol{x})}{\mathcal{U}}, \tag{2.1}$$

where $\mathcal{U} := \max_{z\in\Omega} |u(z)|$. While for the material parameters we can define the normalized tensors,

$$\mathsf{K}^*=\mathsf{K}/\mathcal{K}, \quad \mathsf{M}^*=\mathsf{M}/\mathcal{M}, \tag{2.2}$$

where $\mathcal{K}:= \max_{z\in Y_\ell} |\mathsf{K}(z)|$, $\mathcal{M}:= \max_{z\in Y_\ell} |\mathsf{M}(z)|$ with $Y_\ell:=(-\ell/2, \ell/2]^3$ the periodic cell characterizing the body Ω. We can now introduce an additional length scale relation between $\mathcal{K}$ and $\mathcal{M}$ as follows:

$$\mathcal{M} = \ell_{\mathrm{TE}}^2\mathcal{K}. \tag{2.3}$$

The characteristic intrinsic length ℓ_{TE} accounts for scale-size effects in heat conduction problems of heterogeneous media. When it is identically zero Fourier's classical law of heat conduction is recovered.

Remark 2.1. *We chose to work with the above scaling because of its physical interpretation. The scaling indicates that the size of the heterogeneities are comparable to the order of the period. Naturally, one could consider a different scaling than the one proposed above and arrive at different mascroscopic heat conduction problems. We will not address other type of scalings here. We leave the interested reader to consult the work in [34] for different type of scalings and their influence on effective equations within the context of second gradient elasticity. Moreover, the works in [1, 21] provide a theoretical framework as to why such internal lengths are needed and how they can account for thermal scale-size effects, while the works in [18, 19] provide an experimental justification.*

Thus, the scaled heat flux becomes:

$$q_i = \sum_{j=1}^{3}\left(\mathcal{K}\frac{\mathcal{U}}{\mathrm{L}}\mathsf{K}^*_{ij}\frac{\partial u^*}{\partial x^*_j} + \sum_{k,l=1}^{3}\mathcal{K}\mathcal{U}\Big(\frac{\ell_{\mathrm{TE}}}{\mathrm{L}}\Big)^2\frac{\partial}{\partial x^*_j}\left(\mathsf{M}^*_{ijkl}\frac{\partial^2 u^*}{\partial x^*_k\partial x^*_l}\right)\right). \tag{2.4}$$

If we use the notation, $\boldsymbol{q}^*:=(\mathcal{K}\mathcal{U})^{-1}\boldsymbol{q}$ then we have a scaled form of the heat flux,

$$\boldsymbol{q}^* = \frac{1}{\mathrm{L}}\mathsf{K}^*\nabla^*u^* + \Big(\frac{\ell_{\mathrm{TE}}}{\mathrm{L}}\Big)^2\operatorname{div}^*(\mathsf{M}^*:\nabla^*\nabla^*u^*)\,. \tag{2.5}$$

To simplify our presentation, henceforth, we absorb the factor $1/\mathsf{L}$ into the notation K^*. Moreover, we remark that since the coefficients K and M are Y_ℓ periodic the corresponding scaled coefficients K^* and M^* are Y^* periodic where $Y^*{:=}\frac{\ell}{\mathrm{L}}Y$ with $Y{:=}(-1/2, 1/2]^3$. Finally, hereon, if no confusion arises we will drop the $*$ notation in order to expedite our presentation.

2.2. The microscopic problem

We consider a material with a periodic microstructure of period $\varepsilon{:=}\ell/\mathrm{L}{\ll}1$ occupying a region $\Omega \subset \mathbb{R}^3$. The region Ω that the heterogeneous material occupies is assumed to be a uniformly Lipschitz open set (see [17, Definition 2.65]). The exterior boundary component will be denoted by $\Sigma{:=}\partial\Omega$ while the vector $\boldsymbol{n}$ will denote the unit normal on Σ pointing in the outward direction. The ε periodic problem, generated by defining the non-dimensional number ε as the ratio of ℓ/L, will permit us to obtain an effective equation when $\varepsilon \to 0$. However, unlike in classical homogenization problems, different cases ought to be considered depending on how the intrinsic length scale ℓ_{TE} scales with ℓ (or L). Here, since we are interested in recovering Fourier's classical law of heat conduction as an effective limit, we will only consider the scaling,

$$\ell_{\mathrm{TE}}/\ell \sim 1. \tag{2.6}$$

The physical meaning of the above scaling, is that the intrinsic length ℓ_{TE} is comparable with the length of the heterogeneities. Naturally, other type of scalings are possible, however, we will not address other cases here. We refer the reader to [34] for different type of scalings in the context of generalized continuum mechanics.

Therefore, under the scaling in Eq (2.6), the (generalized) heat flux becomes,

$$\boldsymbol{q}^\varepsilon = \mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon}).\nabla u_\varepsilon + \varepsilon^2 \mathrm{div}\left(\mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon}){:}\nabla\nabla u_\varepsilon\right). \tag{2.7}$$

The microscopic problem is then characterized by the following equation and boundary conditions,

$$\begin{aligned}
&-\mathrm{div}\left(\mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon}).\nabla u_\varepsilon - \varepsilon^2 \mathrm{div}\left(\mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon}){:}\nabla\nabla u_\varepsilon\right)\right) = f && \text{in } \Omega,\\
&\varepsilon^2 \mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon})\nabla\nabla u_\varepsilon{:}\boldsymbol{n}\otimes\boldsymbol{n} = 0 && \text{on } \Sigma,\\
&u_\varepsilon = 0 && \text{on } \Sigma,
\end{aligned} \tag{2.8}$$

where f is some given source that belongs in $\mathrm{L}^2(\Omega)$. We remark, that prescribing a homogeneous Dirichlet boundary condition, as is usually the case, is no longer sufficient. We require, additionally, to prescribe a zero heat flux for what we refer to as a *normal double heat flux* that is directly related to the *spatial retardation* coefficient M. It describes that the internal structure of the material has an effect on the heat flow. It is connected to the choice of the scaling ε^2 in front of the higher gradient term in the flux. It plays here the role of a *natural* boundary condition as one can see at the level of the weak formulation of the problem. It is also a convenient choice of boundary condition as it cancels any surface or line integrals. In direct analogy with second-gradient elasticity, such a term is referred to as normal double traction (see, in particular, [24, 25, 30]).

2.2.1. Notation and assumptions

- We employ the Einstein notation of repeated indices unless otherwise stated.
- Throughout the work we assume that the uniform strong ellipticity condition holds, i.e., there exist positive (generic) constants c_1 and c_2 such that:

$$\begin{gathered} c_1|\boldsymbol{w}|^2 \leq \boldsymbol{w}.\mathsf{K}(\boldsymbol{x}).\boldsymbol{w} \leq c_2|\boldsymbol{w}|^2, \\ c_1|\boldsymbol{w}|^2|\boldsymbol{q}|^2 \leq \boldsymbol{w}\otimes\boldsymbol{q}:\mathsf{M}(\boldsymbol{x}):\boldsymbol{w}\otimes\boldsymbol{q} \leq c_2|\boldsymbol{w}|^2|\boldsymbol{q}|^2, \end{gathered} \tag{2.9}$$

for all $\boldsymbol{w}, \boldsymbol{q} \in \mathbb{R}^3 - \{\mathbf{0}\}$.

2.2.2. Auxiliary formulas

For the readers' convenience and for the expediency of our results, we introduce certain formulas that we will make use of in obtaining the variational formulation of (2.8). These formulas, among others, can also be found in [24, Appendix].

For any smooth enough scalar function ξ defined on Σ or on a neighborhood of Σ, the tangential and normal components of $\nabla\xi$ are,

$$(\nabla\xi)_\tau = -\boldsymbol{n}\times(\boldsymbol{n}\times\nabla\xi) = \nabla\xi - (\nabla\xi)_n\boldsymbol{n}, \quad (\nabla\xi)_n := \nabla\xi.\boldsymbol{n}. \tag{2.10}$$

Moreover, we introduce the surface gradient of ξ using the projection operator $\Pi := \mathrm{I} - \boldsymbol{n}\otimes\boldsymbol{n}$,

$$\nabla_s\xi = (\mathrm{I} - \boldsymbol{n}\otimes\boldsymbol{n})\nabla\xi = \Pi\nabla\xi. \tag{2.11}$$

Thus, we can write down a useful integration by parts formula on surfaces,

$$\int_\Sigma \nabla_s\xi \, d\sigma = \int_\Sigma \xi(\operatorname{div}\boldsymbol{n})\boldsymbol{n}\, d\sigma + \int_{\partial\Sigma} [\![\xi\boldsymbol{\nu}]\!] \, d\lambda, \tag{2.12}$$

where,

$$\nu_i = \boldsymbol{\epsilon}_{ijk} t_j n_k \tag{2.13}$$

are the components of the unit normal vector on $\partial\Sigma$ and tangent to Σ, $\boldsymbol{t}$ is the unit tangent vector to $\partial\Sigma$, and $\boldsymbol{\epsilon}$ is the Levi-Civita tensor. Lastly, we remark, the jump term on Eq (2.12) is on a ridge, i.e., the line on Σ where the tangent plane of Σ is discontinuous.

Remark 2.2. *The above formulas are used with a high degree of frequency in emulsions and capillary fluids (see, e.g., [35]). We refer the reader to the appendix of reference [24] or [25] for an excellent exposition of the above formulae and related topics.*

2.3. Weak formulation

The primary setting for the variational formulation of (2.8) is the space $\mathrm{H}^2(\Omega) \cap \mathrm{H}^1_0(\Omega)$ where the Sobolev space $\mathrm{H}^2(\Omega)$ is a Hilbert space with norm,

$$\|u\|_{\mathrm{H}^2(\Omega)} = \left(\|u\|^2_{\mathrm{L}^2(\Omega)} + \|\nabla u\|^2_{\mathrm{L}^2(\Omega,\mathbb{R}^3)} + \|\nabla\nabla u\|^2_{\mathrm{L}^2(\Omega,\mathbb{R}^{3\times3})}\right)^{1/2}. \tag{2.14}$$

Since the variational formulation of (2.8) is not a standard one, we write down the details for the readers convenience using the notation introduced in Section 2.2.2. Hence, if we multiply (2.8) by a test function $v \in \{\phi \in C^\infty(\overline{\Omega}) \mid \phi = 0 \text{ on } \Sigma\}$ and integrate by parts several times (including integration by parts on surfaces using formula (2.12)) we obtain,

$$
\begin{aligned}
&-\int_\Sigma \Big(\mathsf{K}_{ij}(\frac{\boldsymbol{x}}{\varepsilon})\partial_{x_j}u_\varepsilon - \varepsilon^2\partial_{x_k}\Big(\mathsf{M}_{ikpq}(\frac{\boldsymbol{x}}{\varepsilon})\partial^2_{x_px_q}u_\varepsilon\Big)\Big)n_i v\, d\sigma \\
&+\int_\Omega \mathsf{K}_{ij}(\frac{\boldsymbol{x}}{\varepsilon})\partial_{x_j}u_\varepsilon\partial_{x_j}v\, d\boldsymbol{x} - \varepsilon^2\Big\{\int_\Sigma \mathsf{M}_{ikpq}(\frac{\boldsymbol{x}}{\varepsilon})\partial^2_{x_px_q}u_\varepsilon n_k n_m n_i \partial_{x_m}v\, d\sigma \\
&+\int_{\partial\Sigma} \Big[\!\!\Big[\mathsf{M}_{ikpq}(\frac{\boldsymbol{x}}{\varepsilon})\partial^2_{x_px_q}u_\varepsilon n_k \Pi_{i\ell}\nu_\ell v\Big]\!\!\Big]\, d\lambda - \int_\Sigma \Pi_{\ell m}\partial_{x_m}(\mathsf{M}_{ikpq}(\frac{\boldsymbol{x}}{\varepsilon})\partial^2_{x_px_q}u_\varepsilon n_k \Pi_{i\ell})v\, d\sigma\Big\} \\
&+\varepsilon^2\int_\Omega \mathsf{M}_{ikpq}(\frac{\boldsymbol{x}}{\varepsilon})\partial^2_{x_px_q}u_\varepsilon\partial^2_{x_ix_k}v\, d\boldsymbol{x} = \int_\Omega f\, v\, d\boldsymbol{x}.
\end{aligned}
\tag{2.15}
$$

Using the fact that we have imposed a homogeneous Dirichlet boundary condition and a zero normal double heat flux for the spatial retardation on Σ, we can see that the variational formulation (in vectorial form) reduces to the following: Find $u_\varepsilon \in \mathrm{H}^2(\Omega) \cap \mathrm{H}^1_0(\Omega)$ such that,

$$
\int_\Omega \mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon})\nabla u_\varepsilon \boldsymbol{.} \nabla v\, d\boldsymbol{x} + \varepsilon^2\int_\Omega \mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon})\nabla\nabla u_\varepsilon : \nabla\nabla v\, d\boldsymbol{x} = \int_\Omega f\, v\, d\boldsymbol{x}, \tag{2.16}
$$

for all $v \in \mathrm{H}^2(\Omega) \cap \mathrm{H}^1_0(\Omega)$.

Remark 2.3. *The weak form in Eq* (2.15) *also provides a way for recovering the strong form of problem* (2.8) *in the sense of distributions. For more details, the interested reader can consult [34].*

Remark 2.4. *Existence and uniqueness of a solution in Eq* (2.16) *that belongs in* $\mathrm{H}^2(\Omega) \cap \mathrm{H}^1_0(\Omega)$ *is a matter of applying the Lax-Milgram lemma together with Poincaré's inequality in* $\mathrm{H}^1_0(\Omega)$ *and the assumptions regarding the ellipticity of the tensors in Section 2.2.1. Hence, immediately, we can derive the following estimate from Eq* (2.16)*,*

$$
\Big(\|u_\varepsilon\|^2_{\mathrm{H}^1(\Omega)} + \varepsilon^2\ \|\nabla\nabla u_\varepsilon\|^2_{\mathrm{L}^2(\Omega,\mathbb{R}^{3\times3})}\Big)^{1/2} \le c(\Omega)\,\|f\|_{\mathrm{L}^2(\Omega)}\,. \tag{2.17}
$$

2.4. Variational formulation

The weak solution to Eq (2.16) can be classified as the unique minimum of the functional $\mathcal{J}_\varepsilon(\theta)$,

$$
u_\varepsilon = \underset{\theta\in\mathrm{H}^2(\Omega)\cap\mathrm{H}^1_0(\Omega)}{\arg\min}\ \mathcal{J}_\varepsilon(\theta), \tag{2.18}
$$

where

$$
\mathcal{J}_\varepsilon(\theta) := \frac{1}{2}\int_\Omega \mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon})\nabla\theta\boldsymbol{.}\nabla\theta\, d\boldsymbol{x} + \frac{1}{2}\int_\Omega \varepsilon^2\mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon})\nabla\nabla\theta : \nabla\nabla\theta\, d\boldsymbol{x} - \int_\Omega f\,\theta\, d\boldsymbol{x}. \tag{2.19}
$$

A standard computation of the variational derivative of $\mathcal{J}_\varepsilon$ will recover Eq (2.16) and the Euler-Lagrange equations in succession.

3. Main results

3.1. Homogenization via unfolding Γ–convergence

We define the following domain decompositions (see [12–14, 16]):

$$K_\varepsilon^- := \left\{\ell \in \mathbb{Z}^d \mid \varepsilon(\ell + Y) \subset \overline{\Omega}\right\}, \ \Omega_\varepsilon^- := \mathrm{int}\left(\cup_{\ell \in K_\varepsilon^-} \varepsilon(\ell + Y)\right), \ \Lambda_\varepsilon^- := \Omega \backslash \Omega_\varepsilon^-. \tag{3.1}$$

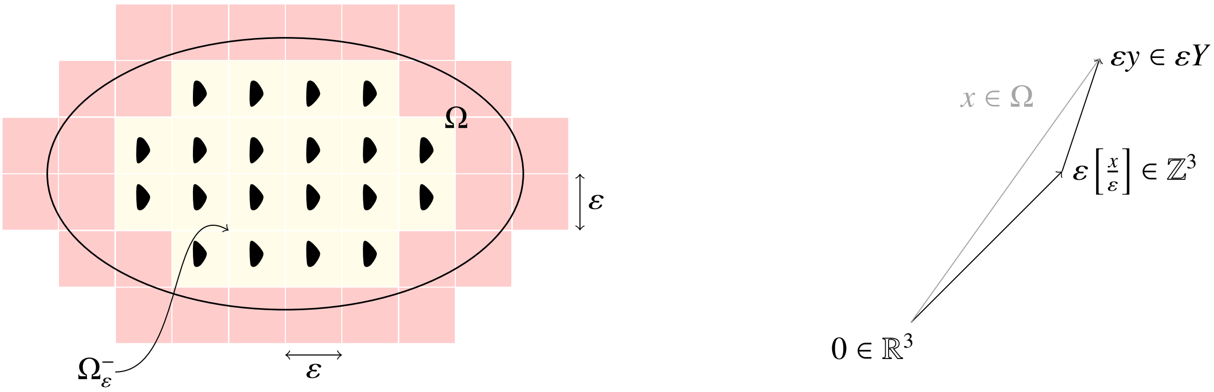

Figure 1. Unfolding operator on a periodic grid.

Let $[z]_Y = (\lfloor z_1 \rfloor, \lfloor z_2 \rfloor, \lfloor z_3 \rfloor)$ denote the integer part of $z \in \mathbb{R}^3$ and denote by $\{z\}_Y$ the difference $z - [z]_Y$ which belongs to Y. Regarding our multiscale problem that depends on a small length parameter $\varepsilon > 0$, we can decompose any $\boldsymbol{x} \in \mathbb{R}^3$ using the maps $[\cdot]_Y : \mathbb{R}^3 \mapsto \mathbb{Z}^3$ and $\{\cdot\}_Y : \mathbb{R}^3 \mapsto Y$ the following way (see Figure 1 (right)),

$$\boldsymbol{x} = \varepsilon\left(\left[\frac{\boldsymbol{x}}{\varepsilon}\right]_Y + \left\{\frac{\boldsymbol{x}}{\varepsilon}\right\}_Y\right). \tag{3.2}$$

Definition 3.1. *([13, Def. 2.1, pp. 1588]) For any Lebesgue measurable function φ on Ω we define the periodic unfolding operator by,*

$$\mathcal{T}_\varepsilon(\varphi)(\boldsymbol{x}, \boldsymbol{y}) = \begin{cases} \varphi\left(\varepsilon\left[\frac{\boldsymbol{x}}{\varepsilon}\right]_Y + \varepsilon \boldsymbol{y}\right) & \text{for a.e. } (\boldsymbol{x}, \boldsymbol{y}) \in \Omega_\varepsilon^- \times Y \\ 0 & \text{for a.e. } (\boldsymbol{x}, \boldsymbol{y}) \in \Lambda_\varepsilon^- \times Y. \end{cases} \tag{3.3}$$

Regarding properties of the unfolding operator, the reader can consult [12–14, 16].

Definition 3.2. *([8, Def. 12 and Prop. 14, pp. 458]) Let $F_\varepsilon : \mathrm{L}^p(\Omega) \to \overline{\mathbb{R}}$ be a sequence of functionals and $F : \mathrm{L}^p(\Omega \times Y) \to \overline{\mathbb{R}}$ ($p > 1$). We say that F_ε unfolding Γ-converges to F if for all $u \in \mathrm{L}^p(\Omega \times Y)$:*

1. *For every sequence $u_\varepsilon \in \mathrm{L}^p(\Omega)$ such that $\mathcal{T}_\varepsilon(u_\varepsilon) \rightharpoonup u$ in $\mathrm{L}^p(\Omega \times Y)$ one has,*

$$F(u) \leq \liminf_{\varepsilon \to 0} F_\varepsilon(u_\varepsilon); \tag{3.4}$$

2. *there exists a sequence $u_\varepsilon \in \mathrm{L}^p(\Omega)$ such that $\mathcal{T}_\varepsilon(u_\varepsilon) \rightharpoonup u$ in $\mathrm{L}^p(\Omega \times Y)$ and*

$$F(u) = \lim_{\varepsilon \to 0} F_\varepsilon(u_\varepsilon). \tag{3.5}$$

Theorem 3.1. *The sequence of functionals $\mathcal{J}_\varepsilon$ unfolding Γ-converge in the weak topology of* $\mathrm{H}^2(\Omega) \cap \mathrm{H}^1_0(\Omega)$ *to* $\mathcal{J}_{\mathrm{eff}}$ *as* $\varepsilon \to 0$,

$$\mathcal{J}_\varepsilon \xrightarrow{\Gamma} \mathcal{J}_{\mathrm{eff}}, \tag{3.6}$$

where

$$\mathcal{J}_{\mathrm{eff}}(\theta){:=}\frac{1}{2}\int_\Omega \mathsf{K}^{\mathrm{eff}}\nabla\theta\boldsymbol{.}\nabla\theta\, d\boldsymbol{x} - \int_\Omega f\theta\, d\boldsymbol{x}, \tag{3.7}$$

$$\mathsf{K}^{\mathrm{eff}}_{ik}{:=}\int_Y \mathsf{K}(\boldsymbol{y})(\nabla_y w_k - \boldsymbol{e}_k)\boldsymbol{.}(\nabla_y w_i - \boldsymbol{e}_i) + \mathsf{M}(\boldsymbol{y})\nabla_y\nabla_y w_k{:}\nabla_y\nabla_y w_i\, d\boldsymbol{y}, \tag{3.8}$$

with $w_k \in \mathrm{H}^2(Y)$, $k = 1, 2, 3$ *the Y-periodic local solution to,*

$$-\mathrm{div}_y\Big(\mathsf{K}(\boldsymbol{y})\boldsymbol{.}(\nabla_y w_k - \boldsymbol{e}_k) - \mathrm{div}_y(\mathsf{M}(\boldsymbol{y}){:}\nabla_y\nabla_y w_k)\Big) {=} 0 \text{ in } Y. \tag{3.9}$$

Remark 3.1. *The first part of Eq* (3.8) *is what one would expect as a result from the homogenization of second order linear elliptic equations while the second part is new, specific to the inclusion of the second-gradient thermal effects.*

Theorem 3.2. *Let* u_ε *and* u *be the unique minimizers of* (2.19) *and* (3.7)*, respectively. Moreover, for* $\tilde{u}_1 \in \mathrm{L}^s(\Omega)$*, let* $f{:=}\mathrm{div}\, \boldsymbol{F}$, $\boldsymbol{F} \in \mathrm{L}^3(\Omega, \mathbb{R}^3)$ *then,*

$$\nabla u_\varepsilon - \nabla u - \nabla_y \hat{u}(\cdot, \frac{\cdot}{\varepsilon}) \to 0 \text{ in } \mathrm{L}^2(\Omega, \mathbb{R}^3), \tag{3.10}$$

as $\varepsilon \to 0$ *with*

$$\hat{u}(\boldsymbol{x}, \boldsymbol{y}) = -w_k(\boldsymbol{y})\frac{\partial u}{\partial x_k}(\boldsymbol{x}) + \tilde{u}_1(\boldsymbol{x}). \tag{3.11}$$

Remark 3.2. *We note in the above theorem, the assumptions that* $\nabla_y w_k \in \mathrm{L}^r$ *and* $\nabla u \in \mathrm{L}^s$ *with* $1/r + 1/s = 1/2$ *are no longer needed. Furthermore, if we compare Eq* (3.11) *with G. Griso's result in Eq* (1.9)*, we see that Eq* (3.11) *is more accessible to computations, hence, more practical. Note that* $\hat{u} \in \mathrm{L}^2(\Omega, \mathrm{H}^1_{\mathrm{per}}(Y))$.

3.2. Remarks on the homogenized coefficients

3.2.1. Symmetry

Since we work within a variational framework, the homogenized coefficients inherit the symmetry that is imposed on them from the framework. If one were to obtain the effective tensor through a multiple scale expansion then the tensor would have the following, non-symmetric, form:

$$\mathsf{K}^{\mathrm{eff}}_{ik}{:=}\int_Y \mathsf{K}_{ij}(\boldsymbol{y})(\delta_{jk} - \frac{\partial w_k}{\partial y_j})\, d\boldsymbol{y}. \tag{3.12}$$

Naturally, the two forms, (3.8) and (3.12), are equivalent (since the tensors K and M are assumed to be isotropic). The proof is virtually identical to the classical case (see [39]), however, we feel it should be included here since it is a higher-gradient generalization of the classical case: Multiply with a test function $v \in \mathrm{H}^2_{\mathrm{per}}(Y)$ equation (3.9) and integrate by parts to obtain,

$$0 = \int_Y \mathsf{M}_{mjpq} \frac{\partial^2 w_k}{\partial y_p \partial y_q} \frac{\partial^2 v}{\partial y_m \partial y_j}\, d\boldsymbol{y} + \int_Y \mathsf{K}_{mj} \frac{\partial (w_k - y_k)}{\partial y_j} \frac{\partial v}{\partial y_m}\, d\boldsymbol{y}. \tag{3.13}$$

Selecting $v = w_i$ we have,

$$0 = \int_Y \mathsf{M}_{mjpq} \frac{\partial^2 w_k}{\partial y_p \partial y_q} \frac{\partial^2 w_i}{\partial y_m \partial y_j}\, d\boldsymbol{y} + \int_Y \mathsf{K}_{mj} \frac{\partial (w_k - y_k)}{\partial y_j} \frac{\partial w_i}{\partial y_m}\, d\boldsymbol{y}. \tag{3.14}$$

If we add and subtract coordinate y_i on the w_i term of the second integral we obtain,

$$\begin{aligned} &\int_Y \mathsf{K}_{ij}(\boldsymbol{y})(\delta_{jk} - \frac{\partial w_k}{\partial y_j})\, d\boldsymbol{y} \\ &\quad = \int_Y \mathsf{M}_{mjpq} \frac{\partial^2 w_k}{\partial y_p \partial y_q} \frac{\partial^2 w_i}{\partial y_m \partial y_j}\, d\boldsymbol{y} + \int_Y \mathsf{K}_{mj} \frac{\partial (w_k - y_k)}{\partial y_j} \frac{\partial (w_i - y_i)}{\partial y_m}\, d\boldsymbol{y}. \end{aligned} \tag{3.15}$$

3.2.2. Variational characterization of the higher-order effective tensor

From equation (3.8), we can see that $\mathsf{K}^{\mathrm{eff}}$ is symmetric as well, and is determined in its entirety from the knowledge of the quadratic form $\mathsf{K}^{\mathrm{eff}}\boldsymbol{\xi} \cdot \boldsymbol{\xi}$ for any constant vector $\boldsymbol{\xi} \in \mathbb{R}^3$. Using definition (3.8) one can check that,

$$\mathsf{K}^{\mathrm{eff}}\boldsymbol{\xi} \cdot \boldsymbol{\xi} = \int_Y \mathsf{K}(\boldsymbol{y})(-\boldsymbol{\xi} + \nabla_y w_\xi).(-\boldsymbol{\xi} + \nabla_y w_\xi)\, d\boldsymbol{y} + \int_Y \mathsf{M}(\boldsymbol{y}) \nabla_y \nabla_y w_\xi : \nabla_y \nabla_y w_\xi\, d\boldsymbol{y}, \tag{3.16}$$

where w_ξ is the solution of the following cell problem,

$$\begin{cases} -\mathrm{div_y}\left(\mathsf{K}\left(\nabla_y w_\xi - \boldsymbol{\xi}\right) - \mathrm{div_y}\left(\mathsf{M} : \nabla_y \nabla_y w_\xi\right)\right) = 0 \text{ in } Y, \\ \boldsymbol{y} \mapsto w_\xi(\boldsymbol{y}) \text{ is } Y - \text{periodic}. \end{cases} \tag{3.17}$$

Using completely standard techniques stemming from the calculus of variations we can write for our case,

$$\mathsf{K}^{\mathrm{eff}}\boldsymbol{\xi} \cdot \boldsymbol{\xi} = \inf_{v \in \mathrm{H}^2_{\mathrm{per}}(Y)} \left(\int_Y \mathsf{K}(\boldsymbol{y})(\nabla_y v - \boldsymbol{\xi}).(\nabla_y v - \boldsymbol{\xi})\, d\boldsymbol{y} + \int_Y \mathsf{M}(\boldsymbol{y}) \nabla_y \nabla_y v : \nabla_y \nabla_y v\, d\boldsymbol{y} \right), \tag{3.18}$$

with $\mathrm{H}^2_{\mathrm{per}}(Y) := \{v \in \mathrm{H}^2(Y) \mid v \text{ is } Y - \textit{periodic}\}$. It follows immediately that the effective coefficients are elliptic (they satisfy the Legendre condition), i.e., $\mathsf{K}^{\mathrm{eff}}\boldsymbol{\xi} \cdot \boldsymbol{\xi} \geq \mathcal{K}|\boldsymbol{\xi}|^2$ where $\mathcal{K} = \int_Y K(\boldsymbol{y})\, d\boldsymbol{y}$.

4. Proof of the main results

4.1. Proof of Theorem 3.1

Theorem 3.1. *The sequence of functionals $\mathcal{J}_\varepsilon$ unfolding Γ-converge in the weak topology of $\mathrm{H}^2(\Omega) \cap \mathrm{H}^1_0(\Omega)$ to $\mathcal{J}_{\mathrm{eff}}$ as $\varepsilon \to 0$,*

$$\mathcal{J}_\varepsilon \xrightarrow{\Gamma} \mathcal{J}_{\mathrm{eff}}, \tag{3.6}$$

where

$$\mathcal{J}_{\mathrm{eff}}(\theta):=\frac{1}{2}\int_\Omega \mathsf{K}^{\mathrm{eff}}\nabla\theta.\nabla\theta\, d\boldsymbol{x} - \int_\Omega f\theta\, d\boldsymbol{x}, \tag{3.7}$$

$$\mathsf{K}^{\mathrm{eff}}_{ik}:=\int_Y \mathsf{K}(\boldsymbol{y})(\nabla_y w_k - \boldsymbol{e}_k).(\nabla_y w_i - \boldsymbol{e}_i) + \mathsf{M}(\boldsymbol{y})\nabla_y\nabla_y w_k:\nabla_y\nabla_y w_i\, d\boldsymbol{y}, \tag{3.8}$$

with $w_k \in \mathrm{H}^2(Y)$, $k = 1, 2, 3$ *the* Y*-periodic local solution to,*

$$-\mathrm{div}_y\Big(\mathsf{K}(\boldsymbol{y}).(\nabla_y w_k - \boldsymbol{e}_k) - \mathrm{div}_y(\mathsf{M}(\boldsymbol{y}):\nabla_y\nabla_y w_k)\Big)=0 \text{ in } Y. \tag{3.9}$$

Proof. Define,

$$\mathcal{E}_\varepsilon(\theta):=\begin{cases}\frac{1}{2}a(\theta,\theta) & \text{if } \theta\in \mathrm{H}^2(\Omega)\cap \mathrm{H}^1_0(\Omega)\\ +\infty & \text{if } \theta\in \mathrm{L}^2(\Omega)\backslash \mathrm{H}^2(\Omega)\cap \mathrm{H}^1_0(\Omega),\end{cases} \tag{4.1}$$

with

$$a(\theta,\theta):=\int_\Omega \mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon})\nabla\theta.\nabla\theta\, d\boldsymbol{x}+\int_\Omega \varepsilon^2\mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon})\nabla\nabla\theta:\nabla\nabla\theta\, d\boldsymbol{x}, \tag{4.2}$$

and

$$\mathcal{E}_{\mathrm{eff}}(\theta):=\begin{cases}\frac{1}{2}\int_\Omega \mathsf{K}^{\mathrm{eff}}\nabla\theta.\nabla\theta\, d\boldsymbol{x} & \text{if } \theta\in \mathrm{H}^1_0(\Omega)\\ +\infty & \text{if } \theta\in \mathrm{L}^2(\Omega)\backslash \mathrm{H}^1_0(\Omega).\end{cases} \tag{4.3}$$

It suffices to show that $\mathcal{E}_\varepsilon \xrightarrow{\Gamma} \mathcal{E}_{\mathrm{eff}}$ where the energy $\mathcal{E}_\varepsilon$ is finite. Γ-limit inferior inequality. Let $u_\varepsilon \in \mathrm{H}^2(\Omega)\cap\mathrm{H}^1_0(\Omega)$ be a solution to (2.8) then based on the estimates in (2.17) and properties of the periodic unfolding operator $\mathcal{T}_\varepsilon$ (see Definition 3.1) we have,

- $\mathcal{T}_\varepsilon(u_\varepsilon) \rightharpoonup u$ in $\mathrm{L}^2(\Omega, \mathrm{H}^2(Y))$
- $\mathcal{T}_\varepsilon(\nabla u_\varepsilon) \rightharpoonup \nabla_x u + \nabla_y \hat{u}$ in $\mathrm{L}^2(\Omega, \mathrm{H}^1(Y, \mathbb{R}^3))$
- $\mathcal{T}_\varepsilon(\varepsilon\nabla\nabla u_\varepsilon) \rightharpoonup \nabla_y\nabla_y\hat{u}$ in $\mathrm{L}^2(\Omega\times Y, \mathbb{R}^{3\times 3})$.

Then, for all $\boldsymbol{\varphi} \in \mathrm{L}^2(\Omega, \mathrm{C}^1_{\mathrm{per}}(Y, \mathbb{R}^3))$ we have,

$$\begin{aligned}0\leq&\frac{1}{2}\int_\Omega \mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon})(\nabla u_\varepsilon-\boldsymbol{\varphi}(\boldsymbol{x},\frac{\boldsymbol{x}}{\varepsilon})).(\nabla u_\varepsilon-\boldsymbol{\varphi}(\boldsymbol{x},\frac{\boldsymbol{x}}{\varepsilon}))\, d\boldsymbol{x}\\ &+\frac{1}{2}\int_\Omega \varepsilon^2\mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon})(\nabla\nabla u_\varepsilon-\nabla\boldsymbol{\varphi}(\boldsymbol{x},\frac{\boldsymbol{x}}{\varepsilon})):(\nabla\nabla u_\varepsilon-\nabla\boldsymbol{\varphi}(\boldsymbol{x},\frac{\boldsymbol{x}}{\varepsilon}))\, d\boldsymbol{x}.\end{aligned} \tag{4.4}$$

Opening up the parentheses in the above expression, we obtain

$$\begin{aligned}
\mathcal{E}_\varepsilon(u_\varepsilon) \geq & \int_\Omega \mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon})\nabla u_\varepsilon.\boldsymbol{\varphi}\, d\boldsymbol{x} - \frac{1}{2}\int_\Omega \mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon})\boldsymbol{\varphi}.\boldsymbol{\varphi}\, d\boldsymbol{x} \\
& + \int_\Omega \varepsilon^2 \mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon})\nabla\nabla u_\varepsilon : \nabla\boldsymbol{\varphi}\, d\boldsymbol{x} - \frac{1}{2}\int_\Omega \varepsilon^2 \mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon})\nabla\boldsymbol{\varphi}:\nabla\boldsymbol{\varphi}\, d\boldsymbol{x} \\
& = \int_{\Omega\times Y} \mathsf{K}(\boldsymbol{y})\mathcal{T}_\varepsilon(\nabla u_\varepsilon).\mathcal{T}_\varepsilon(\boldsymbol{\varphi})\, d\boldsymbol{y}d\boldsymbol{x} - \frac{1}{2}\int_{\Omega\times Y} \mathsf{K}(\boldsymbol{y})\mathcal{T}_\varepsilon(\boldsymbol{\varphi}).\mathcal{T}_\varepsilon(\boldsymbol{\varphi})\, d\boldsymbol{y}d\boldsymbol{x} \\
& + \int_{\Omega\times Y} \varepsilon^2 \mathsf{M}(\boldsymbol{y})\mathcal{T}_\varepsilon(\nabla\nabla u_\varepsilon):\mathcal{T}_\varepsilon(\nabla\boldsymbol{\varphi})\, d\boldsymbol{y}d\boldsymbol{x} - \frac{1}{2}\int_{\Omega\times Y} \varepsilon^2 \mathsf{M}(\boldsymbol{y})\mathcal{T}_\varepsilon(\nabla\boldsymbol{\varphi}):\mathcal{T}_\varepsilon(\nabla\boldsymbol{\varphi})\, d\boldsymbol{y}d\boldsymbol{x} \\
& \overset{\varepsilon\to 0}{\to} \int_{\Omega\times Y} \mathsf{K}(\boldsymbol{y})(\nabla_x u + \nabla_y \hat{u}).\boldsymbol{\varphi}\, d\boldsymbol{y}d\boldsymbol{x} - \frac{1}{2}\int_{\Omega\times Y} \mathsf{K}(\boldsymbol{y})\boldsymbol{\varphi}.\boldsymbol{\varphi}\, d\boldsymbol{y}d\boldsymbol{x} \\
& + \int_{\Omega\times Y} \mathsf{M}(\boldsymbol{y})\nabla_y\nabla_y \hat{u}:\nabla_y\boldsymbol{\varphi}\, d\boldsymbol{y}d\boldsymbol{x} - \frac{1}{2}\int_{\Omega\times Y} \mathsf{M}(\boldsymbol{y})\nabla_y\boldsymbol{\varphi}:\nabla_y\boldsymbol{\varphi}\, d\boldsymbol{y}d\boldsymbol{x}.
\end{aligned} \tag{4.5}$$

Since the space $\mathrm{L}^2(\Omega, \mathrm{C}^1_{\mathrm{per}}(Y, \mathbb{R}^3))$ is dense in $\mathrm{L}^2(\Omega\times Y, \mathbb{R}^3)$, the above inequality holds for a sequence of regular functions of the form $\boldsymbol{\varphi}_\varepsilon(\boldsymbol{x}, \boldsymbol{y})$ Y-periodic in $\boldsymbol{y}$ with the following convergence properties,

- $\mathcal{T}_\varepsilon(\boldsymbol{\varphi}_\varepsilon) \rightharpoonup \nabla_x u + \nabla_y \hat{u}$ in $\mathrm{L}^2(\Omega\times Y, \mathbb{R}^3)$
- $\mathcal{T}_\varepsilon(\varepsilon\nabla\boldsymbol{\varphi}_\varepsilon) \rightharpoonup \nabla_y\nabla_y \hat{u}$ in $\mathrm{L}^2(\Omega\times Y, \mathbb{R}^{3\times 3})$.

Upon extracting a (non-relabeled) sub-sequence, we obtain in the limit inferior of (4.5),

$$\begin{aligned}
\liminf_{\varepsilon\to 0} \mathcal{E}_\varepsilon(u_\varepsilon) \geq & \frac{1}{2}\int_{\Omega\times Y} \Big(\mathsf{K}(\boldsymbol{y})(\nabla_x u + \nabla_y \hat{u}).(\nabla_x u + \nabla_y \hat{u}) \\
& + \mathsf{M}(\boldsymbol{y})\nabla_y\nabla_y \hat{u}:\nabla_y\nabla_y \hat{u}\Big)\, d\boldsymbol{y}d\boldsymbol{x} \\
& \geq \frac{1}{2}\int_\Omega \inf_{v\in \mathrm{H}^2_{\mathrm{per}}(Y)} \int_Y \Big(\mathsf{K}(\boldsymbol{y})(\nabla_x u + \nabla_y v).(\nabla_x u + \nabla_y v) \\
& + \mathsf{M}(\boldsymbol{y})\nabla_y\nabla_y v:\nabla_y\nabla_y v\Big) d\boldsymbol{y}d\boldsymbol{x} \\
& = \frac{1}{2}\int_\Omega \mathsf{K}^{\mathrm{eff}}\nabla_x u.\nabla_x u\, d\boldsymbol{x}
\end{aligned}$$

<u>Γ-limit superior inequality.</u>

We will construct the recovery sequence for smooth functions initially and then use a diagonalization argument to complete the proof.

Let $\boldsymbol{u} \in \mathrm{H}^2(\Omega)\cap \mathrm{H}^1_0(\Omega)$. Relying on the density of $\mathrm{C}^\infty_0(\Omega)$ into $\mathrm{H}^2(\Omega)\cap \mathrm{H}^1_0(\Omega)$ we can suppose without loss of generality that $u \in \mathrm{C}^\infty_0(\Omega)$. Furthermore, let $\hat{u} \in \mathrm{C}^2_{\mathrm{per}}(Y)$ be a minimizer of,

$$\inf_{v\in \mathrm{H}^2_{\mathrm{per}}(Y)} \left\{ \int_Y \mathsf{K}(\boldsymbol{y})(\nabla_x u + \nabla_y v).(\nabla_x u + \nabla_y v)\, d\boldsymbol{y} + \mathsf{M}(\boldsymbol{y})\nabla_y\nabla_y v:\nabla_y\nabla_y v \right\}. \tag{4.6}$$

Existence of such a minimizer is shown using classical arguments of coercivity and lower semi-continuity of,

$$v \mapsto \inf_{v\in \mathrm{H}^2_{\mathrm{per}}(Y)} \left(\int_Y \mathsf{K}(\boldsymbol{y})(\nabla_y v - \boldsymbol{\xi}).(\nabla_y v - \boldsymbol{\xi})\, d\boldsymbol{y} + \int_Y \mathsf{M}(\boldsymbol{y})\nabla_y\nabla_y v:\nabla_y\nabla_y v\, d\boldsymbol{y} \right). \tag{4.7}$$

Define the sequence,

$$u_\varepsilon(\boldsymbol{x}) = u(\boldsymbol{x}) + \varepsilon\hat{u}(\frac{\boldsymbol{x}}{\varepsilon}). \tag{4.8}$$

Then,

- $\mathcal{T}_\varepsilon(u_\varepsilon) \to u$ in $\mathrm{L}^2(\Omega, \mathrm{H}^2(Y))$
- $\mathcal{T}_\varepsilon(\nabla u_\varepsilon) \to \nabla_x u + \nabla_y \hat{u}$ in $\mathrm{L}^2(\Omega, \mathrm{H}^1(Y, \mathbb{R}^3))$
- $\mathcal{T}_\varepsilon(\varepsilon\nabla\nabla u_\varepsilon) \to \nabla_y\nabla_y\hat{u}$ in $\mathrm{L}^2(\Omega \times Y)$.

Thus,

$$\begin{aligned}\mathcal{E}_\varepsilon(u_\varepsilon) &= \frac{1}{2}\int_\Omega \Big(\mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon})\nabla u_\varepsilon . \nabla u_\varepsilon + \varepsilon^2 \mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon})\nabla\nabla u_\varepsilon : \nabla\nabla u_\varepsilon\Big)\, d\boldsymbol{y}d\boldsymbol{x} \\ &= \frac{1}{2}\int_{\Omega\times Y} \Big(\mathsf{K}(\boldsymbol{y})\mathcal{T}(\nabla u_\varepsilon) . \mathcal{T}(\nabla u_\varepsilon) + \varepsilon^2 \mathsf{M}(\boldsymbol{y})\mathcal{T}(\nabla\nabla u_\varepsilon) : \mathcal{T}(\nabla\nabla u_\varepsilon)\Big)\, d\boldsymbol{y}d\boldsymbol{x}.\end{aligned} \tag{4.9}$$

Hence, passing to the limit as $\varepsilon \to 0$ in the expression above we obtain,

$$\begin{aligned}&\lim_{\varepsilon\to 0} \mathcal{E}_\varepsilon(u_\varepsilon) \\ &= \int_{\Omega\times Y} \Big(\mathsf{K}(\boldsymbol{y})(\nabla_x u + \nabla_y \hat{u}) . (\nabla_x u + \nabla_y \hat{u}) + \mathsf{M}(\boldsymbol{y})\nabla_y\nabla_y\hat{u} : \nabla_y\nabla_y\hat{u}\Big)\, d\boldsymbol{y}d\boldsymbol{x} \\ &= \frac{1}{2}\int_\Omega \inf_{v\in \mathrm{H}^2_{\mathrm{per}}(Y)} \int_Y \Big(\mathsf{K}(\boldsymbol{y})(\nabla_x u + \nabla_y v) . (\nabla_x u + \nabla_y v) + \mathsf{M}(\boldsymbol{y})\nabla_y\nabla_y v : \nabla_y\nabla_y v\Big)\, d\boldsymbol{y}d\boldsymbol{x} \\ &= \frac{1}{2}\int_\Omega \mathsf{K}^{\mathrm{eff}}\nabla_x u . \nabla_x u\, d\boldsymbol{x}\end{aligned} \tag{4.10}$$

We can conclude the proof using a density and diagonalization argument. □

Remark 4.1. *The Euler-Lagrange equation of* (3.7) *is,*

$$\int_\Omega \mathsf{K}^{\mathrm{eff}}\nabla u . \nabla\phi\, d\boldsymbol{x} = \int_\Omega f\,\phi\, d\boldsymbol{x} \tag{4.11}$$

for all $\phi \in \mathrm{H}^1_0(\Omega)$. *In the sense of distributions we can recover,*

$$\begin{aligned}-\mathrm{div}\Big(\mathsf{K}^{\mathrm{eff}} . \nabla u\Big) &= f \text{ in } \mathcal{D}(\Omega), \\ u &= 0 \text{ on } \partial\Omega,\end{aligned} \tag{4.12}$$

with $\mathsf{K}^{\mathrm{eff}}$ *given in Eq* (3.8).

The above equation is precisely the limit problem that has been obtained countless times in the homogenization literature. The difference in this work is that the local solution used to construct the effective tensor $\mathsf{K}^{\mathrm{eff}}$ *satisfies a higher-gradient problem with* $w_k \in \mathrm{H}^2_{\mathrm{per}}(Y)$ *(and not only in* $\mathrm{H}^1(Y)$*). This newly found local solution regularity is combined with the theorem below to prove the classical corrector convergence result.*

The next theorem is included only for completion purposes and is a consequence of G. Stampacchia's interpolation theorem [40]. Practically, it allows one to control the L^p norm of the gradient of the weak solution of a second order elliptic system with constant coefficients, for $p \in [2, \infty)$, by controlling the integrability of the data. We refer the interested reader to [4, Thm. 3.28, pp. 76] (and references therein) for a modern treatment on the subject. Our aim here is to apply the theorem below to the second order elliptic system with constant coefficients in (4.12) to obtain the necessary integrability for the homogenized solution to compensate for the remaining regularity that is needed in the classical corrector convergence theorem.

Theorem 4.1. *Let $u \in \mathrm{H}^1_0(\Omega, \mathbb{R}^3)$ be a weak solution of the Dirichlet problem*

$$-\mathrm{div}(\mathbb{A}\nabla u) = -\mathrm{div}\, \boldsymbol{F}, \tag{4.13}$$

where the constant coefficients $\mathbb{A}_{ij\alpha\beta}$ satisfy the Legendre-Hadamard condition, and $\boldsymbol{F} \in \mathrm{L}^p(\Omega, \mathbb{R}^3)$ for some $2 \le p < \infty$. Then, $\nabla u \in \mathrm{L}^p(\Omega, \mathbb{R}^{3\times 3})$ and

$$\|\nabla u\|_{\mathrm{L}^p(\Omega,\mathbb{R}^{3\times 3})} \le c\, \|\boldsymbol{F}\|_{\mathrm{L}^p(\Omega,\mathbb{R}^3)} \tag{4.14}$$

A proof of this theorem can be found in [26, Thm. 7.1, pp. 138] and [4, Thm. 3.29, pp. 79 and discussion on Sect. 3.5, pp. 78].

4.2. Proof of Theorem 3.2

Theorem 3.2. *Let u_ε and u be the unique minimizers of* (2.19) *and* (3.7)*, respectively. Moreover, for $\tilde{u}_1 \in \mathrm{L}^s(\Omega)$, let $f{:=}\mathrm{div}\, \boldsymbol{F}$, $\boldsymbol{F} \in \mathrm{L}^3(\Omega, \mathbb{R}^3)$ then,*

$$\nabla u_\varepsilon - \nabla u - \nabla_y \hat{u}(\cdot, \frac{\cdot}{\varepsilon}) \to 0 \text{ in } \mathrm{L}^2(\Omega, \mathbb{R}^3), \tag{3.10}$$

as $\varepsilon \to 0$ with

$$\hat{u}(\boldsymbol{x}, \boldsymbol{y}) = -w_k(\boldsymbol{y}) \frac{\partial u}{\partial x_k}(\boldsymbol{x}) + \tilde{u}_1(\boldsymbol{x}). \tag{3.11}$$

Proof. The main idea of the proof essentially amounts to a compensated regularity argument, where the burden of regularity is split (un-equally) between the local solution and the homogenized solution. We argue as follows: by the assumption on the body force f we can apply Theorem 4.1 and obtain $\nabla u \in \mathrm{L}^3(\Omega, \mathbb{R}^3)$. Moreover, since the local solution belongs in $\mathrm{H}^2_{\mathrm{per}}(Y)$, $w_k \in \mathrm{H}^2_{\mathrm{per}}(Y)$, we extend it by periodicity to the entire space. By applying standard Sobolev embedding theory we can obtain $\nabla_y w_k \in \mathrm{L}^6(\mathbb{R}^3, \mathbb{R}^3)$ (see e.g. [17, Theorem 2.31]). Therefore, the above compensated regularity argument makes the expression $\nabla u_\varepsilon - \nabla u - \nabla_y \hat{u}(\cdot, \frac{\cdot}{\varepsilon})$ well defined in the L^2 norm and hence, we can prove Proposition 9.12 in [10, pp. 185] directly. In what follows, we provide the actual steps of the argument that is given in [10, Proposition 9.12, pp. 185] with the appropriate adjustments that the second-gradient thermal effects introduce.

Embarking from the ellipticity of the second order tensor K we are led to,

$$
\begin{aligned}
& c_1 \left\| \nabla u_\varepsilon(\boldsymbol{x}) - \nabla u(\boldsymbol{x}) - \nabla_y \hat{u}(\boldsymbol{x}, \frac{\boldsymbol{x}}{\varepsilon}) \right\|^2_{L^2(\Omega,\mathbb{R}^3)} \\
& \leq \int_\Omega \mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon})(\nabla u_\varepsilon(\boldsymbol{x}) - \nabla u(\boldsymbol{x}) - \nabla_y \hat{u}(\boldsymbol{x}, \frac{\boldsymbol{x}}{\varepsilon})).(\nabla u_\varepsilon(\boldsymbol{x}) - \nabla u(\boldsymbol{x}) - \nabla_y \hat{u}(\boldsymbol{x}, \frac{\boldsymbol{x}}{\varepsilon}))\, d\boldsymbol{x} \\
& \leq \int_\Omega \mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon})(\nabla u_\varepsilon(\boldsymbol{x}) - \nabla u(\boldsymbol{x}) - \nabla_y \hat{u}(\boldsymbol{x}, \frac{\boldsymbol{x}}{\varepsilon})).(\nabla u_\varepsilon(\boldsymbol{x}) - \nabla u(\boldsymbol{x}) - \nabla_y \hat{u}(\boldsymbol{x}, \frac{\boldsymbol{x}}{\varepsilon}))\, d\boldsymbol{x} \\
& + \int_\Omega \mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon})(\varepsilon \nabla\nabla u_\varepsilon - \nabla_y \nabla_y \hat{u}(\boldsymbol{x}, \frac{\boldsymbol{x}}{\varepsilon})) : (\varepsilon \nabla\nabla u_\varepsilon - \nabla_y \nabla_y \hat{u}(\boldsymbol{x}, \frac{\boldsymbol{x}}{\varepsilon}))\, d\boldsymbol{x},
\end{aligned} \tag{4.15}
$$

where the last inequality is due to the ellipticity condition of the tensor M. Hence, opening up the expression above, using the structure of Eq (2.8), and the symmetry of the tensors K and M we have,

$$
\begin{aligned}
& c_1 \left\| \nabla u_\varepsilon(\boldsymbol{x}) - \nabla u(\boldsymbol{x}) - \nabla_y \hat{u}(\boldsymbol{x}, \frac{\boldsymbol{x}}{\varepsilon}) \right\|^2_{L^2(\Omega,\mathbb{R}^3)} \\
& \leq \int_\Omega f u_\varepsilon \, d\boldsymbol{x} - 2 \int_\Omega \mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon}) \nabla u_\varepsilon . (\nabla u + \nabla_y \hat{u}) d\boldsymbol{x} + \int_\Omega \mathsf{K}(\frac{\boldsymbol{x}}{\varepsilon})(\nabla u + \nabla_y \hat{u}).(\nabla u + \nabla_y \hat{u}) d\boldsymbol{x} \\
& -2 \int_\Omega \varepsilon \mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon}) \nabla\nabla u_\varepsilon : \nabla_y \nabla_y \hat{u} d\boldsymbol{x} + \int_\Omega \mathsf{M}(\frac{\boldsymbol{x}}{\varepsilon}) \nabla_y \nabla_y \hat{u} : \nabla_y \nabla_y \hat{u} d\boldsymbol{x}.
\end{aligned} \tag{4.16}
$$

By unfolding, we can see that we are able to pass to the limit in each expression due to estimate (2.17). Thus,

$$
\begin{aligned}
\lim_{\varepsilon \to 0} c_1 \left\| \nabla u_\varepsilon - \nabla u - \nabla_y \hat{u} \right\|^2_{L^2(\Omega,\mathbb{R}^3)} \leq & \int_{\Omega \times Y} f u d\boldsymbol{y} d\boldsymbol{x} \\
& - \int_{\Omega \times Y} \mathsf{K}(\boldsymbol{y})(\nabla u + \nabla_y \hat{u}).(\nabla u + \nabla_y \hat{u}) d\boldsymbol{y} d\boldsymbol{x} \\
& - \int_{\Omega \times Y} \mathsf{M}(\boldsymbol{y}) \nabla_y \nabla_y \hat{u} : \nabla_y \nabla_y \hat{u} d\boldsymbol{y} d\boldsymbol{x} = 0.
\end{aligned} \tag{4.17}
$$

On the last step we made use of Eq (4.10). □

5. Discussion

By enriching a microscopic model with higher-gradient contributions, we have obtained an upscaled Fourier's law of heat conduction, which exhibits thermal effects at varying length scales through the effective conductivity tensor. The inherent higher gradient regularity of the enriched microscopic model is transferred to the local problem, enabling us to use a compensated regularity argument and establish the classical corrector result in homogenization with less stringent regularity assumptions. By and large, we expect that the results can be extended to the time-dependent case, benefiting from the natural gradient flow structure of the problem (see [33]). Most likely the techniques of evolutionary Γ-convergence (see e.g., [29]) would be applicable. Naturally, the technique here can be extended to perforated domains by adjusting the unfolding operator as in [11]. The challenge is to handle interface terms.

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Conflict of interest

The authors declare there is no conflict of interest.

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