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Derivation of an effective model for a phase-field description of solid-liquid transformations in porous media

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Derivation of an effective model for a phase-field description of solid-liquid transformations in porous media

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A phase-field model to describe solid-liquid transformations in porous media is derived for microstructures of size $\varepsilon > 0$.

The existence of weak solutions for the micro-model and a-priori estimates are established, using an extension theorem for periodic functions on connected domains.

Finally, the microscale-model is homogenized via the method of two-scale convergence.

1 Introduction

The phase transition between ice and water is a major contributor to the damage to any structures which are exposed to the environment, and is amongst the most important effects to study when investigating the melting of the polar cap or of permafrost soils.

Basic mathematical models to describe phase transitions are the classical Stefan-problem (see e.g. [Meirmanov, 1992] or [Visintin, 1996]) and phase-field approximations of the Stefan-problem, cf. [Caginalp, 1986] or [Visintin, 1996].

Due to the discontinuous nature of the classical Stefan-problem, it is not very accessible by the usual solution theories for partial differential equations. The phase-field approximations, however, are of parabolic type and can therefore more easily be treated by mathematical analysis.

In this article, we consider phase-change in porous media, modeling e.g. the freezing of water in a concrete structure or the melting of ice in permafrost soil. Due to the aforementioned reasons, the phase-change will be described by phase-field models, in specific by the standard Caginalp phase-field model, see the references cited above.

The microstructure of porous media usually results in very high costs for numerical simulations. The method of mathematical homogenization can be used to derive models, which capture the effective behaviour of the problem, without describing the microstructure, thus yielding a model which can be treated numerically far more easy.

In this article, we present the homogenization of a phase-field model for phase transitions in porous media, via the method of two-scale convergence.

Homogenization of phase-field models for solid-liquid transitions has been studied in several works, amongst others see e.g. [Eck, 2004], [Heida, 2011].

But, to the knowledge of the authors, all homogenizations so far have been performed using the method of formal asymptotic expansion (for an introduction to that method see e.g. [Bensoussan et al., 1978]), and an approach of homogenization via two-scale convergence - as presented in this paper - has not been published so far.

2 The micro-scale model

2.1 Formulation of the microscopic problem

The classical Caginalp phase-field equation (coupled with a heat equation) reads as (cf. e.g. [Caginalp, 1986], [Visintin, 1996, p. 174])

$$\tau\chi' - \xi^2\Delta\chi - \frac{1}{2}(\chi - \chi^3) = 2\theta, \tag{1}$$

$$\theta' - K\Delta\theta + \frac{1}{2}l\chi' = 0. \tag{2}$$

In this article, we consider a porous medium which consists of a solid-matrix and a pore space, both of which we assume to be connected (see [Bear and Bachmat, 1984] for different types of porous media). The pore-space is assumed to be filled by some mixture of ice and water, such that the aforementioned phase-field model applies. Finally, this phase-field model with heat conduction in the pore-space is then coupled to a classical heat equation in the solid-matrix.

We make the following mathematical assumptions and constructions (this concept to model a porous medium in a homogenization setting is quite common, see e.g. [Peter, 2007]):

The whole porous body under consideration, e.g. a piece of concrete or some part of permafrost soil, is represented by a bounded Lipschitz-Domain $\Omega \subset \mathbb{R}^3$. To construct the porous microstructure, we at first consider a reference cell $Y := (0,1)^3$.

This reference cell is assumed to consist of two parts, the solid matrix $Z^{\mathrm{M}} \subset Y$ and the pore space $Z^{\mathrm{S}} \subset Y$ such that $\overline{Y} = \overline{Z^{\mathrm{M}}} \cup \overline{Z^{\mathrm{S}}}$ [1]. The interface between the two sub-regions of Y is denoted by $\Gamma := \partial Z^{\mathrm{M}} \cap \partial Z^{\mathrm{S}}$. Furthermore, we assume that both Z^{M} and Z^{S} are bounded Lipschitz-domains and chosen in such a way that all faces of Y are identical and both $Z^{\mathrm{M}} \subset Y$ and $Z^{\mathrm{S}} \subset Y$ are bounded Lipschitz-domains.

[1] Here the index S indicates that the Stefan-problem is modelled in the pore-space

The periodic microstructure of size ε is then constructed by scaled copies of that reference-cell: We define

$$\Omega_\varepsilon^{\mathrm{M}} := \Omega \cap \operatorname{int}\left(\bigcup_{k\in\mathbb{Z}^3} \varepsilon\overline{Z^{\mathrm{M}}{}_k}\right),$$

where $Z^{\mathrm{M}}{}_k$ denotes the translation of Z^{M} by $k \in \mathbb{Z}^3$, and analogously

$$\Omega_\varepsilon^{\mathrm{S}} := \Omega \cap \operatorname{int}\left(\bigcup_{k\in\mathbb{Z}^3} \varepsilon\overline{Z^{\mathrm{S}}{}_k}\right).$$

The periodic interface $\Gamma^\varepsilon := \partial\Omega_\varepsilon^{\mathrm{M}} \cap \partial\Omega_\varepsilon^{\mathrm{S}}$ between $\Omega_\varepsilon^{\mathrm{M}}$ and $\Omega_\varepsilon^{\mathrm{M}}$ is then given by

$$\Gamma^\varepsilon = \overline{\Omega} \cap \left(\bigcup_{k\in\mathbb{Z}^3} \varepsilon\Gamma_k\right).$$

We assume that both $\Omega_\varepsilon^{\mathrm{M}}$ as well as $\Omega_\varepsilon^{\mathrm{S}}$ are Lipschitz-domains for all $\varepsilon > 0$.

The outer boundaries of $\Omega_\varepsilon^{\mathrm{M}}$ and $\Omega_\varepsilon^{\mathrm{S}}$ are denoted by

$$\Gamma_\varepsilon^{\mathrm{M_{ext}}} := \partial\Omega \cap \partial\Omega_\varepsilon^{\mathrm{M}}$$

and

$$\Gamma_\varepsilon^{\mathrm{S_{ext}}} := \partial\Omega \cap \partial\Omega_\varepsilon^{\mathrm{S}}$$

respectively. Finally, let $S = (0, T)$ be a time intervall for some $T > 0$.

We can now state the micro-scale problem, where we assume Robin-boundary conditions for the heat-conduction on both the interface Γ^ε and the outer boundaries $\Gamma_\varepsilon^{\mathrm{M_{ext}}}, \Gamma_\varepsilon^{\mathrm{S_{ext}}}$. Heat exchange between the both regions is modelled, as well as between each region and the exterior (note that we chose to scale the interfacial heat-exchange via Γ^ε by the parameter ε and that we renamed the constants which appeared in equations (1) and (2)):

$$\begin{aligned}
\rho_{\mathrm{M}} u_\varepsilon' - \operatorname{div}(\kappa_{\mathrm{M}} \nabla u_\varepsilon) &= 0 && \text{in} \quad \Omega_\varepsilon^{\mathrm{M}} \times S, \\
\rho_{\mathrm{S}} \theta_\varepsilon' + \lambda \chi_\varepsilon' - \operatorname{div}(\kappa_{\mathrm{S}} \nabla \theta_\varepsilon) &= f && \text{in} \quad \Omega_\varepsilon^{\mathrm{S}} \times S, \\
\mu \chi_\varepsilon' - \operatorname{div}(\nu \nabla \chi_\varepsilon) + \omega_1 \chi_\varepsilon^3 - \omega_2 \chi_\varepsilon &= l\theta_\varepsilon && \text{in} \quad \Omega_\varepsilon^{\mathrm{S}} \times S,
\end{aligned}$$

with the boundary conditions

$$\begin{aligned}
-\kappa_{\mathrm{M}} \nabla u_\varepsilon \cdot \vec{n_{\mathrm{M}}} &= \kappa_{\mathrm{S}} \nabla \theta_\varepsilon \cdot \vec{n_{\mathrm{S}}} && \text{on} \quad \Gamma_\varepsilon \times S, \\
-\kappa_{\mathrm{M}} \nabla u_\varepsilon \cdot \vec{n_{\mathrm{M}}} &= \varepsilon \kappa_{RI} (u_\varepsilon - \theta_\varepsilon) && \text{on} \quad \Gamma_\varepsilon \times S, \\
-\kappa_{\mathrm{M}} \nabla u_\varepsilon \cdot \vec{n_{\mathrm{M}}} &= \kappa_{RE} (u_\varepsilon - \theta_{\mathrm{ext}}) && \text{on} \quad \Gamma_\varepsilon^{\mathrm{M_{ext}}} \times S, \\
-\kappa_{\mathrm{S}} \nabla \theta_\varepsilon \cdot \vec{n_{\mathrm{S}}} &= \kappa_{RE} (\theta_\varepsilon - \theta_{\mathrm{ext}}) && \text{on} \quad \Gamma_\varepsilon^{\mathrm{S_{ext}}} \times S, \\
-\nu \nabla \chi_\varepsilon \cdot \vec{n_{\mathrm{S}}} &= 0 && \text{on} \quad \partial\Omega_\varepsilon^{\mathrm{S}} \times S,
\end{aligned}$$

and the initial conditions

$$\begin{aligned} u_\varepsilon(0) &= u_{0\varepsilon}, \\ \theta_\varepsilon(0) &= \theta_{0\varepsilon}, \\ \chi_\varepsilon(0) &= \chi_{0\varepsilon}. \end{aligned}$$

2.2 Extension operators

In this section we introduce extension operators to extend functions on periodic domains to the whole domain Ω. These will be used to derive a-priori estimates and to handle the nonlinearity in the phase-field equation:

When passing to the limit in the homogenization process, we will need strong convergence of the phase-field variable χ_ε. As this variable is just defined on the periodic domain $\Omega_\varepsilon^{\mathrm{S}}$, it is not even clear how strong convergence could be defined. By the use of extension operators we can circumvent this problem.

For more information on extension operators and their applications, refer, e.g., to [Acerbi et al., 1992] or [Höpker and Böhm, 2014] and the references therein.

Theorem 2.1 (Extension-Operators)**.** *Let Ω be representable by a finite union of axis-parallel cuboids, each of which is assumed to have corner coordinates in $\mathbb{Q}^n$. Let $\varepsilon > 0$ be choosen such that the stretched domain $\frac{1}{\varepsilon}\Omega$ can be represented by a finite union of axis-parallel cuboids with corner coordinates in $\mathbb{Z}^n$.*

Then there exist families of linear operators

$$\begin{aligned} L_\varepsilon^{\mathrm{M}} &: W^{1,p}\left(\Omega_\varepsilon^{\mathrm{M}}\right) \to W^{1,p}(\Omega), \\ L_\varepsilon^{\mathrm{S}} &: W^{1,p}\left(\Omega_\varepsilon^{\mathrm{S}}\right) \to W^{1,p}(\Omega) \end{aligned}$$

such that for every $u_\varepsilon \in W^{1,p}\left(\Omega_\varepsilon^{\mathrm{M}}\right)$ respectively $u_\varepsilon \in W^{1,p}\left(\Omega_\varepsilon^{\mathrm{S}}\right)$

$$\begin{aligned} L_\varepsilon^{\mathrm{M}}(u_\varepsilon) &= u_\varepsilon \quad \text{on} \quad \Omega_\varepsilon^{\mathrm{M}}, \\ \left\| L_\varepsilon^{\mathrm{M}}(u_\varepsilon) \right\|_{W^{1,p}(\Omega)} &\leq C \left\| u_\varepsilon \right\|_{W^{1,p}(\Omega_\varepsilon^{\mathrm{M}})}, \\ &\textit{resp.} \\ L_\varepsilon^{\mathrm{S}}(u_\varepsilon) &= u_\varepsilon \quad \text{on} \quad \Omega_\varepsilon^{\mathrm{S}}, \\ \left\| L_\varepsilon^{\mathrm{S}}(u_\varepsilon) \right\|_{W^{1,p}(\Omega)} &\leq C \left\| u_\varepsilon \right\|_{W^{1,p}(\Omega_\varepsilon^{\mathrm{S}})}, \end{aligned}$$

where the constants $C > 0$ do not depend on ε.

Proof. This follows directly from the results of [Höpker and Böhm, 2014]. □

Lemma 2.2. *The operators constructed in 2.1 also act as extension operators on* L^2-*functions, i.e. for every* $u_\varepsilon \in \mathrm{L}^2\left(\Omega_\varepsilon^{\mathrm{M}}\right)$ *respectively* $u_\varepsilon \in \mathrm{L}^2\left(\Omega_\varepsilon^{\mathrm{S}}\right)$

$$
\begin{aligned}
L_\varepsilon^{\mathrm{M}}(u_\varepsilon) &= u_\varepsilon \quad \textit{on} \quad \Omega_\varepsilon^{\mathrm{M}}, \\
\left\| L_\varepsilon^{\mathrm{M}}(u_\varepsilon) \right\|_{\mathrm{L}^2(\Omega)} &\leq C \left\| u_\varepsilon \right\|_{\mathrm{L}^2(\Omega_\varepsilon^{\mathrm{M}})} \\
&\textit{resp.} \\
L_\varepsilon^{\mathrm{S}}(u_\varepsilon) &= u_\varepsilon \quad \textit{on} \quad \Omega_\varepsilon^{\mathrm{S}}, \\
\left\| L_\varepsilon^{\mathrm{S}}(u_\varepsilon) \right\|_{\mathrm{L}^2(\Omega)} &\leq C \left\| u_\varepsilon \right\|_{\mathrm{L}^2(\Omega_\varepsilon^{\mathrm{S}})}.
\end{aligned}
$$

Proof. This is clear from the proof of theorem 2.1: The local extension operator uses a reflection argument, that of course not just works for $W^{1,p}$-functions, but for L^2-functions as well. ☐

Corollary 2.3. *Under the assumptions of theorem 2.1, there exist families of linear operators*

$$
\begin{aligned}
\mathrm{L}_\varepsilon^{\mathrm{M}} : \left\{ u \in \mathrm{L}^2\left(S, W^{1,p}\left(\Omega_\varepsilon^{\mathrm{M}}\right)\right) | u' \in \mathrm{L}^2\left(S, \mathrm{L}^2\left(\Omega_\varepsilon^{\mathrm{M}}\right)\right) \right\} \\
\to \left\{ u \in \mathrm{L}^2(S, H^1(\Omega)) | u' \in \mathrm{L}^2(S, \mathrm{L}^2(\Omega)) \right\},
\end{aligned}
$$

and

$$
\begin{aligned}
\mathrm{L}_\varepsilon^{\mathrm{S}} : \left\{ u \in \mathrm{L}^2\left(S, W^{1,p}\left(\Omega_\varepsilon^{\mathrm{S}}\right)\right) | u' \in \mathrm{L}^2\left(S, \mathrm{L}^2\left(\Omega_\varepsilon^{\mathrm{S}}\right)\right) \right\} \\
\to \left\{ u \in \mathrm{L}^2(S, H^1(\Omega)) | u' \in \mathrm{L}^2(S, \mathrm{L}^2(\Omega)) \right\},
\end{aligned}
$$

which are bounded uniformly with respect to ε.

Proof. As the integral may be interchanged with linear continuous operators, it is easy to see that the extension of a derivative is the derivative of the extension. ☐

Assumption 2.4. *From now on, we will assume that* Ω *and* ε *either have the properties stated in the corollary above, or that* Ω *satisfies the abstract assumption that for every* ε *there exist extension operators which have the features of those of theorem 2.1, lemma 2.2 and corollary 2.3.*

2.3 Weak formulation of the microscopic problem

Let all the coefficients be positive constants and let $f \in \mathrm{L}^2(S \times \Omega)$. Assume that $\theta_{\text{ext}} \in \mathrm{L}^2\left(S, \mathrm{L}^2(\partial\Omega)\right)$ and that $\theta'_{\text{ext}} \in \mathrm{L}^\infty\left(S, \mathrm{L}^2(\partial\Omega)\right)$.

The weak problem is to find functions

$$
\begin{aligned}
u_\varepsilon &\in \mathrm{L}^2\left(S, H^1\left(\Omega_\varepsilon^{\mathrm{M}}\right)\right), \\
\theta_\varepsilon, \chi_\varepsilon &\in \mathrm{L}^2\left(S, H^1\left(\Omega_\varepsilon^{\mathrm{S}}\right)\right)
\end{aligned}
$$

with derivatives

$$\begin{aligned} u'_\varepsilon &\in \mathrm{L}^2\left(S, \mathrm{L}^2\left(\Omega_\varepsilon^{\mathrm{M}}\right)\right), \\ \theta'_\varepsilon, \chi'_\varepsilon &\in \mathrm{L}^2\left(S, \mathrm{L}^2\left(\Omega_\varepsilon^{\mathrm{S}}\right)\right) \end{aligned}$$

such that

$$\begin{aligned} &\int_{\Omega_\varepsilon^{\mathrm{M}}} \rho_{\mathrm{M}} u'_\varepsilon(t) v \mathrm{d}x + \int_{\Omega_\varepsilon^{\mathrm{M}}} \kappa_{\mathrm{M}} \nabla u_\varepsilon(t) \cdot \nabla v \mathrm{d}x \\ &\qquad + \varepsilon \int_{\Gamma^\varepsilon} \kappa_{RI}(u_\varepsilon(t) - \theta_\varepsilon(t)) v \mathrm{d}\sigma + \int_{\Gamma_\varepsilon^{\mathrm{M}_{\mathrm{ext}}}} \kappa_{RE} u_\varepsilon(t) v \mathrm{d}\sigma \\ &\qquad\qquad = \int_{\Gamma_\varepsilon^{\mathrm{M}_{\mathrm{ext}}}} \kappa_{RE} \theta_{\mathrm{ext}}(t) v \mathrm{d}\sigma \end{aligned}$$

for all $v \in H^1\left(\Omega_\varepsilon^{\mathrm{M}}\right)$ and a.a. $t \in S$,

$$\begin{aligned} &\int_{\Omega_\varepsilon^{\mathrm{S}}} \rho_{\mathrm{S}} \theta'_\varepsilon(t) v \mathrm{d}x + \int_{\Omega_\varepsilon^{\mathrm{S}}} \lambda \chi'_\varepsilon(t) v \mathrm{d}x + \int_{\Omega_\varepsilon^{\mathrm{S}}} \kappa_{\mathrm{S}} \nabla \theta_\varepsilon(t) \cdot \nabla v \mathrm{d}x \\ &\qquad + \varepsilon \int_{\Gamma^\varepsilon} \kappa_{RI}(\theta_\varepsilon(t) - u_\varepsilon(t)) v \mathrm{d}\sigma + \int_{\Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}} \kappa_{RE} \theta_\varepsilon(t) v \mathrm{d}\sigma \\ &\qquad\qquad = \int_{\Omega_\varepsilon^{\mathrm{S}}} f(t) v \mathrm{d}x + \int_{\Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}} \kappa_{RE} \theta_{\mathrm{ext}}(t) v \mathrm{d}\sigma \end{aligned}$$

for all $v \in H^1\left(\Omega_\varepsilon^{\mathrm{S}}\right)$ and a.a. $t \in S$,

$$\begin{aligned} &\int_{\Omega_\varepsilon^{\mathrm{S}}} \mu \chi'_\varepsilon(t) v \mathrm{d}x + \int_{\Omega_\varepsilon^{\mathrm{S}}} \nu \nabla \chi_\varepsilon(t) \cdot \nabla v \mathrm{d}x \\ &\qquad + \int_{\Omega_\varepsilon^{\mathrm{S}}} \omega_1 \chi_\varepsilon^3(t) v \mathrm{d}x - \int_{\Omega_\varepsilon^{\mathrm{S}}} \omega_2 \chi_\varepsilon(t) v \mathrm{d}x = \int_{\Omega_\varepsilon^{\mathrm{S}}} l \theta_\varepsilon(t) v \mathrm{d}x \end{aligned}$$

for all $v \in H^1\left(\Omega_\varepsilon^{\mathrm{S}}\right)$, a.a. $t \in S$ such that the initial conditions

$$\begin{aligned} u_\varepsilon(0) &= u_{0\varepsilon} \in H^1\left(\Omega_\varepsilon^{\mathrm{M}}\right), \\ \theta_\varepsilon(0) &= \theta_{0\varepsilon} \in H^1\left(\Omega_\varepsilon^{\mathrm{S}}\right), \\ \chi_\varepsilon(0) &= \chi_{0\varepsilon} \in H^1\left(\Omega_\varepsilon^{\mathrm{S}}\right). \end{aligned}$$

are satisfied.

Note that, as all considerations take place in the dimension $d = 3$, the embedding $H^1\left(\Omega_\varepsilon^{\mathrm{S}}\right) \hookrightarrow \mathrm{L}^6\left(\Omega_\varepsilon^{\mathrm{S}}\right)$ is continuous and therefore $\chi^3 \in \mathrm{L}^2\left(\Omega_\varepsilon^{\mathrm{S}}\right)$ for all $\chi \in H^1\left(\Omega_\varepsilon^{\mathrm{S}}\right)$. Thus the integrals above are well defined.

Theorem 2.5. *Assume that*

$$\left\|u_{0\varepsilon}\right\|_{H^1(\Omega_\varepsilon^{\mathrm{M}})}, \left\|\theta_{0\varepsilon}\right\|_{H^1(\Omega_\varepsilon^{\mathrm{S}})}, \left\|\chi_{0\varepsilon}\right\|_{H^1(\Omega_\varepsilon^{\mathrm{S}})} \leq C$$

and

$$\varepsilon \int_{\Gamma^\varepsilon} (u_{0\varepsilon} - \theta_{0\varepsilon})^2 \mathrm{d}\sigma \leq C.$$

Then there exist solutions

$$\begin{aligned} u_\varepsilon &\in \mathrm{L}^\infty\left(S, H^1\left(\Omega_\varepsilon^{\mathrm{M}}\right)\right) \cap \mathrm{H}^1\left(S, \mathrm{L}^2\left(\Omega_\varepsilon^{\mathrm{M}}\right)\right), \\ \theta_\varepsilon &\in \mathrm{L}^\infty\left(S, H^1\left(\Omega_\varepsilon^{\mathrm{S}}\right)\right) \cap \mathrm{H}^1\left(S, \mathrm{L}^2\left(\Omega_\varepsilon^{\mathrm{M}}\right)\right), \\ \chi_\varepsilon &\in \mathrm{L}^\infty\left(S, H^1\left(\Omega_\varepsilon^{\mathrm{S}}\right)\right) \cap \mathrm{H}^1\left(S, \mathrm{L}^2\left(\Omega_\varepsilon^{\mathrm{M}}\right)\right) \end{aligned}$$

to the weak problem which satisfy the a-priori estimates

$$\|u_\varepsilon\|_{\mathrm{L}^\infty(S,H^1(\Omega_\varepsilon^{\mathrm{M}}))}, \|\theta_\varepsilon\|_{\mathrm{L}^\infty(S,H^1(\Omega_\varepsilon^{\mathrm{S}}))}, \|\chi_\varepsilon\|_{\mathrm{L}^\infty(S,H^1(\Omega_\varepsilon^{\mathrm{S}}))} \leq C$$

and

$$\left\|{u_\varepsilon}'\right\|_{\mathrm{L}^2(S,\mathrm{L}^2(\Omega_\varepsilon^{\mathrm{M}}))}, \left\|{\theta_\varepsilon}'\right\|_{\mathrm{L}^2(S,\mathrm{L}^2(\Omega_\varepsilon^{\mathrm{S}}))}, \left\|{\chi_\varepsilon}'\right\|_{\mathrm{L}^2(S,\mathrm{L}^2(\Omega_\varepsilon^{\mathrm{S}}))} \leq C.$$

Proof. The proof is an adaption and extension of the proofs of the theorems 2.1 and 2.2. in [Schimperna, 2000] to the setting of porous media.

Though we can proceed quite similar to [Schimperna, 2000], we have to take special care of the estimates, as we will need the a-priori estimates independently of ε.

In this paper, we will abstain from presenting the complete proof of existence and derivation of the a-priori estimates. That proof is quite long and contains many detailed estimates. It will be presented in whole in a forthcoming publication.

We will, however, comment on one important estimate which makes use of the extension operators:

There exists a constant C, independently of ε, such that for all $v \in H^1\left(\Omega_\varepsilon^{\mathrm{M}}\right)$ the estimate

$$\|v\|_{\mathrm{L}^2\left(\Gamma_\varepsilon^{\mathrm{M}_{\mathrm{ext}}}\right)} \leq C\,\|v\|_{H^1(\Omega_\varepsilon^{\mathrm{M}})}$$

holds.

To prove this estimate, we use the extension operator $\mathrm{L}_\varepsilon : H^1\left(\Omega_\varepsilon^{\mathrm{M}}\right) \to H^1(\Omega)$, whose norm is independent of ε. With this extension operator at hand, we can estimate

$$\|v\|_{\mathrm{L}^2\left(\Gamma_\varepsilon^{\mathrm{M}_{\mathrm{ext}}}\right)} = \|\mathrm{L}_\varepsilon(v)\|_{\mathrm{L}^2\left(\Gamma_\varepsilon^{\mathrm{M}_{\mathrm{ext}}}\right)} \leq \|\mathrm{L}_\varepsilon(v)\|_{\mathrm{L}^2(\partial\Omega)} \leq C\,\|\mathrm{L}_\varepsilon(v)\|_{H^1(\Omega)}$$

where in the last inequality we used the continuity of the trace operator $\gamma : H^1(\Omega) \to \mathrm{L}^2(\partial\Omega)$ which is independent of ε. By the boundedness of the extension operator L_ε, independently of ε, we can now deduce the desired estimate

$$\|v\|_{\mathrm{L}^2\left(\Gamma_\varepsilon^{\mathrm{M}_{\mathrm{ext}}}\right)} \leq C\,\|\mathrm{L}_\varepsilon(v)\|_{H^1(\Omega)} \leq \widehat{C}\,\|v\|_{H^1(\Omega_\varepsilon^{\mathrm{M}})}.$$

□

3 Homogenization

3.1 Preliminaries

With the a-priori estimates from theorem 2.5 at hand, passing to the limit in the volume terms and on the the internal boundary Γ^ε can be done similarly as in [Peter, 2007].

To deal with the limit of the integrals on the outer boundaries $\Gamma_\varepsilon^{\mathrm{M}_{\mathrm{ext}}}$ and $\Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}$ of the ε-periodic domains, we prove a result on the weak convergence of the respective characeristic functions, which (in the case of 'cuboidal domains', see the assumptions in theorem 2.1), provides us with an explicit expression for the limit.

We use the fact, that, as time appears just as a parameter, all theorems for stationary two-scale convergence can easily be transfered to the time-dependent case.

We use the extension operators from corollary 2.3 to find extensions

$$\begin{aligned}\widehat{u_\varepsilon} &\in \mathrm{L}^2\left(S, H^1(\Omega)\right),\\ \widehat{\theta_\varepsilon} &\in \mathrm{L}^2\left(S, H^1(\Omega)\right),\\ \widehat{\chi_\varepsilon} &\in \mathrm{L}^\infty\left(S, H^1(\Omega)\right),\end{aligned}$$

where

$$\begin{aligned}\widehat{u_\varepsilon}' &\in \mathrm{L}^2\left(S, \mathrm{L}^2(\Omega)\right),\\ \widehat{\theta_\varepsilon}' &\in \mathrm{L}^2\left(S, \mathrm{L}^2(\Omega)\right),\\ \widehat{\chi_\varepsilon}' &\in \mathrm{L}^2\left(S, \mathrm{L}^2(\Omega)\right).\end{aligned}$$

The boundedness of the extension operator implies that the extended functions remain bounded independently of ε.

3.2 Convergence on the outer boundary

3.2.1 General observations

We consider the characteristic function $\mathbb{1}_{\Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}}$ of the outer boundary of $\Omega_\varepsilon^{\mathrm{S}}$. For now we call $\Omega_\varepsilon^{\mathrm{S}}$ the pore part of Ω. Obviously $\mathbb{1}_{\Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}} \in \mathrm{L}^2(\partial\Omega)$ is bounded independently of ε. Thus there exists a subsequence and a function $g \in \mathrm{L}^2(\partial\Omega)$ such that $\mathbb{1}_{\Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}} \rightharpoonup g$. The pore part of the area of each surface-measurable set $A \subset \partial\Omega$ can be calculated by

$$\mu_\varepsilon^S(A) := \left|A \cap \Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}\right| = \int_{\partial\Omega} \mathbb{1}_A \mathbb{1}_{\Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}} \mathrm{d}\sigma = \int_A \mathbb{1}_{\Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}} \mathrm{d}\sigma.$$

Thus $\mathbb{1}_{\Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}}$ is the Radon-Nikodym density of the surface-porosity measure. The weak convergence implies that

$$\lim_{\varepsilon\to 0} \mu_\varepsilon^S(A) = \lim_{\varepsilon\to 0} \int_A \mathbb{1}_{\Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}} \mathrm{d}\sigma = \int_A g \mathrm{d}\sigma =: \mu^S(A).$$

As the set $\{u \in \mathrm{L}^2(\partial\Omega) : 0 \le u \le 1\}$ is obviously closed and convex, it is also weakly closed. Thus $0 \le g \le 1$.

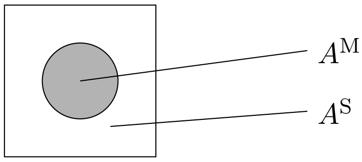

Figure 1: Schematic of one face of the unit-cell

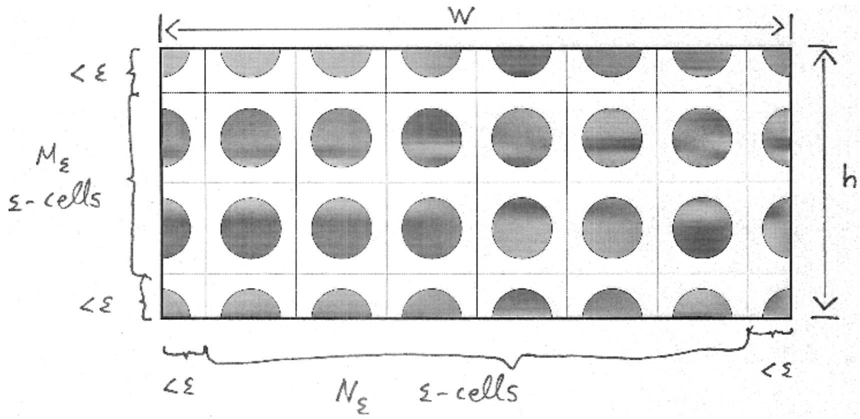

Figure 2: A rectangle R on one face of Ω

Hence the function g can be interpreted as the Radon-Nikodym density of the homogenized surface-porosity measure μ^S.

We can, of course, make a similar observation for $\mathbb{1}_{\Gamma_\varepsilon^{\mathrm{M}_{\mathrm{ext}}}}$.

3.2.2 A convergence theorem

Theorem 3.1. *Let Ω and ε be given as in the assumptions of the extension theorem 2.1. Then the weak convergences*

$$\begin{aligned} \chi_{\Gamma^{\mathrm{M}}_{ext_\varepsilon}} &\rightharpoonup \left|A^{\mathrm{M}}\right| \quad in \quad \mathrm{L}^2\left(S, \mathrm{L}^2(\partial\Omega)\right), \\ \chi_{\Gamma^{\mathrm{S}}_{ext_\varepsilon}} &\rightharpoonup \left|A^{\mathrm{S}}\right| \quad in \quad \mathrm{L}^2\left(S, \mathrm{L}^2(\partial\Omega)\right), \end{aligned}$$

of the characteristic functions of the outer boundaries $\Gamma_\varepsilon^{\mathrm{M}_{\mathrm{ext}}}$ and $\Gamma_\varepsilon^{\mathrm{S}_{\mathrm{ext}}}$ hold, where A^{M}, respectively A^{S}, denote the outer boundaries of Z^{M} and Z^{S} on one face of the unit cell (see figure 1).

Proof. Due to the assumptions of theorem 2.1, for every $\varepsilon > 0$, there exists a finite set I_ε such that $\partial\Omega = \bigcup_{i\in I_\varepsilon} A_\varepsilon^i$, where each A_ε^i is one face of a ε-scaled and translated unit-cell, and the A_ε^i are mutually disjoint.

The area of the outer boundary $\Gamma_\varepsilon^{\mathrm{M}_{\mathrm{ext}}}$ on each such face is given by $\left|A^{\mathrm{M}}\right| \varepsilon^2$.

Let R be an admissable rectangle on one of the faces of Ω, i.e. its sides are parallel to the edges of Ω. Let $2\varepsilon < \min\{w, h\}$, where w is the width of R and h its height.

Then there are $N_\varepsilon \cdot M_\varepsilon$ faces of ε-cells in R, such that $N_\varepsilon \varepsilon = w - \eta_\varepsilon^1$, where $\eta_\varepsilon^1 < 2\varepsilon$ (otherwise we could fit in another column of ε-cells) and $M_\varepsilon \varepsilon = h - \eta_\varepsilon^2$, where $\eta_\varepsilon^2 < 2\varepsilon$. For a visualization see figure 2.

The area of the outer boundary $\Gamma_\varepsilon^{\mathrm{M}_{\mathrm{ext}}}$ in R is then given by

$$\left|\Gamma^{\mathrm{M}}_{\mathrm{ext}_\varepsilon} \cap R\right| = N_\varepsilon \cdot M_\varepsilon \cdot \left|A^{\mathrm{M}}\right| \varepsilon^2 + \mathrm{rest}(\varepsilon)$$

where $|\mathrm{rest}(\varepsilon)| \leq h\eta_\varepsilon^1 + w\eta_\varepsilon^2 < 2h\varepsilon + 2w\varepsilon \to 0$. Hence

$$\left|\Gamma^{\mathrm{M}}_{\mathrm{ext}_\varepsilon} \cap R\right| = (w - \eta_\varepsilon^1) \cdot (h - \eta_\varepsilon^2) \cdot \left|A^{\mathrm{M}}\right| + \mathrm{rest}(\varepsilon) \to wh \left|A^{\mathrm{M}}\right| = \left|A^{\mathrm{M}}\right| |R|.$$

Thus

$$\int_{\partial\Omega} \chi_{\Gamma^{\mathrm{M}}_{\mathrm{ext}_\varepsilon}} \chi_R \mathrm{d}\sigma \to \int_{\partial\Omega} \left|A^{\mathrm{M}}\right| \chi_R \mathrm{d}\sigma$$

Let ϕ be a step-function on $\partial\Omega$. W.l.o.g there is a finite amount of admissable rectangles R_i such that

$$\phi = \sum_i \alpha_i \chi_{R_i}.$$

We calculate

$$\int_{\partial\Omega} \chi_{\Gamma^{\mathrm{M}}_{\mathrm{ext}_\varepsilon}} \phi \mathrm{d}\sigma = \sum_i \alpha_i \int_{\partial\Omega} \chi_{\Gamma^{\mathrm{M}}_{\mathrm{ext}_\varepsilon}} \chi_{R_i} \mathrm{d}\sigma \to \sum_i \alpha_i \int_{\partial\Omega} \left|A^{\mathrm{M}}\right| \chi_{R_i} \mathrm{d}\sigma = \int_{\partial\Omega} \left|A^{\mathrm{M}}\right| \phi \mathrm{d}\sigma$$

We have thus verified the weak-convergence condition on a dense subset of $\mathrm{L}^2(\partial\Omega)$. Since the sequence $\chi_{\Gamma^{\mathrm{M}}_{\mathrm{ext}_\varepsilon}}$ is bounded in $\mathrm{L}^2(\partial\Omega)$, this is sufficient for the weak convergence

$$\chi_{\Gamma^{\mathrm{M}}_{\mathrm{ext}_\varepsilon}} \rightharpoonup \left|A^{\mathrm{M}}\right| \quad \text{in} \quad \mathrm{L}^2(\partial\Omega).$$

Again, by first using stepfunctions, one can easily show that

$$\chi_{\Gamma^{\mathrm{M}}_{\mathrm{ext}_\varepsilon}} \rightharpoonup \left|A^{\mathrm{M}}\right| \quad \text{in} \quad \mathrm{L}^2\left(S, \mathrm{L}^2(\partial\Omega)\right).$$

Of course, by similar arguments it can be shown that the result also holds for $\chi_{\Gamma^{\mathrm{S}}_{\mathrm{ext}_\varepsilon}}$. □

Assumption 3.2. *For the rest of this article, we assume that the geometry is given as in the assumptions of theorem 2.1. This simplifies the homogenized problem as the limits of the characteristic functions of the external boundaries are explicitely known.*

3.3 Two-scale convergence

To pass to the limit in the microscale equations, we will use the notion of two-scale convergence. The foundations of two-scale convergence have been established in [Nguetseng, 1989] and have then been further developed and formalized in [Allaire, 1992].

We define the periodic Sobolev space $W^{1,2}_{\#}(Y)$ as the closure of $C^{\infty}_{\#}\left(\overline{Y}\right)$ - the space of smooth and Y-periodic functions - with respect to the $W^{1,2}$-norm. Furthermore we denote by $W^{1,2}_{\overline{\#}}(Y)$ the space of those functions $u \in W^{1,2}_{\#}(Y)$ which have zero mean-value.

We now introduce the notion of two-scale convergence for time-dependent sequences (see e.g. [Peter, 2007] or [Pavliotis and Stuart, 2008]):

Definition 3.3. *A sequence u_ε in $\mathrm{L}^p(S \times \Omega)$ is said to two-scale converge to $u \in \mathrm{L}^p(S \times \Omega \times Y)$ if*

$$\lim_{\varepsilon \to 0} \int_S \int_\Omega u_\varepsilon(t,x)\phi\left(t,x,\frac{x}{\varepsilon}\right) \mathrm{d}x\mathrm{d}t = \int_S \int_\Omega \int_Y u(t,x,y)\phi(t,x,y)\mathrm{d}y\mathrm{d}x\mathrm{d}t \tag{3}$$

for all testfunctions $\phi \in \mathrm{L}^{p'}\left(S \times \Omega, C_{\#}\left(\overline{Y}\right)\right)$, where $C_{\#}\left(\overline{Y}\right)$ denotes the space of continuous and Y-periodic functions. We use the notation $u_\varepsilon \stackrel{2}{\rightarrow} u$.

The following theorem provides some important results about two-scale convergence:

Theorem 3.4. *1. Two-scale convergent sequences are bounded.*

2. For every bounded sequence u_ε in $\mathrm{L}^2(S \times \Omega)$ there exists a subsequence ε and an element $u \in \mathrm{L}^2(S \times \Omega \times Y)$ such that

$$u_\varepsilon \stackrel{2}{\rightarrow} u.$$

3. Let $u_\varepsilon \in \mathrm{L}^2(S, H^1(\Omega))$ be a bounded sequence. Then there exist a subsequence ε as well as functions $u \in \mathrm{L}^2(S, H^1(\Omega)), u_1 \in \mathrm{L}^2\left(S \times \Omega, W^{1,2}_{\overline{\#}}(Y)\right)$ which satisfy

$$\begin{aligned} u_\varepsilon &\rightharpoonup u \ \textit{in}\ \mathrm{L}^2(S, H^1(\Omega)),\\ u_\varepsilon &\stackrel{2}{\rightarrow} u,\\ \nabla_x u_\varepsilon &\stackrel{2}{\rightarrow} \nabla_x u + \nabla_y u_1. \end{aligned}$$

Proof. See e.g. [Lukkassen et al., 2002], where the theorem is proven for stationary two-scale convergence. However, as time enters two-scale convergence merely as a parameter, the results can directly be adapted to the time-dependent setting. □

The following result is part of [Allaire et al., 1995, proposition 2.6], again extended to time dependent functions:

Theorem 3.5. *Let u_ε be a sequence of functions in $\mathrm{L}^2\left(S, H^1(\Omega)\right)$ such that*

$$\|u_\varepsilon\|_{\mathrm{L}^2(S,\mathrm{L}^2(\Omega))} + \varepsilon \|\nabla u_\varepsilon\|_{\mathrm{L}^2(S,\mathrm{L}^2(\Omega))} \leq C.$$

Then, the estimate

$$\varepsilon \int_S \int_{\Gamma^\varepsilon} |u_\varepsilon(t,\sigma)|^2 \mathrm{d}\sigma\mathrm{d}t \leq C$$

holds, and, up to a subsequence

$$\lim_{\varepsilon\to 0} \varepsilon \int_S \int_{\Gamma_\varepsilon} u_\varepsilon \phi^\varepsilon \mathrm{d}\sigma\mathrm{d}t = \int_S \int_\Omega \int_\Gamma u_0(t,x,\sigma)\phi(t,x,\sigma)\mathrm{d}\sigma\mathrm{d}x\mathrm{d}t$$

for all $\phi(t,x,y) \in C_0^\infty\left(S, C^\infty\left(\bar{\Omega}; C_\#^\infty(Y)\right)\right)$ *where* u_0 *is the trace on* Γ *of the two-scale limit of* u_ε *(that exists in* $\mathrm{L}^2\left(S\times\Omega, W_\#^{1,2}(Y)\right)$ *by part (ii) of [Allaire, 1992, proposition 1.14]).*

3.4 Passing to the limit

We consider exemplary the sequence $\widehat{\chi_\varepsilon}$, which is bounded in $\mathrm{L}^2\left(S, H^1(\Omega)\right)$. Thus there exist - according to theorem 3.4 - a subsequence as well as functions $\chi \in \mathrm{L}^2\left(S, H^1(\Omega)\right)$ and $\chi_1 \in \mathrm{L}^2\left(S\times\Omega, W_\#^{1,2}(Y)\right)$ such that

$$\begin{aligned} \widehat{\chi_\varepsilon} &\xrightarrow{2} \chi, \\ \nabla\widehat{\chi_\varepsilon} &\xrightarrow{2} \nabla_x\chi + \nabla_y\chi_1, \\ \widehat{\chi_\varepsilon} &\rightharpoonup \chi \quad \text{in} \quad \mathrm{L}^2\left(S, H^1(\Omega)\right), \\ \widehat{\chi_\varepsilon}' &\rightharpoonup \chi' \quad \text{in} \quad \mathrm{L}^2\left(S, \mathrm{L}^2(\Omega)\right). \end{aligned}$$

Analogous convergences hold for the extensions $\widehat{u_\varepsilon}$,$\widehat{\theta_\varepsilon}$ of u_ε and θ_ε respectively.

Lemma 3.6. *The following holds for the limit* χ*:*

$$\begin{aligned} \chi &\in \mathrm{L}^6(S\times\Omega), \\ \widehat{\chi_\varepsilon}^3 &\xrightarrow{2} \chi^3 \quad \mathit{in} \quad \mathrm{L}^{\frac{4}{3}}(S\times\Omega). \end{aligned}$$

up to a subsequence.

Proof. As $H^1(\Omega) \hookrightarrow\hookrightarrow \mathrm{L}^4(\Omega)$ (compact embedding), we have by the Lions-Aubin Lemma (cf. [Simon, 1986]) the existence of a further subsequence such that

$$\widehat{\chi_\varepsilon} \to \psi \quad \text{in} \quad \mathrm{L}^4(S\times\Omega)$$

for some $\psi \in \mathrm{L}^4(S\times\Omega)$. But as this convergence also holds in $\mathrm{L}^2(S\times\Omega)$ and strong convergence implies two-scale convergence (see e.g. [Lukkassen et al., 2002]), we have that

$$\psi = \chi.$$

Additionally we know that $\widehat{\chi_\varepsilon}$ is bounded in $\mathrm{L}^6(S\times\Omega)$ (continuity of embedding operator, but not compact for $q=6$). Hence there exists a weakly convergent subsequence

$$\widehat{\chi_\varepsilon} \rightharpoonup \mu \quad \text{in} \quad \mathrm{L}^6(S\times\Omega)$$

and thus also

$$\widehat{\chi_\varepsilon} \rightharpoonup \mu \quad \text{in} \quad \mathrm{L}^4(S \times \Omega).$$

By uniqueness of the weak limit this implies that $\chi = \mu$ and hence

$$\chi \in \mathrm{L}^6(S \times \Omega).$$

The strong convergence in $\mathrm{L}^4(S \times \Omega)$ finally implies

$$\widehat{\chi_\varepsilon}^3 \to \chi^3 \quad \text{in} \quad \mathrm{L}^{\frac{4}{3}}(S \times \Omega)$$

and thus

$$\widehat{\chi_\varepsilon}^3 \overset{2}{\to} \chi^3 \quad \text{in} \quad \mathrm{L}^{\frac{4}{3}}(S \times \Omega).$$

□

We state a convergence result for the traces of the extensions:

Lemma 3.7. *There exists a subsequence such that*

$$\widehat{u_\varepsilon} \to u \quad \textit{in} \quad \mathrm{L}^2(S \times \partial\Omega)$$

and a similar result holds for the sequence $\widehat{\theta_\varepsilon}$.

Proof. The functions $\widehat{u_\varepsilon}$ are bounded in the space

$$\mathcal{W} := \left\{ u \in \mathrm{L}^2(S, H^1(\Omega)) : u' \in \mathrm{L}^2(S, \mathrm{L}^2(\Omega)) \right\},$$

hence there exists a weakly convergent subsequence $\widehat{u_\varepsilon} \rightharpoonup w$ in $\mathcal{W}$, for some $w \in \mathcal{W}$. For every $v \in \mathrm{L}^2(S, H^{-1}(\Omega))$, $\langle F, u \rangle := \langle v, u \rangle$ defines a linear, continuous functional on $\mathcal{W}$. Thus

$$\langle v, \widehat{u_\varepsilon} \rangle \to \langle v, w \rangle \quad \forall v \in \mathrm{L}^2(S, H^{-1}(\Omega))$$

which, by definition, implies

$$\widehat{u_\varepsilon} \rightharpoonup w \quad \text{in} \quad \mathrm{L}^2(S, H^1(\Omega)).$$

By the uniqueness of the weak limit this implies $w = u$, i.e.

$$\widehat{u_\varepsilon} \rightharpoonup u \quad \text{in} \quad \mathcal{W}.$$

The compactness of the trace operator $\gamma : \mathcal{W} \to \mathrm{L}^2\left(S, \mathrm{L}^2(\partial\Omega)\right)$ (see Siegfried Carl, Nonsmooth Variational Problems and their Inequalities) now implies that the traces of the functions converge strongly in $\mathrm{L}^2\left(S, \mathrm{L}^2(\partial\Omega)\right)$, i.e.

$$\widehat{u_\varepsilon} \to u \quad \text{in} \quad \mathrm{L}^2(S \times \partial\Omega).$$

Of course, the same argumentation can be done for the sequence $\widehat{\theta_\varepsilon}$. □

The following lemma will allow us to pass to the limit on the interface Γ^ε:

Lemma 3.8. *For every $\phi_0(t,x) \in C_0^\infty\left(S, C^\infty\left(\bar{\Omega}\right)\right)$ and the sequences of extended functions $\widehat{u_\varepsilon}$ and $\widehat{\theta}_\varepsilon$ we have the convergence*

$$\lim_{\varepsilon\to 0} \varepsilon \int_S \int_{\Gamma_\varepsilon} \left(\widehat{u_\varepsilon}(t,\sigma) - \widehat{\theta}_\varepsilon(t,\sigma)\right) \phi_0(t,\sigma) \mathrm{d}\sigma \mathrm{d}t = |\Gamma| \int_S \int_\Omega \left(u(t,x) - \theta(t,x)\right) \phi_0(t,x) \mathrm{d}x \mathrm{d}t.$$

Proof. From theorem 3.5, we can deduce, as the two-scale limit of the temperature $\widehat{u_\varepsilon}$, as well as ϕ_0, do not depend on y, that

$$\lim_{\varepsilon\to 0} \varepsilon \int_S \int_{\Gamma_\varepsilon} \widehat{u_\varepsilon}(t,\sigma)\phi_0(t,\sigma) \mathrm{d}\sigma \mathrm{d}t = |\Gamma| \int_S \int_\Omega u(t,x)\phi_0(t,x) \mathrm{d}x \mathrm{d}t$$

and analogous for $\widehat{\theta}_\varepsilon$. This directly implies the claim. □

Define the space $C_\#^\infty\left(\overline{Z^{\mathrm{M}}}\right)$ as the 1-periodic C^∞-functions on the 1-periodic extension of $\overline{Z^{\mathrm{M}}}$.

We now choose testfunctions

$$\begin{aligned} \phi_0(t,x) &\in C_0^\infty\left(S, C^\infty\left(\bar{\Omega}\right)\right), \\ \phi_{1,\mathrm{M}}(t,x,y) &\in C_0^\infty\left(S, C^\infty\left(\bar{\Omega}; C_\#^\infty\left(\overline{Z^{\mathrm{M}}}\right)\right)\right). \end{aligned}$$

Obviously, the function (where we extended $\phi_{1,\mathrm{M}}$ by 0 outside of Z^{M})

$$\mathbb{1}_{Z^{\mathrm{M}}}(y)\phi_{1,\mathrm{M}}(t,x,y)$$

is Y-periodic (for fixed (t,x)) and continuous - even smooth - in (t,x), for fixed y. Hence, by [Zhikov, 2004], it can be used as a two-scale testfunction.

The unit cell $Y = (0,1)^3$ can be decomposed into the two parts Z^{M} and Z^{S} which we identify with their 1-periodic extensions. To be precise, by the periodic extension we mean the set

$$\operatorname{int}\left(\bigcup_{k\in\mathbb{Z}^3} \overline{Z^{\mathrm{M}}{}_k}\right).$$

Thus

$$x \in \Omega_\varepsilon^{\mathrm{M}} \Leftrightarrow \left(\frac{x}{\varepsilon} \in Z^{\mathrm{M}}, x \in \Omega\right)$$

and hence

$$\mathbb{1}_{\Omega_\varepsilon^{\mathrm{M}}}(x) = \mathbb{1}_{Z^{\mathrm{M}}}\left(\frac{x}{\varepsilon}\right) \quad \text{for all } x \in \Omega.$$

Completely analogous we define $\phi_{1,\mathrm{S}}$ and $\mathbb{1}_{Z^{\mathrm{S}}}$.

We now test the weak formulation of the microscopic with the testfunction

$$\phi_0(t,x) + \varepsilon\phi_{1,\mathrm{M}}\left(t,x,\frac{x}{\varepsilon}\right) = \phi_0 + \varepsilon\phi_{1,\mathrm{M}}^\varepsilon$$

respectively

$$\phi_0(t,x) + \varepsilon\phi_{1,\mathrm{S}}\left(t,x,\frac{x}{\varepsilon}\right) = \phi_0 + \varepsilon\phi_{1,\mathrm{S}}^\varepsilon$$

and integrate over time.

The first equation reads

$$\begin{aligned}\int_S\int_\Omega \rho_{\mathrm{M}} \widehat{u_\varepsilon}' \mathbb{1}_{Z^{\mathrm{M}}}\left(\frac{x}{\varepsilon}\right)\left(\phi_0+\varepsilon\phi_{1,\mathrm{M}}^\varepsilon\right)\mathrm{d}x\mathrm{d}t\\ +\int_S\int_\Omega \kappa_{\mathrm{M}}\nabla\widehat{u_\varepsilon}\mathbb{1}_{Z^{\mathrm{M}}}\left(\frac{x}{\varepsilon}\right)\cdot\left(\nabla_x\phi_0+\nabla_y\phi_{1,\mathrm{M}}^\varepsilon+\varepsilon\nabla_x\phi_{1,\mathrm{M}}^\varepsilon\right)\mathrm{d}x\mathrm{d}t\\ +\varepsilon\int_S\int_{\Gamma_\varepsilon}\kappa_{RI}\left(\widehat{u_\varepsilon}-\widehat{\theta_\varepsilon}\right)\left(\phi_0+\varepsilon\phi_{1,\mathrm{M}}^\varepsilon\right)\mathrm{d}\sigma\mathrm{d}t+\int_S\int_{\partial\Omega}\kappa_{RE}\widehat{u_\varepsilon}\mathbb{1}_{\Gamma_\varepsilon^{\mathrm{M}}\mathrm{ext}}\left(\phi_0+\varepsilon\phi_{1,\mathrm{M}}^\varepsilon\right)\mathrm{d}\sigma\mathrm{d}t\\ =\int_S\int_{\partial\Omega}\kappa_{RE}\theta_{\mathrm{ext}}\mathbb{1}_{\Gamma_\varepsilon^{\mathrm{M}}\mathrm{ext}}\left(\phi_0+\varepsilon\phi_{1,\mathrm{M}}^\varepsilon\right)\mathrm{d}\sigma\mathrm{d}t.\end{aligned}$$

First, we consider the term with the time-derivative and calculate

$$\begin{aligned}\int_S\int_{\Omega_\varepsilon^{\mathrm{M}}}\rho_{\mathrm{M}}u_\varepsilon'\phi_0(t,x)\mathrm{d}x\mathrm{d}t &= -\int_S\int_{\Omega_\varepsilon^{\mathrm{M}}}\rho_{\mathrm{M}}u_\varepsilon\phi_0'(t,x)\mathrm{d}x\mathrm{d}t\\ &= -\int_S\int_\Omega\rho_{\mathrm{M}}\widehat{u_\varepsilon}\mathbb{1}_{Z^{\mathrm{M}}}\left(\frac{x}{\varepsilon}\right)\phi_0'(t,x)\mathrm{d}x\mathrm{d}t\\ &\to -\int_S\int_\Omega\int_Y\rho_{\mathrm{M}}u(t,x)\chi_{Z^{\mathrm{M}}}(y)\phi_0'(t,x)\mathrm{d}y\mathrm{d}x\mathrm{d}t\\ &= -\left|Z^{\mathrm{M}}\right|\int_S\int_\Omega\rho_{\mathrm{M}}u(t,x)\phi_0'(t,x)\mathrm{d}x\mathrm{d}t\\ &= \left|Z^{\mathrm{M}}\right|\int_S\int_\Omega\rho_{\mathrm{M}}u'(t,x)\phi_0(t,x)\mathrm{d}x\mathrm{d}t.\end{aligned}$$

The limit of the second term can easily be computed by using the two-scale convergence

$$\nabla_x\widehat{u_\varepsilon}\xrightarrow{2}\nabla_x u+\nabla_y u_1$$

which yields

$$\begin{aligned}&\int_S\int_\Omega\kappa_{\mathrm{M}}\nabla\widehat{u_\varepsilon}\mathbb{1}_{Z^{\mathrm{M}}}\left(\frac{x}{\varepsilon}\right)\cdot\left(\nabla_x\phi_0+\nabla_y\phi_{1,\mathrm{M}}^\varepsilon+\varepsilon\nabla_x\phi_{1,\mathrm{M}}^\varepsilon\right)\mathrm{d}x\mathrm{d}t\\ &\to\int_S\int_\Omega\int_{Z^{\mathrm{M}}}\kappa_{\mathrm{M}}\left(\nabla_x u(t,x)+\nabla_y u_1(t,x,y)\right)\cdot\left(\nabla_x\phi_0(t,x)+\nabla_y\phi_{1,\mathrm{M}}(t,x,y)\right)\mathrm{d}y\mathrm{d}x\mathrm{d}t.\end{aligned}$$

The limit of the third term is known from lemma 3.8:

$$\varepsilon\int_S\int_{\Gamma^\varepsilon}\kappa_{RI}\left(\widehat{u_\varepsilon}-\widehat{\theta_\varepsilon}\right)\left(\phi_0+\varepsilon\phi_{1,\mathrm{M}}^\varepsilon\right)\mathrm{d}\sigma\mathrm{d}t\to|\Gamma|\int_S\int_\Omega\kappa_{RI}(u-\theta)\phi_0\mathrm{d}x\mathrm{d}t.$$

With the knowledge of the strong convergence of the trace of $\widehat{u}$ (see lemma 3.7) and the weak convergence of the characteristic function of the outer boundary (see theorem 3.1), we can easily compute the convergence of the last two terms:

$$\int_S\int_{\partial\Omega}\kappa_{RE}\widehat{u_\varepsilon}\mathbb{1}_{\Gamma_\varepsilon^{\mathrm{M}}\mathrm{ext}}\left(\phi_0+\varepsilon\phi_{1,\mathrm{M}}^\varepsilon\right)\mathrm{d}\sigma\mathrm{d}t\to\left|A^{\mathrm{M}}\right|\int_S\int_{\partial\Omega}\kappa_{RE}u\phi_0\mathrm{d}\sigma\mathrm{d}t$$

and

$$\int_S \int_{\partial\Omega} \kappa_{RE}\theta_{\text{ext}} \mathbb{1}_{\Gamma_\varepsilon^{\text{M}_{\text{ext}}}} \left(\phi_0 + \varepsilon\phi_{1,\text{M}}^\varepsilon\right) \mathrm{d}\sigma\mathrm{d}t \to \left|A^{\text{M}}\right| \int_S \int_{\partial\Omega} \kappa_{RE}\theta_{\text{ext}}\phi_0 \mathrm{d}\sigma\mathrm{d}t.$$

The complete limit equation for the homogenized temperature u is thus given as

$$\begin{aligned}
&\left|Z^{\text{M}}\right| \int_S \int_\Omega \rho_{\text{M}} u'(t,x)\phi_0(t,x)\mathrm{d}x\mathrm{d}t \\
&\quad + \int_S \int_\Omega \int_{Z^{\text{M}}} \kappa_{\text{M}}(\nabla_x u(t,x) + \nabla_y u_1(t,x,y)) \cdot (\nabla_x\phi_0(t,x) + \nabla_y\phi_{1,\text{M}}(t,x,y))\mathrm{d}y\mathrm{d}x\mathrm{d}t \\
&\qquad + |\Gamma| \int_S \int_\Omega \kappa_{RI}(u-\theta)\phi_0(t,x)\mathrm{d}x\mathrm{d}t + \left|A^{\text{M}}\right| \int_S \int_{\partial\Omega} \kappa_{RE}(u-\theta_{\text{ext}})\phi_0\mathrm{d}\sigma\mathrm{d}t = 0.
\end{aligned}$$

Passing to the limit in the second equation can be done similarly as for the first equation and yields the limit equation

$$\begin{aligned}
&\left|Z^{\text{S}}\right| \int_S \int_\Omega \rho_{\text{S}}\theta'\phi_0\mathrm{d}x\mathrm{d}t + \left|Z^{\text{S}}\right| \int_S \int_\Omega \lambda\chi'\phi_0\mathrm{d}x\mathrm{d}t \\
&\quad + \int_S \int_\Omega \int_{Z^{\text{S}}} \kappa_{\text{S}}(\nabla_x\theta(t,x) + \nabla_y\theta_1(t,x,y)) \cdot (\nabla_x\phi_0(t,x) + \nabla_y\phi_{1,\text{S}}(t,x,y))\mathrm{d}y\mathrm{d}x\mathrm{d}t \\
&+ |\Gamma| \int_S \int_\Omega \kappa_{RI}(\theta-u)\phi_0\mathrm{d}x\mathrm{d}t + \left|A^{\text{S}}\right| \int_S \int_{\partial\Omega} \kappa_{RE}(\theta-\theta_{\text{ext}})\phi_0\mathrm{d}\sigma\mathrm{d}t = \left|Z^{\text{S}}\right| \int_S \int_\Omega f\phi_0\mathrm{d}x\mathrm{d}t
\end{aligned}$$

for the homogenized temperature θ.

Using the lemma 3.6, which ensures two-scale convergence of $\widehat{\chi_\varepsilon}^3$ with respect to $\mathrm{L}^{\frac{4}{3}}$, we can finally pass to the limit in the last equation and deduce the limit equation

$$\begin{aligned}
&\left|Z^{\text{S}}\right| \int_S \int_\Omega \mu\chi'\phi_0\mathrm{d}x\mathrm{d}t \\
&\quad + \int_S \int_\Omega \int_{Z^{\text{S}}} \nu(\nabla_x\chi(t,x) + \nabla_y\chi_1(t,x,y)) \cdot (\nabla_x\phi_0(t,x) + \nabla_y\phi_{1,\text{S}}(t,x,y)\mathrm{d}y\mathrm{d}x\mathrm{d}t \\
&\qquad + \left|Z^{\text{S}}\right| \int_S \int_\Omega \omega_1\chi^3\phi_0\mathrm{d}x\mathrm{d}t - \left|Z^{\text{S}}\right| \int_S \int_\Omega \omega_2\chi\phi_0\mathrm{d}x\mathrm{d}t = \left|Z^{\text{S}}\right| \int_S \int_\Omega l\theta\phi_0\mathrm{d}x\mathrm{d}t.
\end{aligned}$$

for the homogenized phase-field variable χ.

3.5 Derivation of homogenized diffusion tensors

We will now derive a homogenized diffusion tensor to simplify the first homogenized equation. To that end wefine the space $W_\#^{1,2}\left(Z^{\text{M}}\right)$ as the closure of $C_\#^\infty\left(\overline{Z^{\text{M}}}\right)$ w.r.t the norm of $W^{1,2}\left(Z^{\text{M}}\right)$.

Choosing $\phi_0 = 0$ yields:

$$\int_S \int_\Omega \int_{Z^{\text{M}}} \kappa_{\text{M}}(\nabla_x u(t,x) + \nabla_y u_1(t,x,y)) \cdot \nabla_y\phi_{1,\text{M}}(t,x,y)\mathrm{d}y\mathrm{d}x\mathrm{d}t = 0.$$

This implies that

$$\int_{Z^{\mathrm{M}}} (\nabla_x u(t,x) + \nabla_y u_1(t,x,y)) \cdot \nabla_y \phi_{1,\mathrm{M}}(y) \mathrm{d}y = 0$$

a.e. in $S \times \Omega$, by density for all $\phi_{1,\mathrm{M}} \in W^{1,2}_{\#}\left(Z^{\mathrm{M}}\right)$. This relation holds - of course - especially for all $\phi_{1,\mathrm{M}} \in W^{1,2}_{\overline{\#}}\left(Z^{\mathrm{M}}\right)$, by which we denote the functions with mean-value 0 on Z^{M}.

Consider the function $u_1(t,x) \in W^{1,2}_{\#}(Y)$. As in the equation the gradient w.r.t y appears, u_1 is just determined up to a constant and can be chosen such that its mean-value in Z^{M} equals zero. The restriction of u_1 to Z^{M} then lies in $W^{1,2}_{\overline{\#}}\left(Z^{\mathrm{M}}\right)$.

By Poincares inequality for functions with zero mean-value, this implies that every other function $u_2 \in W^{1,2}_{\overline{\#}}\left(Z^{\mathrm{M}}\right)$ that satisfies the above relation equals u_1 a.e. in Z^{M}.

Consider the following cell-problem: Find $\zeta_j \in W^{1,2}_{\overline{\#}}\left(Z^{\mathrm{M}}\right)$ such that

$$\int_{Z^{\mathrm{M}}} (\nabla_y \zeta_j(y) + e_j) \cdot \nabla_y \phi \mathrm{d}y = 0 \quad \forall \phi \in W^{1,2}_{\overline{\#}}\left(Z^{\mathrm{M}}\right).$$

By definition, $W^{1,2}_{\#}\left(Z^{\mathrm{M}}\right)$ is a closed subspace of $W^{1,2}\left(Z^{\mathrm{M}}\right)$ and it is then easy to see that this holds for $W^{1,2}_{\overline{\#}}\left(Z^{\mathrm{M}}\right)$ as well. The well-known theory for monotone operators (under consideration of the Poincare-inequality for functions with zero mean-value) directly gives the existence and uniqueness of a solution of the cell-problem.

Multiplying the cell problem by $\frac{\partial}{\partial x_j} u(t,x)$ and summation of j yields

$$\int_{Z^{\mathrm{M}}} \left(\sum_{j=1}^{3} \frac{\partial}{\partial x_j} u(t,x) \nabla_y \zeta_j(y) + \nabla_x u(t,x) \right) \cdot \nabla_y \phi = 0,$$

and thus

$$\int_{Z^{\mathrm{M}}} \left(\nabla_y \left[\sum_{j=1}^{3} \frac{\partial}{\partial x_j} u(t,x) \zeta_j(y) \right] + \nabla_x u(t,x) \right) \cdot \nabla_y \phi = 0.$$

Hence $\sum_{j=1}^{3} \frac{\partial}{\partial x_j} u(t,x) \zeta_j(y)$ solves the equation derived from the homogenized problem from which we can, recalling the uniqueness of u_1, deduce the identity

$$u_1(t,x,y) = \sum_{j=1}^{3} \frac{\partial}{\partial x_j} u(t,x) \zeta_j(y)$$

a.e. in Z^{M}.

We calculate

$$\begin{aligned}
&\int_S \int_\Omega \int_{Z^{\mathrm{M}}} \kappa_{\mathrm{M}} (\nabla_x u(t,x) + \nabla_y u_1(t,x,y)) \cdot \nabla_x \phi_0(t,x) \mathrm{d}y \mathrm{d}x \mathrm{d}t \\
&= \int_S \int_\Omega \int_{Z^{\mathrm{M}}} \kappa_{\mathrm{M}} \left(\nabla_x u(t,x) + \nabla_y \sum_{j=1}^{3} \frac{\partial}{\partial x_j} u(t,x) \zeta_j(y) \right) \cdot \nabla_x \phi_0(t,x) \mathrm{d}y \mathrm{d}x \mathrm{d}t \\
&= \int_S \int_\Omega \sum_{j=1}^{3} \kappa_{\mathrm{M}} \int_{Z^{\mathrm{M}}} (e_j + \nabla_y \zeta_j(y)) \mathrm{d}y \frac{\partial}{\partial x_j} u(t,x) \cdot \nabla_x \phi_0(t,x) \mathrm{d}x \mathrm{d}t \\
&= \int_S \int_\Omega P^{\mathrm{M}} \nabla_x u(t,x) \cdot \nabla_x \phi_0(t,x) \mathrm{d}x \mathrm{d}t
\end{aligned}$$

with the homogenized diffusion tensor P^{M} where

$$P^{\mathrm{M}}_{jk} = \kappa_{\mathrm{M}} \int_{Z^{\mathrm{M}}} \left(\delta_{jk} + \partial_{y_j} \zeta_k(y) \right) \mathrm{d}y$$

which is independent of t and x.

Of course, similar arguments can be used to derive homogenized diffusion tensors for the elliptic terms in the other two homogenized equations:

We denote by P^{S} and P^{SPF} the homogenized diffusion tensors in the equations for θ and χ, respectively.

3.6 Properties of the homogenized diffusion tensors

In this section we show, by the example of P^{M}, that the homogenized diffusion tensors are symmetric and positive definite. The same results follow for P^{S} and P^{SPF} similarly.

Symmetry can be shown analogous to the procedure in [Pavliotis and Stuart, 2008, p.190]. To show the positive definiteness however, we have to take into account the geometry of the reference cell Y: The arguments could not be used if we had a 'honeycomb' geometry, i.e. $Z^{\mathrm{M}} \subset\subset Y$.

Theorem 3.9. *The homogenized diffusion tensor P^{M} is positiv definite.*

Proof. Let $\xi \in \mathbb{R}^n$. We calculate

$$\begin{aligned}
\xi^{\mathrm{T}} P^{\mathrm{M}} \xi &= \sum_{j,k} \int_{Z^{\mathrm{M}}} (e_k + \nabla_y \zeta_k(y)) \cdot (e_j + \nabla_y \zeta_j(y)) \, \xi_k \xi_j \mathrm{d}y \\
&= \int_{Z^{\mathrm{M}}} \nabla_y \left[\xi \cdot (y + \zeta) \right] \cdot \nabla_y \left[\xi \cdot (y + \zeta) \right] \mathrm{d}y = \int_{Z^{\mathrm{M}}} \left| \nabla_y \left[\xi \cdot (y + \zeta) \right] \right|^2 \mathrm{d}y \geq 0.
\end{aligned}$$

Assume that $\xi^{\mathrm{T}} P^{\mathrm{M}} \xi = 0$, then $\nabla_y \left[\xi \cdot (y + \zeta) \right] = 0$ a.e. in Z^{M}. Thus there is a constant $C \in \mathbb{R}$ such that $\xi \cdot (y + \zeta(y)) = C$ a.e. and hence

$$\xi \cdot \zeta(y) = C - \xi \cdot y \quad \text{a.e.}$$

The domain Z^{M} has a specific structure in our setting: its 1-periodic extension is assumed to be connected. Thus its intersection with ∂Y has a positive 2-dimensional surface measure on all faces of Y, as we assumed the faces of Y to be all identical.

This observation implies that there is, on all faces of Y, a surface with positive 2-dimensional surface measure where ζ is defined. Also, the function ζ is 1-periodic. It hence follows that $\xi = 0$, as the right hand side above is not 1-periodic.

Note that, if Z^{M} would be strictly contained in Y, this argument would not work. □

3.7 The full homogenized problem

We use the density of the testfunctions ϕ_0 to verify that the homogenized equations stay valid for all testfunctions $v \in \mathrm{L}^2\left(S, H^1(\Omega)\right)$ and use the homogenized diffusion tensors to state the full homogeniued problem:

Homogenized heat diffusion in the solid matrix:

$$\begin{aligned} \left|Z^{\mathrm{M}}\right| \int_S \int_\Omega \rho_{\mathrm{M}} u' v \mathrm{d}x\mathrm{d}t + \int_S \int_\Omega P^{\mathrm{M}} \nabla_x u \cdot \nabla_x v \mathrm{d}x\mathrm{d}t \\ + |\Gamma| \int_S \int_\Omega \kappa_{RI} (u - \theta) v \mathrm{d}x\mathrm{d}t + \left|A^{\mathrm{M}}\right| \int_S \int_{\partial\Omega} \kappa_{RE} (u - \theta_{\mathrm{ext}}) v \mathrm{d}\sigma\mathrm{d}t = 0. \end{aligned}$$

Homogenized heat diffusion in the Stefan-Region:

$$\begin{aligned} \left|Z^{\mathrm{S}}\right| \int_S \int_\Omega \rho_{\mathrm{S}} \theta' v \mathrm{d}x\mathrm{d}t + \left|Z^{\mathrm{S}}\right| \int_S \int_\Omega \lambda \chi' v \mathrm{d}x\mathrm{d}t \\ + \int_S \int_\Omega P^{\mathrm{S}} \nabla_x \theta \cdot \nabla_x v \mathrm{d}x\mathrm{d}t + |\Gamma| \int_S \int_\Omega \kappa_{RI} (\theta - u) v \mathrm{d}x\mathrm{d}t \\ + \left|A^{\mathrm{S}}\right| \int_S \int_{\partial\Omega} \kappa_{RE} (\theta - \theta_{\mathrm{ext}}) v \mathrm{d}\sigma\mathrm{d}t = \left|Z^{\mathrm{S}}\right| \int_S \int_\Omega f v \mathrm{d}x\mathrm{d}t. \end{aligned}$$

Homogenized evolution of the phase-field:

$$\begin{aligned} \left|Z^{\mathrm{S}}\right| \int_S \int_\Omega \mu \chi' v \mathrm{d}x\mathrm{d}t + \int_S \int_\Omega P^{SPF} \nabla_x \chi \cdot \nabla_x v \mathrm{d}x\mathrm{d}t \\ + \left|Z^{\mathrm{S}}\right| \int_S \int_\Omega \omega_1 \chi^3 v \mathrm{d}x\mathrm{d}t - \left|Z^{\mathrm{S}}\right| \int_S \int_\Omega \omega_2 \chi v \mathrm{d}x\mathrm{d}t = \left|Z^{\mathrm{S}}\right| \int_S \int_\Omega l \theta v \mathrm{d}x\mathrm{d}t. \end{aligned}$$

This corresponds to the classical formulation

$$\begin{aligned} \left|Z^{\mathrm{M}}\right| \rho_{\mathrm{M}} u' - \operatorname{div}(P^{\mathrm{M}} \nabla_x u) + |\Gamma| \kappa_{RI} (u - \theta) &= 0 && \text{in } \Omega, \\ \left|Z^{\mathrm{S}}\right| \rho_{\mathrm{S}} \theta' + \left|Z^{\mathrm{S}}\right| \lambda \chi' - \operatorname{div}(P^{\mathrm{S}} \nabla_x \theta) + |\Gamma| \kappa_{RI} (\theta - u) &= \left|Z^{\mathrm{S}}\right| f && \text{in } \Omega, \\ \left|Z^{\mathrm{S}}\right| \mu \chi' - \operatorname{div}(P^{SPF} \nabla_x \chi) + \left|Z^{\mathrm{S}}\right| \omega_1 \chi^3 - \left|Z^{\mathrm{S}}\right| \omega_2 \chi &= \left|Z^{\mathrm{S}}\right| l \theta && \text{in } \Omega \end{aligned}$$

with the boundary conditions

$$\begin{aligned} -P^{\mathrm{M}} \nabla u \cdot \vec{n} &= \left|A^{\mathrm{M}}\right| \kappa_{RE} (u - \theta_{\mathrm{ext}}) && \text{on } \partial\Omega, \\ -P^{\mathrm{S}} \nabla \theta \cdot \vec{n} &= \left|A^{\mathrm{M}}\right| \kappa_{RE} (u - \theta_{\mathrm{ext}}) && \text{on } \partial\Omega, \\ -P^{SPF} \nabla \chi \cdot \vec{n} &= 0 && \text{on } \partial\Omega. \end{aligned}$$

By standard methods, it is easy to see that, if the initial values converge weakly in $L^2(\Omega)$, their weak limits are the initial values of the homogenized system.

4 Outlook

Additionally to the results in this article, the authors have already studied the homogenization of systems with different scalings, e.g. of the interfacial width in the phase-field model. Also the derivation of sharp-interface models from the effective models derived in this article has been investigated. Furthermore, the diffusion of chemical species in the pore-space of the porous medium as well as the modeling of mechanical effects due to the change of the phases and the homogenization of the respective models have been studied.

The corresponding results will be published in forthcoming articles.

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