

# Homogenisation in domains with evolving microstructure

Malte A. Peter <sup>a</sup>,

<sup>a</sup>*Centre for Industrial Mathematics, FB 3, University of Bremen, Postfach 330 440, 28334 Bremen, Germany*

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## Abstract

We propose a method which accounts for an evolving microstructure in homogenisation problems. The concept of the method is quite general and can be applied to a number of different problems. It makes use of a transformation to a homogenisable substitute problem on a fixed periodic domain.

## Résumé

**Homogénéisation dans des domaines avec évolution de la micro-structure.** On propose une méthode pour inclure une évolution de la micro-structure en problème d'homogénéisation. L'idée de la méthode est assez générale et peut être employée pour une diversité de problèmes différents. Elle utilise la transformation d'un problème substitué homogénéisé dans un domaine fixé périodique.

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## Version française abrégée

Dans cette note on considère le problème d'homogénéisation d'un système couplé de deux équations aux dérivées partielles paraboliques, dont la micro-structure suit une évolution prescrite en fonction du temps. Les mécanismes motivant l'étude de ce problème sont la réaction, la diffusion et le transport de masse à travers une surface de séparation dans un milieu poreux sec. L'évolution de la micro-structure provient d'une accumulation d'un produit solide. Par ailleurs, la taille des pores diminue, ce qui engendre une réduction de la diffusion dans les pores. Notre méthode peut aussi être employée pour modéliser les changements du volume du film d'eau dans un milieu poreux humide. Le système d'équations considéré a été choisi parce qu'il possède de nombreuses qualités typiques des problèmes en milieu poreux.

L'idée utilisée pour éviter les difficultés introduites par l'évolution de la micro-structure est assez générale. Elle est applicable à beaucoup de situations différentes. Puisque l'évolution n'est pas spatialement homogène, le domaine n'est en général pas périodique pour  $t > 0$ , même si le domaine initial l'était. Par conséquent, les méthodes d'homogénéisation périodique [3,12,4] ne peuvent pas être utilisées

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*Email address:* mpeter@math.uni-bremen.de (Malte A. Peter).

directement. Notre idée est de ramener la description spatiale du problème à un domaine de référence statique. En choisissant ce domaine de référence, dont la micro-structure est périodique, on va montrer de quelle manière l'homogénéisation peut être appliquée. On peut constater que, avec quelques hypothèses additionnelles, il est possible de retrouver, à partir des équations homogénéisées relatives au domaine de référence, les équations relatives au problème initial.

Afin de fixer les idées, on considère la réaction, la diffusion aussi que l'échange à travers une surface de séparation dans un milieu poreux  $\Omega$ , qui ne change pas macroscopiquement avec le temps. Cependant, les domaines de phases (c'est-à-dire l'espace de pores  $\Omega^p(t)$  et la matrice solide  $\Omega^s(t)$ ), qui forment  $\Omega$ , peuvent évoluer. On suppose que  $\Omega$  a une micro-structure  $\varepsilon$ -périodique relative à un volume de référence  $Y$  à  $t = 0$ . Remarquons que l' $\varepsilon$ -périodicité de la micro-structure de  $\Omega$  à  $t = 0$  n'est pas essentielle et peut être évitée. Le volume de référence est constitué du volume occupé par le pore-air,  $Z^p$ , et par la matrice solide,  $Z^s$ . On suppose que l'évolution des différentes parties de  $\Omega$  est donnée par une application préservant l'orientation  $\psi_\varepsilon^i(\cdot, t): \Omega_\varepsilon^i(0) \rightarrow \Omega_\varepsilon^i(t)$ ,  $i \in \{p, s\}$ , pour tous  $t \in S$ .

Les équations du modèle pour les concentrations inconnues dans le pore-air et dans la matrice solide sont données par (1). Le problème (1) peut être reformulé dans la description de référence (i.e. en coordonnées lagrangiennes) en utilisant le calcul des corps déformables, [14], cf. (2). Si les fonctions dépendant de la transformation sont bornées, alors des résultats standards démontrent l'existence et l'unicité de la solution de (2) (cf. [10,13]).

Le problème homogénéisé limite pour  $\varepsilon \rightarrow 0$  est obtenu en utilisant la méthode de la convergence à deux échelles [9,1]. Quelques hypothèses sur la transformation, (4) en particulier, sont nécessaires. L'idée-clé est de représenter la transformation de la manière indiquée en (5). Par la passage à la limite  $\varepsilon \rightarrow 0$ , on obtient  $\hat{u}_\varepsilon^p \rightarrow \hat{u}^p = \hat{u}^p(X, t)$  et  $\hat{u}_\varepsilon^s \rightarrow \hat{u}^s = \hat{u}^s(X, Y, t)$ . La formulation forte des équations limite est donnée en (6)–(8). S'il n'y a pas de flux d'excipient (c'est-à-dire pore-air ou matrice solide) par les faces du cube unité, alors une représentation spatiale correspondante peut être obtenue; celle-ci est indiquée en (9)–(11).

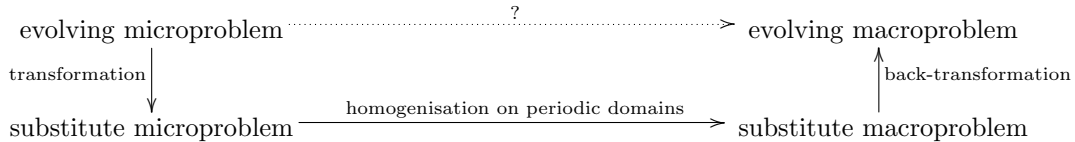
La méthode présentée est particulièrement utile pour considérer des problèmes dont l'évolution de la micro-structure est causée par la réaction et la diffusion. Dans ce cas, les fonctions représentant l'évolution ( $\Psi_\varepsilon^i$  et  $J_\varepsilon^i$ ) peuvent être modélisées en les reliant aux concentrations, par exemple quand la micro-structure est changée par une réaction ou par une précipitation. Ce type des résultats peut être trouvé en [10]. Ils seront exposés dans des publications à venir. La structure des systèmes d'équations résultants peut aussi être utilisée pour des approches à deux échelles (cf. par exemple [8]).

## 1. Introduction

In this note, we consider the homogenisation problem of a coupled system of two parabolic partial differential equations in a two-phase medium, whose microstructure undergoes a given evolution with respect to time. The motivating mechanisms behind this problem are reaction, diffusion and interfacial exchange in a dry porous medium. The evolution of the microstructure originates from an accumulation of solid reaction products. In turn, the pore space shrinks and, thereby, diffusion in the air-filled part of the pores is effectively hindered. The method can also be used to describe changes of water films in wet porous media, e.g. The particular system of equations considered here is chosen because it exhibits many typical features of porous-media problems.

The idea employed to handle the evolution of the microstructure is quite general and is applicable to many different situations. Since the domain may evolve differently at different places, it is generally not periodic anymore for  $t > 0$ , even if it has been periodic initially (i.e. at  $t = 0$ ). Therefore, periodic-homogenisation ideas [3,12,4] cannot be applied directly. Our idea is to transform the spatial description

of the problem to a (static) reference domain (motivated by the notion of motion in classical continuum mechanics, cf. [14], e.g.). Choosing this reference domain to have a periodic microstructure, it is shown that the homogenisation can be performed. It turns out that, under some additional assumptions, it is also possible to transform the homogenised equations given on the reference domain back to an associated evolving domain. The basic idea of the approach is summarised in the following diagram:



In order to fix ideas, we consider reaction, diffusion and interfacial exchange in a porous medium  $\Omega(t)$ . We assume that the evolution of the phase domains (i.e. pore space  $\Omega^p(t)$  and solid matrix  $\Omega^s(t)$ ) is given. It is supposed to be due to an addition of a reaction product to the solid matrix (or precipitation to the solid matrix). Hence, the pore space is deformed and an evolution of the pore air causes a mass flux of concentration of the species under consideration even if it is in diffusive equilibrium. On the other hand, the evolution of the solid matrix is caused by an addition of (clean) carrier substance. Therefore, the model equations for the concentration in pore air and in solid matrix differ by an advection term (cf. (1) below).

The main restriction of the transformation approach is that it requires the transformations to be continuously differentiable with continuously-differentiable inverse in the microscopic or macroscopic variable in order to be able to recover the spatial form of the homogenised problem. In particular, this means that topology changes of the domains cannot be captured. Nevertheless, the method is particularly useful when considering problems where the evolution of the microstructure is induced by the reaction–diffusion problem itself. Here, the functions describing the evolution ( $\Psi_\varepsilon^i$  and  $J_\varepsilon^i$ , cf. below) can be modelled constitutively by relating them to the concentrations, for example if the microstructure is changed by a reaction or precipitation. Results in this direction can be found in [10] and will be presented in forthcoming publications. The structure of the resulting systems of equations can also be used as a starting point for two-scale modelling approaches, cf. [8], for example.

The problem under consideration has been considered for *fixed* periodic microstructure in similar form by several authors, e.g. [2,7,6,11]. The idea how to obtain the substitute problem is similar to that of Hornung [5], who briefly indicated how a homogenisation problem in a non-periodic (time-independent) domain can be transformed to one given in a periodic domain. It is noteworthy that the method of handling the evolving microstructure does not seem to have appeared elsewhere and is of interest even for the simple case of only one equation.

## 2. The system of equations in a time-dependent domain

We begin by formulating some assumptions on the domain  $\Omega(t)$  and its parts:

- The Lipschitz-continuous macroscopic domain  $\Omega(t)$  does not change with time, i.e.  $\Omega(t) \equiv \Omega(0) = \Omega$ , but it consists of two measurable time-dependent subdomains  $\Omega^p(t)$  and  $\Omega^s(t)$ , i.e.  $\bar{\Omega} = \bar{\Omega}^p(t) \cup \bar{\Omega}^s(t)$  with  $\Omega^p(t) \cap \Omega^s(t) = \emptyset$  for all times.
- The domain  $\Omega$  is  $\varepsilon$ -periodic at  $t = 0$ , i.e. there exists a reference cell  $Y$  with  $\bar{Y} = \bar{Z}^p \cup \bar{Z}^s$  and  $Z^p \cap Z^s = \emptyset$  such that  $\Omega_\varepsilon^i(0) = \bar{\Omega} \cap \text{int} \bigcup_{k \in \mathbb{Z}^n} \varepsilon \bar{Z}_k^i$  for  $i \in \{p, s\}$  where  $\Omega_\varepsilon^p(t)$  is connected. We write  $\Gamma_\varepsilon(t) = \partial\Omega_\varepsilon^p(t) \cap \partial\Omega_\varepsilon^s(t)$  for the Lipschitz-continuous internal interface and, in order to avoid technicalities, we assume  $Y$  to be the  $n$ -dimensional unit cube.

— The evolution of the different parts of  $\Omega$  can be described by an orientation-preserving mapping  $\psi_\varepsilon^i(\cdot, t): \Omega_\varepsilon^i(0) \rightarrow \Omega_\varepsilon^i(t)$ ,  $i \in \{p, s\}$ , for each  $t \in S$ .

We denote the coordinates of the reference configuration by upper-case variables,  $X \in \Omega_\varepsilon^i(0)$ , and those of the current configuration by lower-case variables,  $x = \psi_\varepsilon^i(X, t) \in \Omega_\varepsilon^i(t)$ ,  $i \in \{p, s\}$ . Note that the condition that  $\Omega$  has an  $\varepsilon$ -periodic microstructure at  $t = 0$  is not essential and is only chosen for convenience; it is only required that some periodic reference domain exists, to which the subdomains can be mapped by functions  $\psi_\varepsilon^i$ .

We are now in a position to formulate the system of equations under consideration for the unknown concentrations where we account for a (given) evolution of the phases. The problem of reaction, diffusion and interfacial exchange is given by

$$\partial_t u_\varepsilon^p(x, t) - \nabla \cdot (D_\varepsilon^p \nabla u_\varepsilon^p - v_\varepsilon^p u_\varepsilon^p) = f_\varepsilon^p, \quad x \in \Omega_\varepsilon^p(t), \quad t \in S = (0, T), \quad (1a)$$

$$\partial_t u_\varepsilon^s(x, t) - \nabla \cdot (\varepsilon^2 D_\varepsilon^s \nabla u_\varepsilon^s) = f_\varepsilon^s, \quad x \in \Omega_\varepsilon^s(t), \quad t \in S, \quad (1b)$$

$$-(D_\varepsilon^p \nabla u_\varepsilon^p) \cdot N_\varepsilon^p = (\varepsilon^2 D_\varepsilon^s \nabla u_\varepsilon^s + v_\varepsilon^s u_\varepsilon^s) \cdot N_\varepsilon^s = \varepsilon a_\varepsilon(u_\varepsilon^p - u_\varepsilon^s), \quad x \in \Gamma_\varepsilon(t), \quad t \in S, \quad (1c)$$

where  $v_\varepsilon^i(x, t) = \partial_t \psi_\varepsilon^i(\psi_\varepsilon^{i-1}(x, t), t)$  is the velocity due to the deformation and  $N_\varepsilon^i$  is the outward unit normal vector on  $\Omega_\varepsilon^i(t)$ ,  $i \in \{p, s\}$ . System (1) is completed by homogeneous Neumann boundary conditions at the exterior boundaries,  $\partial \Omega_\varepsilon^i(t) \cap \partial \Omega$ , and initial values  $u_\varepsilon^i(0)$ ,  $i \in \{p, s\}$ . This problem is stated on time-dependent domains which are not necessarily  $\varepsilon$ -periodic for  $t > 0$ . It is noteworthy that the model equations for  $u_\varepsilon^p$  and  $u_\varepsilon^s$  differ by the advection term owing to the evolution of  $\Omega_\varepsilon^p(t)$  being due to a deformation and that of  $\Omega_\varepsilon^s(t)$  being due to an addition of solid. Moreover, the function  $\psi_\varepsilon^p(x, \cdot)$  defines the trajectory of the air particle residing at  $x$  at time  $t = 0$ , while the analogue is not true for  $\psi_\varepsilon^s(x, \cdot)$  due to the different physical interpretation.

Problem (1) can be reformulated in the reference (i.e. Lagrangian) description making use of some of the calculus of mechanics of deformable bodies [14]. In particular, we denote the deformation gradient by  $\Psi_\varepsilon^i$ , i.e.  $\Psi_\varepsilon^i = \nabla \psi_\varepsilon^i$ , and its determinant by  $J_\varepsilon^i$ , i.e.  $J_\varepsilon^i = \det \Psi_\varepsilon^i$ ,  $i \in \{p, s\}$ . We use hats to denote the corresponding quantities in the reference description,  $\hat{u}_\varepsilon^i(X, t) = u_\varepsilon^i(\psi_\varepsilon^i(X, t), t)$ ,  $i \in \{p, s\}$ , and analogously for the other quantities. Moreover, we write  $\Omega_\varepsilon^i = \Omega_\varepsilon^i(0)$ ,  $i \in \{p, s\}$ , and  $\Gamma_\varepsilon = \Gamma_\varepsilon(0)$ . In the reference domain, the system of equations (1) reads

$$\partial_t (J_\varepsilon^p \hat{u}_\varepsilon^p) - \nabla \cdot (J_\varepsilon^p \Psi_\varepsilon^{p-1} \hat{D}_\varepsilon^p \Psi_\varepsilon^{p-T} \nabla u_\varepsilon^p) = J_\varepsilon^p \hat{f}_\varepsilon^p, \quad x \in \Omega_\varepsilon^p, \quad t \in S, \quad (2a)$$

$$\partial_t (J_\varepsilon^s \hat{u}_\varepsilon^s) - \nabla \cdot (J_\varepsilon^s \Psi_\varepsilon^{s-1} (\varepsilon^2 \hat{D}_\varepsilon^s \Psi_\varepsilon^{s-T} \nabla \hat{u}_\varepsilon^s + \hat{v}_\varepsilon^s \hat{u}_\varepsilon^s)) = J_\varepsilon^s \hat{f}_\varepsilon^s, \quad x \in \Omega_\varepsilon^s, \quad t \in S, \quad (2b)$$

$$\begin{aligned} -(J_\varepsilon^p \Psi_\varepsilon^{p-1} \hat{D}_\varepsilon^p \Psi_\varepsilon^{p-T} \nabla \hat{u}_\varepsilon^p) \cdot N_\varepsilon^p &= J_\varepsilon^s \Psi_\varepsilon^{s-1} (\varepsilon^2 \hat{D}_\varepsilon^s \Psi_\varepsilon^{s-T} \nabla \hat{u}_\varepsilon^s + \hat{v}_\varepsilon^s \hat{u}_\varepsilon^s) \cdot N_\varepsilon^s \\ &= \varepsilon \hat{a}_\varepsilon \|\Psi_\varepsilon^{-T} N_\varepsilon\| J_\varepsilon (\hat{u}_\varepsilon^p - \hat{u}_\varepsilon^s), \quad x \in \Gamma_\varepsilon, \quad t \in S, \end{aligned} \quad (2c)$$

$t \in S$ , and analogously for the initial and boundary values at the exterior boundary, where  $\|\cdot\|$  denotes the Euclidean norm.

For ease of notation, we write  $\psi_\varepsilon = \chi_\varepsilon^p \psi_\varepsilon^p + \chi_\varepsilon^s \psi_\varepsilon^s$ , where  $\chi_\varepsilon^i$  is the characteristic function of  $\Omega_\varepsilon^i$ ,  $i \in \{p, s\}$ , and, analogously, for  $D_\varepsilon$ . The functions  $J_\varepsilon$  and  $\Psi_\varepsilon^{-1} \hat{D}_\varepsilon \Psi_\varepsilon^{-T}$  are assumed to be bounded away from zero and uniformly elliptic, respectively, and, together with  $\partial_t J_\varepsilon^i$ , are assumed to be bounded from above with all bounds independent of  $\varepsilon$ . Then, standard results yield existence and uniqueness of a solution of (2) (cf. [10,13], e.g.). Moreover, the unknowns and their gradients satisfy the standard a-priori estimates, i.e.

$$\int_{\Omega_\varepsilon^p} |\hat{u}_\varepsilon^p|^2 dx + \int_{\Omega_\varepsilon^s} |\hat{u}_\varepsilon^s|^2 dx + \int_0^t \int_{\Omega_\varepsilon^p} |\nabla \hat{u}_\varepsilon^p|^2 dx dt + \varepsilon^2 \int_0^t \int_{\Omega_\varepsilon^s} |\nabla \hat{u}_\varepsilon^s|^2 dx dt + \varepsilon \int_0^t \int_{\Gamma_\varepsilon} |\hat{u}_\varepsilon^p - \hat{u}_\varepsilon^s|^2 d\sigma_x dt \leq C \quad (3)$$

a.e. in  $(0, T)$ , where  $C$  is independent of  $\varepsilon$ .

### 3. Macroscopic equations for given evolution

We want to discuss the homogenised macroscopic limit equations corresponding to  $\varepsilon \rightarrow 0$  for a given evolution  $\psi_\varepsilon$ . In particular, we would like to investigate if there is a relation between the limit problems and the transformation  $\psi_\varepsilon$  of the  $\varepsilon$ -periodic domains.

Using the method of two-scale convergence [9,1], the homogenised limit problem can be obtained. The two-scale limit functions of  $J_\varepsilon$  and  $\Psi_\varepsilon^{-1}$  are denoted by  $J = J(X, Y, t)$  and  $\Psi^{-1} = \Psi^{-1}(X, Y, t)$ , respectively. In order to pass to the limit in products of the type  $J_\varepsilon^i u_\varepsilon^i$  and  $J_\varepsilon \Psi_\varepsilon^{-1} \hat{D}_\varepsilon^i \Psi_\varepsilon^{-T} \nabla u_\varepsilon^i$  where  $u_\varepsilon^i$  and  $\nabla u_\varepsilon^i$  two-scale converge, we require

$$\lim_{\varepsilon \rightarrow 0} \|\Psi_\varepsilon^{-1}\|_{L^2(\Omega \times S)} = \|\Psi^{-1}\|_{L^2(\Omega \times Y \times S)} \quad \text{and} \quad \lim_{\varepsilon \rightarrow 0} \|J_\varepsilon\|_{L^2(\Omega \times S)} = \|J\|_{L^2(\Omega \times Y \times S)}, \quad (4)$$

cf. [1]. For this, it suffices that  $\Psi_\varepsilon^{-1}$  and  $J_\varepsilon$  are sums of functions belonging to the following classes,

- functions being continuous with respect to one space variable,
- functions being a product of functions which depend on one space variable and time only.

Moreover, we assume that the right-hand sides  $f_\varepsilon^p$  and  $f_\varepsilon^s$  have two-scale limits  $f^p$  and  $f^s$ , respectively. The key idea is to represent the transformation as

$$\psi_\varepsilon(X, t) = [X/\varepsilon]_Y + \varepsilon \psi_X(\{X/\varepsilon\}_Y, t), \quad (5)$$

where  $[X]_Y$  denotes the unique integer combination  $\sum_{i=1}^n k_i e_i$  of the periods such that  $\{X\}_Y = X - [X]_Y$  belongs to  $Y$  (where  $e_i$  is the  $i$ th unit vector), and  $\psi_X$  is the transformation in the cell located at the point  $X$ .

In the limit, we obtain  $\hat{u}_\varepsilon^p \rightarrow \hat{u}^p = \hat{u}^p(X, t)$  and  $\hat{u}_\varepsilon^s \rightarrow \hat{u}^s = \hat{u}^s(X, Y, t)$  and the strong form of the limit equations reads

$$\partial_t \left( \int_{Z^p} J dY \hat{u}^p(X, t) \right) - \nabla_X \cdot (P^p \nabla_X \hat{u}^p) = \int_{Z^p} J \hat{f}^p dY - \int_\Gamma \hat{a} \|\Psi^{-T} N\| J (\hat{u}^p - \hat{u}^s) d\sigma_Y, \quad X \in \Omega, \quad (6a)$$

$$\partial_t (J \hat{u}^s(X, Y, t)) - \nabla_Y \cdot (J \Psi^{-1} (\hat{D} \Psi^{-T} \nabla_Y \hat{u}^s + \hat{v}^s \hat{u}^s)) = \hat{f}^s, \quad X \in \Omega, Y \in Z^s, \quad (6b)$$

$$-J \Psi^{s-1} (\hat{D} \Psi^{s-T} \nabla_Y \hat{u}^s + \hat{v}^s \hat{u}^s) \cdot N^s = -\hat{a} \|\Psi^{-T} N\| J (\hat{u}^p - \hat{u}^s), \quad X \in \Omega, Y \in \Gamma, \quad (6c)$$

where  $\hat{v}^s = \partial_t \psi_X^s(Y, t)$ . The homogeneous Neumann boundary conditions at the exterior boundary are recovered and  $\hat{u}^s$  is subject to periodic boundary conditions on  $\partial Z^s \cap \partial Y$ . The macroscopic diffusion tensor  $P^p = [p_{ij}^p]_{ij}$  is given by

$$p_{ij}^p(X, t) = \int_{Z^p} J \Psi^{-1} \hat{D} \Psi^{-T} (\nabla_Y \hat{\zeta}_i^p + e_i) (\nabla_Y \hat{\zeta}_j^p + e_j) dY \quad (7)$$

and the  $Y$ -periodic cell solutions  $\hat{\zeta}_j^p(X, Y, t) = \zeta_j^p(X, Y, t)$ ,  $j = 1, \dots, n$ , satisfy

$$-\nabla_Y \cdot (J \Psi^{-1} \hat{D} \Psi^{-T} (\nabla_Y \hat{\zeta}_j^p + e_j)) = 0, \quad Y \in Z^p. \quad (8)$$

Under some additional assumptions on the transformation, it is possible to interpret the functions  $\Psi$  and  $J$  as related to a transformation and recover spatial representations of the homogenised limit problems. If there is no flux of carrier substance (i.e. pore air or solid matrix) across the faces of the unit cube,  $\partial Y$ , the two-scale limit of the deformation gradient  $\nabla_X \psi_\varepsilon(X, t)$  is given by  $\nabla_Y \psi_X(Y, t)$ , i.e.  $\Psi = \nabla_Y \psi_X(Y, t)$ . Having this in mind, the spatial representation of the macroscopic problems can be determined. In particular, we obtain  $x = X$  in the limit. The corresponding spatial representation of (6) reads

$$\partial_t(|Z^P(t)|u^P(x,t)) - \nabla_x \cdot (P^P \nabla_x u^P) = \int_{Z^P(t)} f^P dy - \int_{\Gamma(t)} a(u^P - u^S) d\sigma_y, \quad x \in \Omega, \quad (9a)$$

$$\partial_t u^S(x,y,t) - \nabla_y \cdot (D^S \nabla_y u^S) = f^S, \quad x \in \Omega, y \in Z^S(t), \quad (9b)$$

$$-(D^S \nabla_y u^S + v^S u^S) \cdot n^S = -a(u^P - u^S), \quad x \in \Omega, y \in \Gamma(t). \quad (9c)$$

Similarly, the tensor elements can be written in terms of the spatial representation,

$$p_{ij}^P(x,t) = \int_{Z^P(t)} (\nabla_y \zeta_j^P(x,y,t) + \Psi^{-T} e_j)^T D (\nabla_y \zeta_i^P(x,y,t) + \Psi^{-T} e_i) dy, \quad (10)$$

where the cell problem is given by

$$-\nabla_y \cdot (D (\nabla_y \zeta_j^P(x,y,t) + \Psi^{-T} e_j)) = 0, \quad y \in Z^P(t). \quad (11)$$

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