

Rate of convergence for a Galerkin scheme approximating a two-scale reaction-diffusion system with nonlinear transmission condition

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Rate of convergence for a Galerkin scheme
approximating a two-scale reaction-diffusion
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by

A. Muntean, O. Lakkis



Centre for Analysis, Scientific computing and Applications
Department of Mathematics and Computer Science
Eindhoven University of Technology
P.O. Box 513
5600 MB Eindhoven, The Netherlands
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RATE OF CONVERGENCE FOR A GALERKIN SCHEME APPROXIMATING A TWO-SCALE REACTION-DIFFUSION SYSTEM WITH NONLINEAR TRANSMISSION CONDITION

ADRIAN MUNTEAN AND OMAR LAKKIS

ABSTRACT. We study a two-scale reaction-diffusion system with nonlinear reaction terms and a nonlinear transmission condition (remotely resembling Henry's law) posed at air-liquid interfaces. We prove the rate of convergence of the two-scale Galerkin method proposed in [7] for approximating this system in the case when both the microstructure and macroscopic domain are two-dimensional. The main difficulty is created by the presence of a boundary nonlinear term entering the transmission condition. Besides using the particular two-scale structure of the system, the ingredients of the proof include two-scale interpolation-error estimates, an interpolation-trace inequality, and improved regularity estimates.

1. INTRODUCTION

Reaction and transport phenomena in porous media are the governing processes in many natural and industrial systems. Not only do these reaction and transport phenomena occur at different space and time scales, but it is also the porous medium itself which is heterogeneous with heterogeneities present at many spatial scales. The mathematical challenge in this context is to understand and then control the interplay between nonlinear production terms with intrinsic multiple-spatial structure and structured transport in porous media. To illustrate this scenario, we consider a large domain with randomly distributed heterogeneities where complex two-phase-two-component processes are relevant only in a small (local) subdomain. This subdomain (which sometimes is referred to as *distributed microstructure*¹ following the terminology of R. E. Showalter) needs fine resolution as the complex processes are governed by small-scale effects. The PDEs used in this particular context need to incorporate two distinct spatial scales: a macroscale (for the large domain, say Ω) and a microscale (for the microstructure, say Y). Usually, $x \in \Omega$ and $y \in Y$ denote macro and micro variables.

1.1. Problem statement. Let S be the time interval $]0, T[$ for a given fixed $T > 0$. We consider the following two-spatial-scale PDE system describing the evolution of the the vector (U, u, v) :

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Key words and phrases. Two-scale reaction-diffusion system, nonlinear transmission conditions, Galerkin method, rate of convergence, distributed-microstructure model.

¹Further keywords are: Barenblatt's parallel-flow models, totally-fissured and partially-fissured media, or double(dual-)-porosity models.

$$(1.1) \quad \theta \partial_t U(t, x) - D \Delta U(t, x) = - \int_{\Gamma_R} b(U(t, x) - u(t, x, y)) d\lambda_y^2 \quad \text{in } S \times \Omega,$$

$$(1.2) \quad \partial_t u(t, x, y) - d_1 \Delta_y u(t, x, y) = -k\eta(u(t, x, y), v(t, x, y)) \quad \text{in } S \times \Omega \times Y,$$

$$(1.3) \quad \partial_t v(t, x, y) - d_2 \Delta_y v(t, x, y) = -\alpha k\eta(u(t, x, y), v(t, x, y)) \quad \text{in } S \times \Omega \times Y,$$

with macroscopic non-homogeneous Dirichlet boundary condition

$$(1.4) \quad U(t, x) = U^{ext}(t, x) \quad \text{on } S \times \partial\Omega,$$

and microscopic homogeneous Neumann boundary conditions

$$(1.5) \quad \nabla_y u(t, x, y) \cdot n_y = 0 \quad \text{on } S \times \Omega \times \Gamma_N,$$

$$(1.6) \quad \nabla_y v(t, x, y) \cdot n_y = 0 \quad \text{on } S \times \Omega \times \Gamma.$$

The coupling between the micro- and the macro-scale is made by the following nonlinear transmission condition on Γ_R

$$(1.7) \quad -\nabla_y u(t, x, y) \cdot n_y = -b(U(t, x) - u(t, x, y)) \quad \text{on } S \times \Omega \times \Gamma_R.$$

The initial conditions

$$(1.8) \quad U(0, x) = U_I(x) \quad \text{in } \Omega,$$

$$(1.9) \quad u(0, x, y) = u_I(x, y) \quad \text{in } \Omega \times Y,$$

$$(1.10) \quad v(0, x, y) = v_I(x, y) \quad \text{in } \Omega \times Y,$$

close the system of mass-balance equations.

Continuing along the lines of [7], the central theme of this paper is understanding the role of the nonlinear term $b(\cdot)$ in what the *a priori* and *a posteriori* error analyses of (1.1)–(1.10) are concerned. Within the frame of this paper, we focus on the *a priori* analysis and consequently prepare a functional framework for the *a posteriori* analysis which is still missing for such situations. Since our problem is new, the existing well-established literature on *a priori error* estimates for linear two-scale problems (cf. e.g. [6]) cannot guess the rate of convergence of the Galerkin approximants to the weak solution to (1.1)–(1.10). Therefore, a new analysis approach is needed. Notice that the main difficulty is created by the presence of a boundary nonlinear term entering the transmission condition (1.7). Here we prove the rate of convergence of the two-scale Galerkin method proposed in [7] for approximating this system in the case when both the microstructure and macroscopic domain are two-dimensional, see Theorem 3.5. Nevertheless, we expect that the results can be extended to the 3D case under stronger assumptions, for instance, on the regularity of Γ_R and data. Besides using the particular two-scale structure of the system, the ingredients of the proof include two-scale interpolation-error estimates, an interpolation-trace inequality, and improved regularity estimates.

The paper is structured in the following fashion:

CONTENTS

1. Introduction	1
1.1. Problem statement	1
1.2. Geometry of the domain	3
1.3. Physical interpretation of (1.1)–(1.10)	3

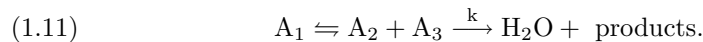
2. Technical preliminaries	4
2.1. Assumptions on data, parameters, and spatial domains Ω, Y	4
2.2. Weak formulation. Known results	4
2.3. Galerkin approximation. Basic (semi-discrete) estimates	5
3. Estimating the rate of convergence: The case $Y \subset \Omega \subset \mathbb{R}^2$	7
3.1. Approximation of smooth two-scale functions	7
3.2. Main result. Proof of Theorem 3.5	9
Acknowledgments	13
References	13

1.2. Geometry of the domain. We assume the domains Ω and Y to be connected in \mathbb{R}^3 with Lipschitz continuous boundaries. We denote by λ^k the k -dimensional Lebesgue measure ($k \in \{2, 3\}$), and assume that $\lambda^3(\Omega) \neq 0$ and $\lambda^3(Y) \neq 0$. Here, Ω is the macroscopic domain, while Y denotes the part of a standard pore associated with microstructures within Ω . To be more precise, Y represents the wet part of the pore. The boundary of Y is denoted by Γ , and consists of two distinct parts

$$\Gamma = \Gamma_R \cup \Gamma_N.$$

Here $\Gamma_R \cap \Gamma_N = \emptyset$, and $\lambda_y^2(\Gamma_R) \neq 0$. Note that Γ_N is the part of ∂Y that is isolated with respect to transfer of mass (i.e. Γ_N is a Neumann boundary), while Γ_R is the gas/liquid interface along which the mass transfer takes place. Throughout the paper λ_y^k ($k \in \{1, 2\}$) denotes the k -dimensional Lebesgue measure on the boundary ∂Y of the microstructure.

1.3. Physical interpretation of (1.1)–(1.10). U , u , and v are the mass concentrations assigned to the chemical species A_1 , A_2 , and A_3 involved in the reaction mechanism



For instance, the natural carbonation of stone follows the mechanism (1.11), where $A_1 := \text{CO}_2(\text{g})$, $A_2 := \text{CO}_2(\text{aq})$, and $A_3 := \text{Ca}(\text{OH})_2(\text{aq})$, while the product of reaction is in this case $\text{CaCO}_3(\text{aq})$. We refer the reader to [1] for details on the mathematical analysis of a (macroscopic) reaction-diffusion system with free boundary describing the evolution of (1.11) in concrete.

Besides overlooking what happens with the produced $\text{CaCO}_3(\text{aq})$, the PDE system also indicates that we completely neglect the water as reaction product in (1.11) as well as its motion inside the microstructure Y . A correct modeling of the role of water is possible. However, such an extension of the model would essentially complicate the structure of the PDE system and would bring us away from our initial goal. On the other hand, it is important to observe that the sink/source term

$$(1.12) \quad - \int_{\Gamma_R} b(U - u) d\lambda_y^2$$

models the contribution in the effective equation (1.1) coming from mass transfer between air and water regions at microscopic level. Surface integral terms like (1.12) have been obtained in the context of two-scale models (for the so-called Henry and Raoult laws [3] – linear choices of $b(\cdot)$!) by various authors; see for instance [5]

and references cited therein. The parameter k is the reaction constant for the competitive reaction between the species A_2 and A_3 , while α is the ratio of the molecular weights of these two species. Furthermore, we denote by θ the porosity of the medium.

2. TECHNICAL PRELIMINARIES

2.1. Assumptions on data, parameters, and spatial domains Ω, Y . For the transport coefficients, we assume that

$$(A1) \quad D > 0, d_1 > 0, d_2 > 0.$$

Concerning the micro-macro transfer and the reaction terms, we suppose:

$$(A2) \quad \text{The sink/source term } b : \mathbb{R} \rightarrow \mathbb{R}_+ \text{ is globally Lipschitz, and } b(z) = 0 \text{ if } z \leq 0. \text{ This implies that it exists a constant } \hat{c} > 0 \text{ such that } b(z) \leq \hat{c}z \text{ if } z > 0;$$

$$(A3) \quad \eta : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}_+ \text{ is defined by } \eta(r, s) := R(r)Q(s), \text{ where } R, Q \text{ are globally Lipschitz continuous, with Lipschitz constants } c_R \text{ and } c_Q \text{ respectively. Furthermore, we assume that } R(r) > 0 \text{ if } r > 0 \text{ and } R(r) = 0 \text{ if } r \leq 0, \text{ and similarly, } Q(s) > 0 \text{ if } s > 0 \text{ and } Q(s) = 0 \text{ if } s \leq 0.$$

Finally, we have $k > 0$, and $\alpha > 0$.

For the initial and boundary functions, we assume

$$(A4) \quad U^{ext} \in H^1(S, H^2(\Omega)) \cap H^2(S, L^2(\Omega)) \cap L_+^\infty(S \times \Omega), \quad U_I \in H^2(\Omega) \cap L_+^\infty(\Omega), \\ U_I - U^{ext}(0, \cdot) \in H_0^1(\Omega), \quad u_I, v_I \in L^2(\Omega, H^2(Y)) \cap L_+^\infty(\Omega \times Y).$$

For the approximation with piecewise linear functions (finite elements), we assume:

$$(A5) \quad \Omega \text{ and } Y \text{ are convex domains in } \mathbb{R}^2 \text{ with sufficiently smooth boundaries;}$$

$$(A6) \quad h^2 \max\{\gamma_1, \gamma_3\} < 1, \text{ where } h, \gamma_1, \text{ and } \gamma_3 \text{ are strictly positive constants entering the statement of Lemma 3.1.}$$

2.2. Weak formulation. Known results. Our concept of weak solution is given in the following.

Definition 2.1. A triplet of functions (U, u, v) with $(U - U^{ext}) \in L^2(S, H_0^1(\Omega))$, $\partial_t U \in L^2(S \times \Omega)$, $(u, v) \in L^2(S, L^2(\Omega, H^1(Y)))^2$, $(\partial_t u, \partial_t v) \in L^2(S \times \Omega \times Y)^2$, is called a weak solution of (1.1)–(1.10) if for a.e. $t \in S$ the following identities hold

$$(2.1) \quad \frac{d}{dt} \int_{\Omega} \theta U \varphi + \int_{\Omega} D \nabla U \nabla \varphi + \int_{\Omega} \int_{\Gamma_R} b(U - u) \varphi d\lambda_y^2 dx = 0 \\ \frac{d}{dt} \int_{\Omega \times Y} u \phi + \int_{\Omega \times Y} d_1 \nabla_y u \nabla_y \phi - \int_{\Omega} \int_{\Gamma_R} b(U - u) \phi d\lambda_y^2 dx$$

$$(2.2) \quad + k \int_{\Omega \times Y} \eta(u, v) \phi = 0$$

$$(2.3) \quad \frac{d}{dt} \int_{\Omega \times Y} v \psi + \int_{\Omega \times Y} d_2 \nabla_y v \nabla_y \psi + \alpha k \int_{\Omega \times Y} \eta(u, v) \psi = 0,$$

for all $(\varphi, \phi, \psi) \in H_0^1(\Omega) \times L^2(\Omega; H^1(Y))^2$, and

$$U(0) = U_I \text{ in } \Omega, \quad u(0) = u_I, \quad v(0) = v_I \text{ in } \Omega \times Y.$$

Theorem 2.2. *It exists a globally-in-time unique positive and essentially bounded solution (U, u, v) in the sense of Definition 2.1.*

Proof. We refer the reader to [7] for the proof of this result. \square

2.3. Galerkin approximation. Basic (semi-discrete) estimates. Following the lines of [7, 9], we introduce the Schauder bases: Let $\{\xi_i\}_{i \in \mathbb{N}}$ be a basis of $L^2(\Omega)$, with $\xi_j \in H_0^1(\Omega)$, forming an orthonormal system (say o.n.s.) with respect to $L^2(\Omega)$ -norm. Furthermore, let $\{\zeta_{jk}\}_{j,k \in \mathbb{N}}$ be a basis of $L^2(\Omega \times Y)$, with

$$(2.4) \quad \zeta_{jk}(x, y) = \xi_j(x)\eta_k(y),$$

where $\{\eta_k\}_{k \in \mathbb{N}}$ is a basis of $L^2(Y)$, with $\eta_k \in H^1(Y)$, forming an o.n.s. with respect to $L^2(Y)$ -norm.

Let us also define the projection operators on finite dimensional subspaces P_x^N, P_y^N associated to the bases $\{\xi_j\}_{j \in \mathbb{N}}$, and $\{\eta_k\}_{k \in \mathbb{N}}$ respectively. For (φ, ψ) of the form

$$\begin{aligned} \varphi(x) &= \sum_{j \in \mathbb{N}} a_j \xi_j(x), \\ \psi(x, y) &= \sum_{j, k \in \mathbb{N}} b_{jk} \xi_j(x) \eta_k(y), \end{aligned}$$

we define

$$(2.5) \quad (P_x^N \varphi)(x) = \sum_{j=1}^N a_j \xi_j(x),$$

$$(2.6) \quad (P_x^N \psi)(x, y) = \sum_{j=1}^N \sum_{k \in \mathbb{N}} b_{jk} \sigma_j(x) \eta_k(y)$$

$$(2.7) \quad (P_y^N \psi)(x, y) = \sum_{j \in \mathbb{N}} \sum_{k=1}^N b_{jk} \sigma_j(x) \eta_k(y).$$

The bases $\{\sigma_j\}_{j \in \mathbb{N}}$, and $\{\eta_k\}_{k \in \mathbb{N}}$ are chosen such that the projection operators P_x^N, P_y^N are stable with respect to the L^∞ -norm and H^2 -norm; i.e. for a given function the L^∞ -norm and H^2 -norm of the truncations by the projection operators can be estimated by the corresponding norms of the function.

Remark 2.3. Apparently, this choice of bases is rather restrictive. It is worth noting that we can remove the requirement that P_x^N, P_y^N are stable with respect to the L^∞ -norm in the case we work with a globally Lipschitz choice for the mass-transfer term $b(\cdot)$. We will give detailed explanations on this aspect elsewhere.

Now, we look for finite-dimensional approximations of order $N \in \mathbb{N}$ for the functions $U_0 := U - U^{ext}$, u , and v , of the following form

$$(2.8) \quad U_0^N(t, x) = \sum_{j=1}^N \alpha_j^N(t) \xi_j(x),$$

$$(2.9) \quad u^N(t, x, y) = \sum_{j, k=1}^N \beta_{jk}^N(t) \xi_j(x) \eta_k(y),$$

$$(2.10) \quad v^N(t, x, y) = \sum_{j, k=1}^N \gamma_{jk}^N(t) \xi_j(x) \eta_k(y),$$

where the coefficients $\alpha_j^N, \beta_{jk}^N, \gamma_{jk}^N, j, k = 1, \dots, N$ are determined by the following relations:

$$(2.11) \quad \int_{\Omega} \theta \partial_t U_0^N(t) \varphi dx + \int_{\Omega} D \nabla U_0^N(t) \nabla \varphi dx = \\ - \int_{\Omega} \left(\int_{\Gamma_R} b((U_0^N + U^{ext} - u^N)(t)) d\lambda_y^2 + \theta \partial_t U^{ext}(t) + D \Delta U^{ext}(t) \right) \varphi dx$$

$$(2.12) \quad \int_{\Omega \times Y} \partial_t u^N(t) \phi dx dy + \int_{\Omega \times Y} d_1 \nabla_y u^N(t) \nabla_y \phi dx dy = \\ \int_{\Omega} \int_{\Gamma_R} b((U_0^N + U^{ext} - u^N)(t)) \phi d\lambda_y^2 dx - k \int_{\Omega \times Y} \eta(u^N(t), v^N(t)) \phi dy dx$$

$$(2.13) \quad \int_{\Omega \times Y} \partial_t v^N(t) \psi dy dx + \int_{\Omega \times Y} d_2 \nabla_y v^N(t) \nabla_y \psi dy dx = \\ - \alpha k \int_{\Omega \times Y} \eta(u^N(t), v^N(t)) \psi dy dx$$

for all $\varphi \in \text{span}\{\xi_j : j \in \{1, \dots, N\}\}$, and $\phi, \psi \in \text{span}\{\zeta_{jk} : j, k \in \{1, \dots, N\}\}$, and

$$(2.14) \quad \alpha_j^N(0) := \int_{\Omega} (U_I - U^{ext}(0)) \xi_j dx,$$

$$(2.15) \quad \beta_{jk}^N(0) := \int_{\Omega} \int_Y u_I \zeta_{jk} dx dy,$$

$$(2.16) \quad \gamma_{jk}^N(0) := \int_{\Omega} \int_Y v_I \zeta_{jk} dx dy.$$

Theorem 2.4. *Assume that the projection operators P_x^N, P_y^N , defined in (2.5)-(2.7), are stable with respect to the L^∞ -norm and H^2 -norm, and that (A1)-(A4) are satisfied. Then the following statements hold:*

- (i) *The finite-dimensional approximations $U_0^N(t)$, $u^N(t)$, and $v^N(t)$ are positive and uniformly bounded. More precisely, we have for a.e. $(x, y) \in \Omega \times Y$, all $t \in S$, and all $N \in \mathbb{N}$*

$$(2.17) \quad 0 \leq U_0^N(t, x) \leq m_1, \quad 0 \leq u^N(t, x, y) \leq m_2, \quad 0 \leq v^N(t, x, y) \leq m_3,$$

where

$$m_1 := 2 \|U^{ext}\|_{L^\infty(S \times \Omega)} + \|U_I\|_{L^\infty(\Omega)},$$

$$m_2 := \max\{\|u_I\|_{L^\infty(\Omega \times Y)}, m_1\},$$

$$m_3 := \|v_I\|_{L^\infty(\Omega \times Y)}.$$

- (ii) *There exists a constant $c > 0$, independent of N , such that*

$$(2.18) \quad \|U_0^N\|_{L^\infty(S, H^1(\Omega))} + \|\partial_t U_0^N\|_{L^2(S, L^2(\Omega))} \leq c,$$

$$(2.19) \quad \|u^N\|_{L^\infty(S, L^2(\Omega; H^1(Y)))} + \|\partial_t u^N\|_{L^2(S, L^2(\Omega; L^2(Y)))} \leq c,$$

$$(2.20) \quad \|v^N\|_{L^\infty(S, L^2(\Omega; H^1(Y)))} + \|\partial_t v^N\|_{L^2(S, L^2(\Omega; L^2(Y)))} \leq c,$$

- (iii) *Then there exists a constant $c > 0$, independent of N , such that the following estimates hold*

$$(2.21) \quad \|\nabla_x u^N\|_{L^\infty(S, L^2(\Omega \times Y))} + \|\nabla_x v^N\|_{L^\infty(S, L^2(\Omega \times Y))} \leq c$$

$$(2.22) \quad \|\nabla_y \nabla_x u^N\|_{L^2(S, L^2(\Omega \times Y))} + \|\nabla_y \nabla_x v^N\|_{L^2(S, L^2(\Omega \times Y))} \leq c.$$

Proof. This statement combines the information stated in Theorem 6.1 and Theorem 6.2 from [7]. We refer the reader to the cited paper for the proof details. \square

With these estimates in hand, we have enough compactness to establish the convergence of the Galerkin approximates to the weak solution of our problem.

Theorem 2.5. *There exists a subsequence, again denoted by (U_0^N, u^N, v^N) , and a limit $(U_0, u, v) \in L^2(S; H^1(\Omega)) \times [L^2(S; L^2(\Omega; H^1(Y)))]^2$, with $(\partial_t U_0^N, \partial_t u^N, \partial_t v^N) \in L^2(S \times \Omega) \times [L^2(S \times \Omega \times Y)]^2$, such that*

$$\begin{aligned} (U_0^N, u^N, v^N) &\rightharpoonup (U_0, u, v) \text{ weakly in } L^2(S; H^1(\Omega)) \times [L^2(S; L^2(\Omega; H^1(Y)))]^2 \\ (\partial_t U_0^N, \partial_t u^N, \partial_t v^N) &\rightharpoonup (\partial_t U_0, \partial_t u, \partial_t v) \text{ weakly in } L^2 \\ (U_0^N, u^N, v^N) &\rightarrow (U_0, u, v) \text{ strongly in } L^2 \\ u^N|_{\Gamma_R} &\rightarrow u|_{\Gamma_R} \text{ strongly in } L^2(S \times \Omega, L^2(\Gamma_R)) \end{aligned}$$

Proof. See the proof of Theorem 6.3 in [7]. \square

In the next section, we address the question we wish to answer:

How fast do the subsequences mentioned in Theorem 2.4 converge to their unique limit indicated in Theorem 2.5?

3. ESTIMATING THE RATE OF CONVERGENCE: THE CASE $Y \subset \Omega \subset \mathbb{R}^2$

Adapting some of the working ideas mentioned in [10, 8] to this two-spatial-scale scenario, we obtain an *a priori* estimate for the convergence rate of the Galerkin scheme constructed in section 2.3.

3.1. Approximation of smooth two-scale functions. As preparation for the definition of the finite element solution to our problem, we briefly introduce some concepts concerning the approximation of smooth functions in $\Omega, Y \subset \mathbb{R}^2$ (taking into account assumption (A5)); see, for instance, [2] or [10] for more details.

For simplicity, we let h denote the maximum length of the sides of the triangulations \mathcal{T}_h of both Ω and Y . h decreases as triangulations are made finer. Let's assume that we can construct quasiuniform triangulations ([10], p.2) and that the angles of these triangulations are bounded from below by uniformly in h positive constants.

Define $V_h := \text{span}\{\xi_j : j \in \{1, \dots, N\}\}$, and $B_h := \text{span}\{\eta_k : k \in \{1, \dots, N\}\}$ where ξ_j and η_k are defined as in section 2.3. We also introduce $W_h := \text{span}\{\zeta_{jk} : j, k \in \{1, \dots, N\}\}$, where ζ_{jk} are given by (2.4). Note that $W_h := V_h \times B_h$.

A given smooth function φ in Ω vanishing on $\partial\Omega$ may be approximated by the interpolant $I_h\varphi$ in the space of piecewise continuous linear functions vanishing outside $\bigcup \mathcal{T}_h$. Standard interpolation error arguments ensure that for any $\varphi \in H^2(\Omega) \cap H_0^1(\Omega)$, we get

$$\begin{aligned} \|I_h\varphi - \varphi\|_{L^2(\Omega)} &\leq ch^2 \|\varphi\|_{L^2(\Omega)} \\ \|\nabla(I_h\varphi - \varphi)\|_{L^2(\Omega)} &\leq ch \|\varphi\|_{L^2(\Omega)}. \end{aligned}$$

We define the macro and micro-macro Riesz projection operators (i.e. \mathcal{R}_h^M and \mathcal{R}_h^m) in the following manner:

$$(3.1) \quad \mathcal{R}_h^M : H^1(\Omega) \rightarrow V_h,$$

$$(3.2) \quad \mathcal{R}_h^m : L^2(\Omega; H^1(Y)) \rightarrow W_h,$$

where R_h^M is the standard single-scale Riesz projection, while \mathcal{R}_h^m is the tensor product of the projection operators

$$(3.3) \quad P^{\ell 0} : L^2(\Omega) \rightarrow V_h$$

$$(3.4) \quad P^{\ell 1} : H^1(Y) \rightarrow B_h.$$

Note that this construction of the micro-macro Riesz projection is quite similar to the one proposed in [6] (cf. especially the proof of Lemma 3.1 *loc. cit.*). The only difference is that we do not require any periodic distribution of the microstructure Y . Consequently, if one assumes a periodic covering of Ω by replicates of Y sets, then one recovers the situation dealt with in [6].

Lemma 3.1. (*Interpolation-error estimates*) *Let \mathcal{R}_h^m and \mathcal{R}_h^M be the micro and, respectively, macro Riesz's projection operators. Then there exist the strictly positive constants γ_ℓ ($\ell \in \{1, 2, 3, 4\}$), which are independent of h , such that the Lagrange interpolants $\mathcal{R}_h^m \phi$ and $\mathcal{R}_h^M \varphi$ satisfy the inequalities:*

$$(3.5) \quad \|\varphi - \mathcal{R}_h^M \varphi\|_{L^2(\Omega)} \leq \gamma_1 h^2 \|\varphi\|_{H^2(\Omega)},$$

$$(3.6) \quad \|\varphi - \mathcal{R}_h^M \varphi\|_{H^1(\Omega)} \leq \gamma_2 h \|\varphi\|_{H^2(\Omega)},$$

$$(3.7) \quad \|\varphi - \mathcal{R}_h^m \phi\|_{L^2(\Omega; L^2(Y))} \leq \gamma_3 h^2 (\|\phi\|_{L^2(\Omega; H^2(Y)) \cap L^2(Y; H^2(\Omega))}),$$

$$(3.8) \quad \|\phi - \mathcal{R}_h^m \phi\|_{L^2(\Omega; H^1(Y))} \leq \gamma_4 h (\|\phi\|_{L^2(\Omega; H^2(Y)) \cap L^2(Y; H^2(\Omega))})$$

for all $(\varphi, \phi) \in H^2(\Omega) \times [L^2(\Omega; H^2(Y)) \cap L^2(Y; H^2(\Omega))]$.

Proof. (3.5) and (3.6) are standard interpolation-error estimates, see [10], e.g., while (3.7) and (3.8) are interpolation-error estimates especially tailored for elliptic problems with two-spatial scales structures; see Lemma 3.1 [6] (and its proof) for a statement referring to the periodic case with $(n-1)$ -spatially separated scales. One of the key ideas of the proof is to see the spaces $L^2(\Omega, L^2(Y))$ and $L^2(\Omega, H^1(Y))$ as tensor products of the spaces $L^2(\Omega)$ and $L^2(Y)$, and respectively of $L^2(\Omega)$ and $H^1(Y)$. \square

Remark 3.2. Note that, without essential differences, this study can be done in terms of two distinct triangulations \mathcal{T}_{h_M} and \mathcal{T}_{h_m} , where h_M and h_m are maximum length of the sides of the corresponding triangulation of the macro and micro domains (Ω and Y).

Unless otherwise specified, the expressions $|\cdot|$ and $\|\cdot\|$ denote the L^2 and H^1 norms, respectively, in the corresponding function spaces.

3.2. Main result. Proof of Theorem 3.5.

Definition 3.3. (Weak solution of semi-discrete formulation) The triplet (U_0^h, u^h, v^h) is called weak solution of the semi-discrete formulation (2.12)-(2.13) if and only if

$$(3.9) \quad \int_{\Omega} \theta \partial_t U_0^h(t) \varphi dx + \int_{\Omega} D \nabla U_0^h(t) \nabla \varphi dx = \\ - \int_{\Omega} \left(\int_{\Gamma_R} b((U_0^h + U^{ext} - u^h)(t)) d\lambda_y^1 + \theta \partial_t U^{ext}(t) + D \Delta U^{ext}(t) \right) \varphi dx$$

$$(3.10) \quad \int_{\Omega \times Y} \partial_t u^h(t) \phi dx dy + \int_{\Omega \times Y} d_1 \nabla_y u^N(t) \nabla_y \phi dx dy = \\ \int_{\Omega} \int_{\Gamma_R} b((U_0^h + U^{ext} - u^h)(t)) \phi d\lambda_y^1 dx - k \int_{\Omega \times Y} \eta(u^h(t), v^h(t)) \phi dy dx$$

$$(3.11) \quad \int_{\Omega \times Y} \partial_t v^h(t) \psi dy dx + \int_{\Omega \times Y} d_2 \nabla_y v^h(t) \nabla_y \psi dy dx = \\ - \alpha k \int_{\Omega \times Y} \eta(u^h(t), v^h(t)) \psi dy dx$$

for all $\varphi \in V_h$ and $(\phi, \psi) \in W_h \times W_h$ and $U_0^h(0) = U_I \in L^2(\Omega)$ and $u^h(0), v^h(0) \in L^2(\Omega \times Y)$.

Lemma 3.4. (Improved regularity) Assume (A1)–(A5) to hold. Then

$$(3.12) \quad U_0^h \in L^2(S; H^2(\Omega))$$

$$(3.13) \quad u^h, v^h \in L^2(S; L^2(\Omega; H^2(Y))) \cap L^2(S; L^2(Y; H^2(\Omega))).$$

Proof. Assumption (A5) and a standard lifting regularity argument leads to $U_0^h \in L^2(S; H^2(\Omega))$ and $u^h, v^h \in L^2(S \times \Omega; H^2(Y))$. Employing difference quotients with respect to the variable x (quite similarly to the proof of Theorem 6.2 [7]), we can show that $u^h, v^h \in L^2(S \times Y; H^2(\Omega))$. We omit the proof details. \square

Theorem 3.5. (Rate of convergence) Assume (A1)–(A5) are satisfied. If additionally, assumption (A6) holds, then it exists a constant $\mathcal{K} > 0$, which is independent of h , such that

$$(3.14) \quad \|U_0 - U_0^h\|_{L^2(S; H^1(\Omega))}^2 + \|u - u^h\|_{L^2(S; L^2(\Omega; H^2(Y))) \cap L^2(S; L^2(Y; H^2(\Omega)))}^2 \\ + \|v - v^h\|_{L^2(S; L^2(\Omega; H^2(Y))) \cap L^2(S; L^2(Y; H^2(\Omega)))}^2 \leq \mathcal{K} h^2.$$

Remark 3.6. We will compute the constant \mathcal{K} explicitly; see (3.28).

Proof. (of Theorem 3.5) Firstly, we denote the errors terms by

$$e_U := U_0 - U_0^h \\ e_u := u - u^h \\ e_v := v - v^h.$$

We choose as test functions in Definition 3.3 the triplet

$$(3.15) \quad (\varphi, \phi, \psi) := (r^h - U_0^h, p^h - u^h, q^h - v^h),$$

where the functions r^h , p^h , and q^h will be chosen in a precise way (in terms of Riesz projections of the unknowns) at a later stage. We obtain

$$\begin{aligned}
(3.16) \quad & \frac{\theta}{2} \frac{d}{dt} |U_0 - U^h|^2 + D \|U - U^h\|^2 \leq \int_{\Omega} \theta \partial_t (U_0 - U^h) (U_0 - U^h) \\
& + \int_{\Omega} D \nabla (U_0 - U_0^h) \nabla (U_0 - U^h) \\
& = \theta \int_{\Omega} \partial_t (U_0 - U^h) (U_0 - r^h) + \int_{\Omega} D \nabla (U_0 - U^h) \nabla (U_0 - r^h) \\
& + \theta \int_{\Omega} \partial_t (U_0 - U^h) (r^h - U^h) + \int_{\Omega} D \nabla (U_0 - U^h) \nabla (r^h - U^h).
\end{aligned}$$

Using Cauchy-Schwarz inequality, we have

$$\begin{aligned}
(3.17) \quad & \frac{\theta}{2} \frac{d}{dt} |U_0 - U^h|^2 + D \|U_0 - U^h\|^2 \leq \theta |\partial_t (U_0 - U^h)| |U - r^h| \\
& + D |\nabla (U_0 - U^h)| |\nabla (U_0 - r^h)| \\
& + \theta |\partial_t (U_0 - U^h)| |r^h - U^h| + D |\nabla (U_0 - U^h)| |\nabla (r^h - U^h)| \\
& \leq \theta |\partial_t (U_0 - U^h)| |U - r^h| + D |\nabla (U_0 - U^h)| |\nabla (U_0 - r^h)| \\
& + \int_{\Omega} \int_{\Gamma_R} |b(U_0 - u) - b(U_0^h - u^h)| |r^h - U^h| d\lambda_y^1.
\end{aligned}$$

Noticing that $r^h - U_0 = (r^h - U_0) + (U_0 - U^h)$, (3.17) leads to

$$\begin{aligned}
(3.18) \quad & \frac{\theta}{2} \frac{d}{dt} |e_U|^2 + D \|e_U\|^2 \leq \theta |\partial_t e_U| |U - r^h| + D |\nabla e_U| |\nabla (U_0 - r^h)| \\
& + \hat{c} \int_{\Omega} \int_{\Gamma_R} (|e_U| + |e_u|) (|r^h - U_0| + |e_U|) d\lambda_y^1.
\end{aligned}$$

Proceeding similarly with the remaining two equations, we get:

$$\begin{aligned}
(3.19) \quad & \frac{1}{2} |\partial_t e_u|^2 + d_1 |\nabla_y e_u|^2 \leq |\partial_t (u - u^h)| |u - p^h| + d_1 |\nabla (u - u^h)| |\nabla (u - p^h)| \\
& + |\partial_t (u - u^h)| |p^h - u^h| + d_1 |\nabla (u - u^h)| |\nabla (p^h - u^h)| \\
& \leq |\partial_t e_u| |u - p^h| + d_1 |\nabla_y e_u| |\nabla_y (u - p^h)| \\
& + \int_{\Omega} \int_{\Gamma_R} |b(U_0 - u) - b(U^h - u^h)| |p^h - u^h| d\lambda_y^1 \\
& + k \int_{\Omega \times Y} |\eta(u, v) - \eta(u^h, v^h)| |p^h - u^h| \\
& \leq |\partial_t e_u| |u - p^h| + d_1 |\nabla_y e_u| |\nabla (u - p^h)| \\
& + \hat{c} \int_{\Omega} \int_{\Gamma_R} (|e_U| + |e_u|) (|p^h - u| + |e_u|) d\lambda_y^1 \\
& + k \int_{\Omega \times Y} |R(u)Q(v) - R(u^h)Q(v^h)| (|p^h - u| + |e_u|).
\end{aligned}$$

Finally, we also obtain

$$(3.20) \quad \int_{\Omega \times Y} |\partial_t e_v|^2 + d_2 \int_{\Omega \times Y} |\nabla_y e_v|^2 \leq |\partial_t e_v| |v - q^h| + d_2 |\nabla_y e_v| |\nabla_y (v - q^h)| \\ + \alpha k \int_{\Omega \times Y} |R(u)Q(v) - R(u^h)Q(v^h)| (|q^h - v| + |e_v|).$$

Putting together (3.18), (3.19), and (3.20), we obtain

$$\begin{aligned} \frac{\theta}{2} \frac{d}{dt} |e_U|^2 &+ \frac{1}{2} \frac{d}{dt} |e_u|^2 + \frac{1}{2} \frac{d}{dt} |e_v|^2 + D \|e_U\|^2 \\ &+ d_1 \|e_u\|^2 + d_2 \|e_v\|^2 \leq \theta |\partial_t e_U| |U_0 - r^h| \\ &+ |\partial_t e_u| |u - p^h| + |\partial_t e_v| |v - q^h| + D \|e_U\| |\nabla(U_0 - r^h)| \\ &+ d_1 \|e_v\| |\nabla(v - p^h)| + d_2 \|e_v\| |\nabla_y(v - q^h)| \\ &+ \hat{c} \int_{\Omega} \int_{\Gamma_R} (|e_U| + |e_u|) (|r^h - U_0| + |e_U|) d\lambda_y^1 \\ &+ \hat{c} \int_{\Omega} \int_{\Gamma_R} (|e_U| + |e_u|) (|p^h - u| + |e_u|) d\lambda_y^1 \\ &+ \int_{\Omega \times Y} k(1 + \alpha) |R(u)Q(v) - R(u^h)Q(v^h)| (|p^h - u| + |q^h - v| + |e_u| + |e_v|) \\ &=: \sum_{\ell=1}^4 I_{\ell}, \end{aligned}$$

where the terms I_{ℓ} ($\ell \in \{1, \dots, 4\}$) are given by

$$\begin{aligned} I_1 &:= \theta |\partial_t e_U| |U_0 - r^h| + |\partial_t e_u| |u - p^h| + |\partial_t e_v| |v - q^h| \\ I_2 &:= D |\nabla e_U| |\nabla(U_0 - r^h)| + d_1 |\nabla_y e_u| |\nabla_y(u - p^h)| + d_2 |\nabla_y e_v| |\nabla_y(v - q^h)| \\ I_3 &:= \hat{c} \int_{\Omega} \int_{\Gamma_R} (|e_U| + |e_u|) (|r^h - U_0| + |p^h - u| + |e_U| + |e_u|) d\lambda_y^1 \\ I_4 &:= k(1 + \alpha) \int_{\Omega \times Y} |R(u)Q(v) - R(u^h)Q(v^h)| (|p^h - u| + |q^h - v| + |e_u| + |e_v|). \end{aligned}$$

We choose now r^h , p^h , and q^h to be the respective Riesz projections of U_0^h , u^h , and v^h and estimate each of these I_{ℓ} terms, i.e. we set

$$(3.21) \quad r^h := \mathcal{R}_h^M U^h, \quad p^h := \mathcal{R}_h^m u^h, \quad \text{and} \quad q^h := \mathcal{R}_h^m v^h.$$

The main ingredients used in getting the next estimates are Young's inequality, the interpolation-error estimates stated in Lemma 3.1, the improved regularity estimates from Lemma 3.4, as well as an interpolation-trace inequality (see the appendix in [4], e.g.).

Let us denote for terseness

$$X := L^2(S; L^2(\Omega; H^2(Y))) \cap L^2(S; L^2(Y; H^2(\Omega))).$$

We obtain following estimates:

$$\begin{aligned}
|I_1| &\leq \gamma_1 \theta |\partial_t e_U| h^2 \|U_0\|_{H^2(\Omega)} + \gamma_3 h^2 (|\partial_t e_u + \partial_t e_v|) (\|u\|_X + \|v\|_X) \\
&\leq h^2 \frac{\gamma_1 \theta}{2} \left(|\partial_t e_U|^2 + \|U_0\|_{H^2(\Omega)}^2 \right) + h^2 \frac{\gamma_3}{2} (|\partial_t e_u|^2 + \|u\|_X^2) \\
(3.22) \quad &+ h^2 \frac{\gamma_3}{2} (|\partial_t e_v|^2 + \|v\|_X^2).
\end{aligned}$$

$$\begin{aligned}
|I_2| &\leq \gamma_2 D \|\nabla e_U\| h \|U\|_{H^2(\Omega)} + \gamma_4 d_1 |\nabla_y e_u| h \|u\|_X + \gamma_4 d_2 |\nabla_y e_v| h \|v\|_X \\
&\leq \epsilon \|\nabla e_U\|^2 + h^2 c_\epsilon \gamma_2^2 D^2 \|U_0\|_{H^2(\Omega)}^2 + \epsilon \|\nabla_y e_u\|^2 + h^2 c_\epsilon \gamma_4^2 d_1^2 \|u\|_X^2 \\
&\quad + \epsilon \|\nabla_y e_v\|^2 + h^2 c_\epsilon \gamma_4^2 d_2^2 \|v\|_X^2 \\
&\leq h^2 c^* c_\epsilon (\gamma_2^2 + 2\gamma_4^2) (D^2 + d_1^2 + d_2^2) (\|U_0\|_{H^2(\Omega)} + \|u\|_X^2 + \|v\|_X^2) \\
(3.23) \quad &+ \epsilon \|\nabla e_U\|^2 + \epsilon \|\nabla_y e_u\|^2 + \epsilon \|\nabla_y e_v\|^2,
\end{aligned}$$

where the constant $c^* > 0$ is sufficiently large.

The estimate on $|I_3|$ is a bit delicate. To get it, we repeatedly use the following interpolation-trace estimate

$$(3.24) \quad \|\varphi\|_{L^2(\Omega); L^2(\Gamma_R)}^2 \leq \epsilon \int_{\Omega} |\nabla_y \varphi|_{L^2(Y)}^2 + c(c_\epsilon + 1) \|\varphi\|_{L^2(\Omega; L^2(Y))}^2,$$

for the case when $\varphi \in \{e_u, e_v\}$, where $\epsilon > 0$ and $c, c_\epsilon \in]0, \infty[$ are fixed constants.

We get

$$\begin{aligned}
|I_3| &\leq \hat{c} \lambda(\Gamma_R) \int_{\Omega} |e_U| |r^h - U_0| + \hat{c} \int_{\Omega} |r^h - U_0| \int_{\Gamma_R} |e_u| d\lambda_y^1 \\
&\quad + \int_{\Omega} |e_U| \int_{\Gamma_R} |p^h - u| + \hat{c} \int_{\Omega} \int_{\Gamma_R} |e_u| |p^h - u| d\lambda_y^1 + 2\hat{c} \int_{\Omega} \int_{\Gamma_R} (|e_u|^2 + |e_v|^2) d\lambda_y^1 \\
&\leq \frac{\hat{c} \lambda(\Gamma_R)}{2} \left(\|e_U\|_{H^2(\Omega)}^2 + \gamma_1 h^4 \|U_0\|_{H^2(\Omega)}^2 \right) \\
&\quad + \frac{\hat{c}}{2} \left(\gamma_1 \lambda(\Gamma_R) h^4 \|U_0\|_{H^2(\Omega)}^2 + \|e_u\|_{L^2(\Omega; L^2(\Gamma_R))} \right) \\
&\quad + \frac{\hat{c}}{2} \left(|\lambda(\Gamma_R)| \|e_U\|_{H^2(\Omega)}^2 + \epsilon h^2 \gamma_4^2 \|u\|_X^2 + c(c_\epsilon + 1) \gamma_3 h^4 \|u\|_X^2 \right) \\
&\quad + \frac{\hat{c}}{2} \left(\epsilon \int_{\Omega} |\nabla_y e_u|^2 + c(c_\epsilon + 1) \|e_u\|_{L^2(\Omega; L^2(Y))}^2 + \epsilon h^2 \|u\|_X^2 + c(c_\epsilon + 1) \gamma_3 h^4 \|u\|_X^2 \right) \\
&\quad + 2\hat{c} \lambda(\Gamma_R) |e_U|^2 + \epsilon \int_{\Omega} |\nabla_y e_u|^2 + c(c_\epsilon + 1) \|e_u\|_{L^2(\Omega; L^2(Y))}^2. \\
(3.25)
\end{aligned}$$

In order to estimate from above the term $|I_4|$, we use the structural assumption (A3) on the reaction terms $R(\cdot)$ and $Q(\cdot)$. We obtain

$$\begin{aligned}
|I_4| &\leq k(1 + \alpha) \int_{\Omega \times Y} |R(u) - R(u^h)| |Q(v)| + |Q(v) - Q(v^h)| |R(u^h)| \times \\
&\quad \times (|p^h - u| + |q^h - v| + \|e_u\| + \|e_v\|) \\
&\leq 3h^2 k \gamma_3 (1 + \alpha) (Q_m c_R + R_m c_Q) (\|u\|_X^2 + \|v\|_X^2) \\
(3.26) \quad &+ k(1 + \alpha) (Q_m c_R + R_m c_Q) (|e_u|^2 + |e_v|^2),
\end{aligned}$$

where $R_m := \max_{r \in [0, M_2]} \{R(r)\}$, $Q_m := \max_{s \in [0, M_3]} \{R(s)\}$, while c_R and c_Q are the corresponding Lipschitz constants of R and Q .

Consequently, we obtain

$$\begin{aligned}
\sum_{\ell=1}^3 |I_\ell| &\leq h^2 \left(\frac{\gamma_1}{2} \theta |\partial_t e_U|^2 + \frac{\gamma_3}{2} |\partial_t e_u|^2 + |\partial_t e_v|^2 \right) + h^2 (\mathcal{K} + \mathcal{F}(h)) \\
&\quad + \left[k(1 + \alpha)(Q_m c_R + R_m c_Q) + \left(c + \frac{\hat{c}}{2} \right) \right] (|e_u|^2 + |e_v|^2) \\
(3.27) \quad &\quad + \epsilon |\nabla e_U|^2 + \epsilon \left(2 + \frac{\hat{c}}{2} \right) \int_{\Omega} |\nabla_y e_u|^2 + \epsilon \int_{\Omega} |\nabla_y e_v|^2,
\end{aligned}$$

where

$$\begin{aligned}
\mathcal{K} &:= \frac{\gamma_3}{2} (\|u\|_X^2 + \|v\|_X^2) \\
(3.28) \quad &\quad + \frac{\gamma_1 \theta}{2} \|U_0\|_{H^2(\Omega)}^2 + 3k\gamma_3(1 + \alpha)(Q_m c_R + R_m c_Q) (\|u\|_X^2 + \|v\|_X^2) \\
\frac{\mathcal{F}(h)}{h^2} &:= 2\epsilon\gamma_4 \|u\|_X^2 + \gamma_1 \left(1 + \frac{\hat{c}}{2} \lambda(\Gamma_R) \right) \|U_0\|_{H^2(\Omega)}^2 \\
(3.29) \quad &\quad + 2c(c_\epsilon + 1)\gamma_3 \|u\|_X^2.
\end{aligned}$$

Notice that \mathcal{K} is a finite positive constant that is independent of h , while $F :]0, \infty[\rightarrow]0, \infty[$ is a function of order of $\mathcal{O}(h^2)$ as $h \rightarrow 0$.

By (A6) we can compensate the first term of the r.h.s. of (3.27), while the last three terms from the r.h.s. can be compensated by choosing the value of ϵ as $\epsilon \in \left] 0, \min\{D, d_2, \frac{2d_1}{\hat{c}+4}\} \right[$. Relying on the way we approximate the initial data, we use now Gronwall's inequality to conclude the proof of this theorem. \square

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CENTER FOR ANALYSIS SCIENTIFIC COMPUTING AND APPLICATIONS (CASA), DEPARTMENT OF MATHEMATICS AND COMPUTER SCIENCE, INSTITUTE OF COMPLEX MOLECULAR SYSTEMS (ICMS), EINDHOVEN UNIVERSITY OF TECHNOLOGY, PO BOX 513, 5600 MB, EINDHOVEN, THE NETHERLANDS

E-mail address: `a.muntean@tue.nl`

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF SUSSEX, FALMER, BRIGHTON, BN1 9RF, UK

E-mail address: `o.lakkis@sussex.ac.uk`

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