Homogenization of multi-specie reaction-diffusion systems in domains with rough boundaries

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Abstract. We address the problem of parametrizing the boundary data for reaction-diffusion partial differential equations associated to distributed systems that possess rough boundaries. Using techniques from homogenization theory and multiple-scale analysis we present the effective equation and boundary conditions that are satisfied by the homogenized solution. We present numerical simulations that validate our theoretical results.

Keywords: Reaction-diffusion systems; Homogenization; Multiple-scale analysis
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INTRODUCTION

Reaction-diffusion systems model a large variety of process, such as physical, physiological and ecological phenomena. However, the geometry of the domains where such systems evolve may be quite complex. This poses serious practical as well as theoretical challenges. For example, many sophisticated PDE solvers balk in handling the fine scales of the boundary or the roughness may induce noise and uncertainty in measuring the state variables of the system close to the boundary. Potential applications of the results presented here include ecological systems where one finds a large spatial variability of limnological parameters in connection with boundary complexity [3, 4, 5].

One possible approach to these problems consists in generating an equivalent system, defined on a smoothed layer containing the domain, whose the parameters near the boundary depend on the rough geometry and such that the solution in the interior of the space domain is very close to the one of the original system . To this aim, a natural idea would be analyze rough boundaries with homogenization methods [1, 2, 6].

In this work, a multiple scale analysis method is used to homogenize reaction-diffusion systems in domains with rough boundaries. Our main concern is to develop the formal asymptotics and to validate it through numerical experiments. The approach proposed here follows a previous work where complete proofs of theorems are presented for the scalar case [7]. Convergence of the homogenized solution is then verified by numerical simulations.

THE MODEL

We consider a rectangular domain Ω_ε whose boundary is partly rough with periodic roughness elements Γ_ε. To model this boundary, we shall use the curve $z = h(x/\varepsilon)$ in the (x,z) plane of period ε in x (see Figure 1). Here ε refers to the basic scale where the boundary oscillation takes place and is assumed to be much smaller than the characteristic dimensions of our domain. With [2], we assume that the boundary oscillates between the lines $z = -A$ and $z = 0$. Furthermore, we assume that $z = h(x/\varepsilon)$ is monotone in the semi-period and is a differentiable function.

We assume that the dynamics of the system is described as following:

$$\partial_t \mathbf{U} - \mathbf{D}\Delta\mathbf{U} = \mathbf{G}(\mathbf{U}), \quad (x,z) \text{ in } \Omega_\varepsilon \text{ \& } t \geq 0 \tag{1}$$

where each component of the vector $\mathbf{U} = [U_1(x,z,t),\dots,U_n(x,z,t)]'$ represents the concentration of each substance, $\mathbf{D} = diag\{\sigma_i\}, i = 1,\dots,n$ is the matrix of diffusion coefficients, Δ denotes the Laplace operator and $\mathbf{G} = [g_1(U_1,\dots,U_n),\dots,g_n(U_1,\dots,U_n)]'$ accounts for all local reactions. We consider appropriate boundary conditions of Dirichlet *or* Neumann type. Namely,

$$\text{Dirichlet:} \qquad \mathbf{U} = \mathbf{0} \ , \ (x,z) \text{ on } \Gamma_\varepsilon \ , \tag{2}$$

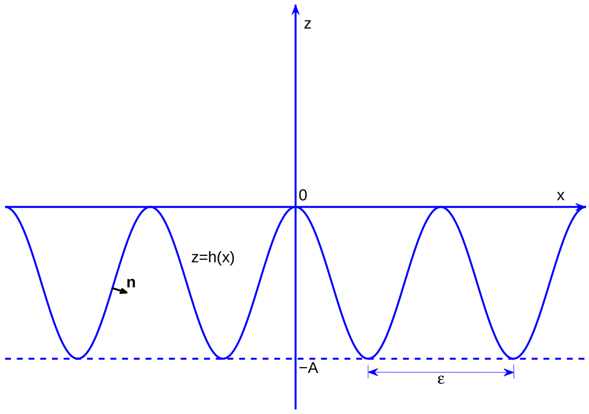

FIGURE 1. Pictorial description of a boundary segment. The upper part ($z > h(x/\varepsilon)$) represent a subset of the internal domain, the periodic curve ($z = h(x)$) is the boundary and the dashed line ($z = -A$) is the external lower boundary.

or

$$\text{Neumann:} \qquad \mathbf{DU_n} = \mathbf{0}\ ,\ (x,z) \text{ on } \Gamma_\varepsilon\ , \tag{3}$$

and suitable smooth initial conditions.
We assume that the system under consideration admits solutions in an interval of time independent of ε and that the nonlinear functions $g_i(\cdot)$ admit Taylor expansions at any point.

MAIN RESULTS

In this section we present the main results concerning the formal homogenization. In particular, two main theorems, accounting for the formal asymptotic analysis of the Neumann and Dirichlet cases, are reported.
Following [2], we introduce $y = x/\varepsilon$ and write U_i as function of x, y, z, t and ε: $U_i(x,z,t,\varepsilon) = u_i(x,y,z,t,\varepsilon)$. Here, u_i is required to be periodic in y with period 1, which is the period of the curve $z = h(y)$. Next, we assume that u_i can be expanded for ε small in the form:

$$u_i(x,x/\varepsilon,z,t,\varepsilon) = \sum_{j=0}^{2} u_i^{(j)}(x,x/\varepsilon,z,t,\varepsilon) + O(\varepsilon^3). \tag{4}$$

Moreover, let us introduce $y_1(z)$ and $y_2(z)$ as two inverses of $z = h(y)$ over one period. The first, $y_1(z)$, increases from $y_1 = 0$ at $z = 0$ to $y_1 = y_1(-A)$ at $z = -A$, and $y_2(z)$ increases from $y_2(-A) = y_1(-A)$ to $y_2(0) = 1$ as z increases from $-A$ to 0.
We can then summarize the main result in the following:

Theorem 1 (Neumann b. c.) *Let $\mathbf{U} = [U_1(x,z,t,\varepsilon),\dots,U_n(x,z,t,\varepsilon)]'$ satisfy the reaction-diffusion system (1) with Neumann boundary condition (3) on $z = h(y)$ a differentiable 1-periodic function. Suppose that $U_i = u_i(x,y,z,t,\varepsilon)$ has the asymptotic form (4), where u_i is 1-periodic in y. Then, $u_i^{(0)}(x,z,t)$ is independent of y for $-A \le z \le 0$ and is a solution of the problem:*

$$\begin{array}{l}
\partial_t \mathbf{u}^{(0)} - \mathbf{D}\Delta \mathbf{u}^{(0)} = \mathbf{F}(\mathbf{u}^{(0)}), \quad z > 0 \\
\partial_t \mathbf{u}^{(0)} - \mathbf{D_{eff}}\partial_{zz}\mathbf{u}^{(0)} = \mathbf{F}(\mathbf{u}^{(0)}), \quad -A < z < 0 \\
\mathbf{u}^{(0)}, \mathbf{D_{eff}}\partial_z \mathbf{u}^{(0)} \qquad \textit{continuous} \quad \textit{at} \quad z = 0 \\
\partial_z \mathbf{u}^{(0)} = 0, \quad z = -A,
\end{array}$$

where $\mathbf{u}^{(0)} = [u_1^{(0)},\ldots,u_n^{(0)}]$, $\mathbf{D} = diag\{\sigma_i\}$, $\mathbf{D_{eff}} = diag\{\sigma_i\partial_z(y_2(z)-y_1(z))/(y_2(z)-y_1(z))\}$ *and* $\mathbf{F}(\mathbf{u}^{(0)}) = [f_1(u_1^{(0)},\ldots,u_n^{(0)}),\ldots,f_n(u_1^{(0)},\ldots,u_n^{(0)})]'$ *with* $f_i(\cdot)$ *a Taylor expansion of* $g_i(\cdot)$ *in (1).*

Theorem 2 (Dirichlet b. c.) *Let* $\mathbf{U} = [U_1(x,z,t,\varepsilon),\ldots,U_n(x,z,t,\varepsilon)]'$ *satisfy the reaction-diffusion system (1) with Dirichlet boundary condition (2) on* $z = h(y)$ *a differentiable* 1*-periodic function. Suppose that* $U_i = u_i(x,y,z,t,\varepsilon)$ *has the asymptotic form (4), where* u_i *is* 1*-periodic in* y*. Then,* $u_i^{(0)}(x,z,t)$ *is independent of* y *for* $-A \le z \le 0$ *and is a solution of the problem:*

$$\begin{aligned}
&\partial_t\mathbf{u}^{(0)} - \mathbf{D}\Delta\mathbf{u}^{(0)} = \mathbf{F}(\mathbf{u}^{(0)}), \quad z > 0\\
&\mathbf{u}^{(0)} = 0, \quad -A \le z \le 0,
\end{aligned}$$

where $\mathbf{u}^{(0)} = [u_1^{(0)},\ldots,u_n^{(0)}]$*,* $\mathbf{D} = diag\{\sigma_i\}$ *and* $\mathbf{F}(\mathbf{u}^{(0)}) = [f_1(u_1^{(0)},\ldots,u_n^{(0)}),\ldots,f_n(u_1^{(0)},\ldots,u_n^{(0)})]'$ *with* $f_i(\cdot)$ *a Taylor expansion of* $g_i(\cdot)$ *in (1).*

The proof of these results follow the one given in [7] for the scalar case and will not be reported for lack of space.
In the next section we apply the theorems to a model describing the dynamics of a predator-prey system. Numerical experiments show that u_i converges to its expansion of the form Equation (4) in Theorems 1 and 2 as $\varepsilon \to 0$.

NUMERICAL VALIDATION

In order to numerically validate the results, we apply the method to an ecological model in a rectangular domain Ω_ε representing a prototypical lake whose boundary is decomposed in $\partial\Omega_\varepsilon = \Gamma_L \cup \Gamma_R \cup \Gamma_T \cup \Gamma_B$, where $\Gamma_T = h_T(x/\varepsilon)$ and $\Gamma_B = h_B(x/\varepsilon)$ are highly oscillating periodic functions (with period ε in x) (see left part of Figure 2) in which we have Neumann or Dirichlet boundary conditions.
We take the dynamics to be described by the Rosenzweig-MacArthur model with a quadratic mortality term [9]:

$$\begin{aligned}
&\frac{\partial U_1}{\partial t} - \nabla\cdot(\sigma_1\nabla U_1) = rU_1\left(1-\frac{U_1}{k}\right) - q\frac{U_1U_2}{W+U_1}\\
&\frac{\partial U_2}{\partial t} - \nabla\cdot(\sigma_2\nabla U_2) = \eta q\frac{U_1U_2}{W+U_1} - U_2^2
\end{aligned}$$

The homogenized domain is described by $\Omega_h = \Omega_O \cup \Omega_T \cup \Omega_B$ where the rough boundaries, Γ_T and Γ_B in the original

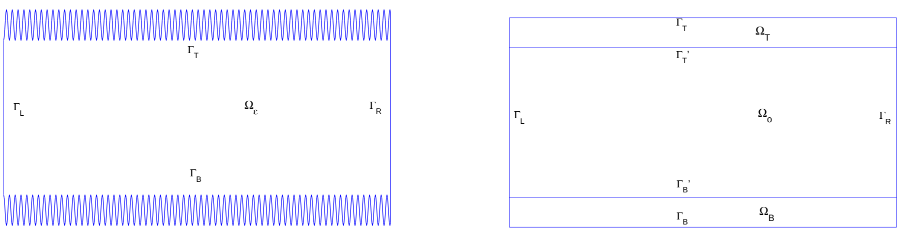

FIGURE 2. The original domain (left) with a partially rough boundary and the homogenized domain (right).

domain, are replaced by two equivalent layers where two modified systems hold (see right part of Figure 2). The coefficients of the equations in these new systems are determined by solving a homogenized problem, as reported in Theorems 1 and 2 for Neumann and Dirichlet boundary conditions, respectively.
Numerical simulations show that, as $\varepsilon \to 0$, $\mathbf{U} \to \mathbf{u}^{(0)}$. Figures 3 reports the spatial MSE between homogenized and exact solutions for each time instant and different values of ε for Neuman case. As we can see from Figure 4, the error decreases as $\varepsilon \to 0$ when the system reaches the steady state.

In conclusion we remark that the present work validates, for certain systems, the results we had obtained before [7] for the case of scalar equations. The proposed approach increases the robustness and stability of the numerical solution

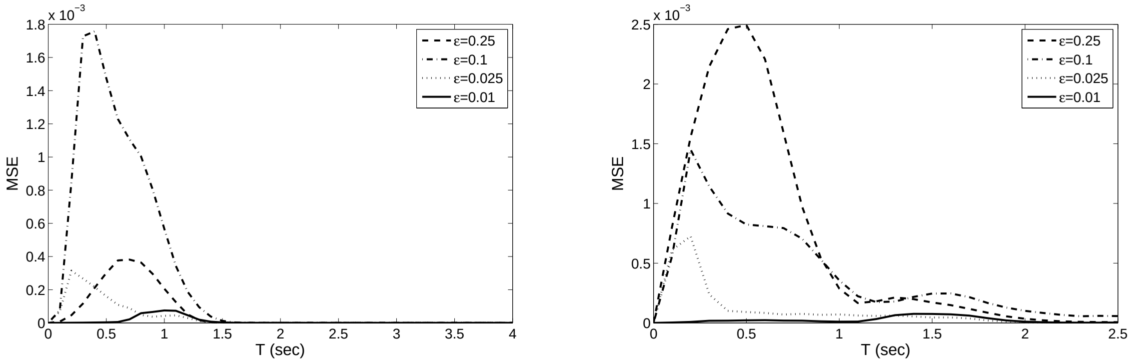

FIGURE 3. MSE between original and homogenized solutions U_1 (left) and U_2 (right) for Neumann boundary conditions.

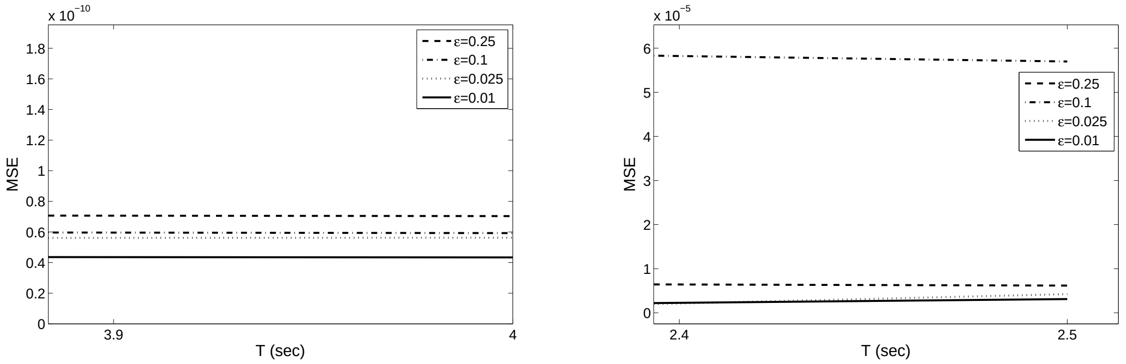

FIGURE 4. Steady state MSE between original and homogenized solutions U_1 (left) and U_2 (right) for Neumann boundary conditions.

methods. Moreover, finding an effective description of the asymptotic behavior of the solutions may help in removing a crucial source of instability.
The authors are currently developing identification techniques for the application of the proposed method to domains with generic rough boundaries.

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