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On upscaling of oscillating boundary analysis and numerics

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On upscaling of oscillating boundary: analysis and numerics

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1 Introduction - Problem sketch

Let Ω be an open connected bounded subset of \mathbb{R}^n and let Γ denote the boundary of Ω . We consider the perturbation of Γ in the sense of an ε order oscillations, henceforth denoted by Γ_ε . Furthermore, these oscillations are assumed to be periodic. Let there be a partial differential equation defined in Ω_ε with boundary conditions defined on Γ_ε . The problem is the following:

Definition 1.1.

$$\begin{aligned} -\Delta u_\varepsilon &= f_\varepsilon & \text{in } \Omega_\varepsilon \\ -\nu_\varepsilon \cdot \nabla u_\varepsilon &= k u_\varepsilon & \text{on } \Gamma_\varepsilon. \end{aligned}$$

Problem: Can we define a problem P defined in Ω such that the solution u is close to u^ε in a certain norm, say in $H^1(\Omega)$?

Intuitively, one can think of several approaches of defining P in Ω . For instance, one can think of defining a diffeomorphism mapping Ψ of domain Ω_ε into Ω ($\Psi : \Omega_\varepsilon \mapsto \Omega$) such that the equations are modified according to the mapping Ψ . Even though this approach looks pretty much intuitive, it is clear that the derivatives of Ψ enter into the equations. If we are not careful about the appropriate mapping, the equations become more complicated. We will show the instances of resulting equations of such scalings in Section 4.

Alternatively, one can use upscaling arguments whereby one retains the equation defined in Ω similar to Ω_ε and introduces a new (modified) boundary condition at Γ so that the problem P is defined in Ω with boundary conditions defined at Γ . The approach becomes more clear if one assigns a physical picture to the model. Let u_ε denote the concentration of some chemical species and we consider a stationary situation. f_ε denotes the reaction term (rate of generation or depletion) in Ω_ε . The boundary conditions are of Robin type and denote the balance between the normal component of the flux incoming to the boundary and the rate of depletion of the chemical species through the boundary. When we replace the oscillating boundary Γ_ε by a straight boundary Γ , essentially, we need to take into account the change in length that has taken place because of this replacement as the rate of depletion through the boundary (or the incoming flux) depends on the measure of the boundary. Thus, during the upscaling procedure, we need to modify the boundary conditions accordingly to account for the change in the incoming flux. Similar analogies can be given for other physical variable, be it the stationary temperature distribution or the stationary potential distribution.

The advantages of such an approach are clear if we would like to compute the solution. The discretization of the domain containing the boundary Γ_ε needs to be fine enough to compute the solution and hence the size of the matrices required to solve the problem becomes very large as the oscillations become fast enough. Instead if the problem is defined

on the domain having flat boundaries, the numerical solution is much easier to compute. Moreover, often we are not interested in the exact details of the oscillatory behaviour near the boundary and the efforts required to compute the fine enough solution near the boundary are not of much use. Actually, one can go a bit further and argue that in the case of very fine oscillations, there is a clear scale separation and one can use upscaling techniques (for example, defining the cell problem) to obtain the solution on a fine scale. Here, we have not dealt with the problem of refining solution at the finer scale.

Such problems can be easily put into the category of multiscale problems with the finer scale being represented by the oscillations and the coarse scale represented by the flat boundary. One specific example of such problems is in the chemical vapor deposition processes with substrates having trenches in it. To enhance the surface area, the trenches are etched on the surface of the silicon substrate. The gases flow over the surface and diffuse through the trenches and deposit on the boundaries. If we neglect the change in the geometry because of the deposition of various layers, we have the setting of the problem identical to the one defined above. The semi-conductor industry hence especially deals with such problems.

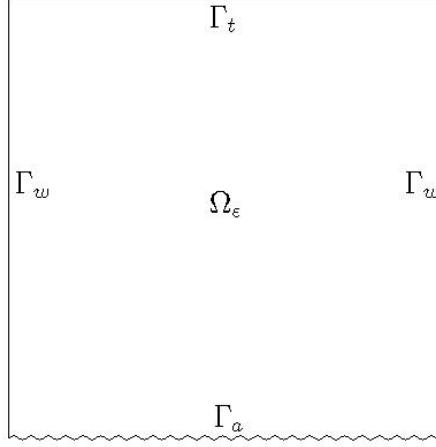
To provide an overview of the work that has been done in this regard we primarily refer to [CFP99] and [NNRM06] and the references therein. Further references in the analysis for the upscaling of oscillating boundary including the non-linear boundary conditions are [AB07], [ABDMG04] and [BG03]. For a general overview of the homogenization, we refer to [HJ91]. For a different application of the formal asymptotic technique being used here see [vN08] and [vN09]. In this direction, [vNPEH10] deals with the upscaling for the case of reactive flow describing the growth of bio-film in a porous media. See [Neu08] for numerical computations for the case of comparison between the upscaled equation and the original equations.

The report is organized in the following way. In Section 2 we deal with the formal asymptotics approach to identify the modified boundary conditions following the approach of Gobbert and Ringhofer [GR98]. The rigorous proof for such an upscaling for a simpler problem is given in Section 2.2. This is followed by numerical computations in Section 3. We provide an instance of domain rescaling in Section 4. We then conclude the report with conclusions and possible future extensions.

2 Formal Asymptotics

2.1 Asymptotic Analysis

Consider the following domain $\Omega_\epsilon \subset \mathbb{R}^2$:



On Ω_ϵ define the following equation:

Definition 2.1.

$$\partial_t \rho = -\text{div}_{x,y} F + R(\rho, x, y, t) \quad (2.1)$$

$$F = -D(x, y, t) \nabla_{x,y} \rho \quad (2.2)$$

$$\rho(x, y, t) = \rho_b(x, y, t), \quad (x, y) \in \Gamma_t \quad (2.3a)$$

$$\nu \cdot F(x, y, t) = 0, \quad (x, y) \in \Gamma_w \quad (2.3b)$$

$$\nu \cdot F(x, y, t) = k \cdot \rho(x, y, t), \quad (x, y) \in \Gamma_a, \quad k \in \mathbb{R}$$

where the surface Γ_a is given by:

$$y = \epsilon h\left(x, \frac{x}{\epsilon}\right)$$

Introduce parameters $\xi = \frac{x}{\epsilon}$ and $\eta = \frac{y}{\epsilon}$. Assume h is periodic in the variable ξ , so

$$h(x, \xi + 1) = h(x, \xi)$$

Now asymptotic analysis is used to derive a boundary condition such that the oscillating boundary can be replaced by a flat boundary. For this purpose make the assumption that the solution can be split in an outer solution and an inner solution, where the outer solution is valid in the area away from the oscillating boundary, and the inner solution in a small layer close to this boundary. Intuitively, the inner and outer solutions should have matching conditions. This hopefully will result in an asymptotic boundary condition for the outer solution.

The following Ansatz is made, where $\bar{\rho}_\epsilon$ and \bar{F}_ϵ represent the solution and flux of the inner solution, and $\tilde{\rho}_\epsilon$ and \tilde{F}_ϵ represent the solution and flux of the outer solution.

Ansatz 2.1.

$$\rho(x, y, t) = \tilde{\rho}_\epsilon(x, y, t) + \bar{\rho}_\epsilon(x, \frac{x}{\epsilon}, \frac{y}{\epsilon}, t) \quad (2.4a)$$

$$\tilde{\rho}_\epsilon = \sum_{j=0}^{\infty} \tilde{\rho}_j(x, y, t) \epsilon^j, \quad \bar{\rho}_\epsilon = \sum_{j=0}^{\infty} \bar{\rho}_j(x, \frac{x}{\epsilon}, \frac{y}{\epsilon}, t) \epsilon^j \quad (2.4b)$$

$$F(x, y, t) = \tilde{F}_\epsilon(x, y, t) + \bar{F}_\epsilon(x, \frac{x}{\epsilon}, \frac{y}{\epsilon}, t) \quad (2.5a)$$

$$\tilde{F}_\epsilon = \sum_{j=0}^{\infty} \tilde{F}_j(x, y, t) \epsilon^j, \quad \bar{F}_\epsilon = \sum_{j=-1}^{\infty} \bar{F}_j(x, \frac{x}{\epsilon}, \frac{y}{\epsilon}, t) \epsilon^j \quad (2.5b)$$

The expansion for \bar{F}_ϵ starts with an order $\frac{1}{\epsilon}$ as it contains the gradient of $\bar{\rho}_\epsilon$. Because the expectation is that the inner solution will only have a contribution close to Γ_a , the following properties should hold:

$$\lim_{\eta \rightarrow \infty} \bar{\rho}_j(x, \xi, \eta, t) = 0 \quad \forall x, \xi, t, j = 0, 1, 2, \dots \quad (2.6a)$$

$$\lim_{\eta \rightarrow \infty} \bar{F}_j(x, \xi, \eta, t) = 0 \quad \forall x, \xi, t, j = -1, 0, 1, \dots \quad (2.6b)$$

On top of that, assume $\bar{\rho}_j$ and \bar{F}_j are periodic in ξ (just like the boundary):

$$\bar{\rho}_j(x, \xi + 1, \eta, t) = \bar{\rho}_j(x, \xi, \eta, t)$$

$$\bar{F}_j(x, \xi + 1, \eta, t) = \bar{F}_j(x, \xi, \eta, t)$$

The expansion can be written as:

$$\begin{aligned} 0 = & \quad \epsilon^{-1} \left(-\text{div}_{\xi, \eta} \bar{F}_{-1} \right) \\ & + \epsilon^0 \left(\partial_t \tilde{\rho}_0 + \partial_t \bar{\rho}_0 + \text{div}_{\xi, \eta} \bar{F}_0 + \text{div}_{x, y} \tilde{F}_0 - R(\tilde{\rho}, x, y, t) \right) \\ & + \epsilon^1 \left(\partial_t \tilde{\rho}_1 + \partial_t \bar{\rho}_1 + \text{div}_{\xi, \eta} \bar{F}_1 + \text{div}_{x, y} \tilde{F}_1 \right) \\ & + O(\epsilon^2) \end{aligned} \quad (2.7)$$

If in equation (2.4a), $\epsilon \rightarrow 0$ and $\eta \rightarrow \infty$, all the $\bar{\rho}$ and $\tilde{\rho}$ disappear except for $\tilde{\rho}_0$. Since equations (2.1) and (2.2) must hold, the following equations are resulting:

$$\partial_t \tilde{\rho}_0 = -\text{div}_{x, y} \tilde{F}_0 + R(\tilde{\rho}_0, x, y, t) \quad (2.8)$$

$$\tilde{F}_0 = -D(x, y, t) \nabla_{x, y} \tilde{\rho}_0 \quad (2.9)$$

The leading-order term of the layer correction, determined by the pair $(\bar{\rho}_0, \bar{F}_{-1})$, can be obtained by letting $\epsilon \rightarrow 0$ and fixing η :

$$\begin{aligned} \operatorname{div}_{\xi,\eta} \bar{F}_{-1} &= 0 \\ \bar{F}_{-1} &= -D(x, 0, t) \nabla_{\xi,\eta} \bar{\rho}_0 \end{aligned}$$

So combining these two equations gives

$$\operatorname{div}_{\xi,\eta} (D(x, 0, t) \nabla_{\xi,\eta} \bar{\rho}_0) = 0 \quad (2.10)$$

Before it is possible to see what the boundary condition on Γ_a (given by equation 2.3c) will become, first the normal vector ν should be rewritten. Therefore ν is given by

$$\nu = \frac{1}{\sigma} (\epsilon \tilde{\nu} + \bar{\nu})$$

where

$$\begin{aligned} \tilde{\nu} &= \begin{pmatrix} \partial_x h \\ 0 \end{pmatrix}, \quad \bar{\nu} = \begin{pmatrix} \partial_\xi h \\ -1 \end{pmatrix} \\ \sigma &= \sqrt{1 + (\epsilon \partial_x h + \partial_\xi h)^2} \end{aligned}$$

Now the boundary condition becomes (in leading $\frac{1}{\epsilon}$ order):

$$\bar{\nu} \cdot \bar{F}_{-1} = 0$$

So

$$\bar{\nu} D \nabla_{\xi,\eta} \bar{\rho}_0 = 0 \text{ for } \eta = h(x, \xi) \quad (2.11)$$

When combining equations (2.10) and (2.11) with the boundary conditions on the wall, and with the conditions given by (2.6a) and (2.6b):

$$\bar{\rho}_0(x, \xi, \eta, t) = 0 \text{ and } \bar{F}_{-1}(x, \xi, \eta, t) = 0 \text{ for all } x, \xi, \eta, t$$

This is important, since it makes sure needed correction of the density close to the surface Γ_a is depending on ϵ in such a way that it gets smaller when $\epsilon \rightarrow 0$. On top of that, the flux will stay bounded as $\epsilon \rightarrow 0$. However, there still can be a significant correction to the flux F close to the surface Γ_a as nothing is known yet with respect to \bar{F}_0 . Therefore the next order term of the layer expansion is brought into play:

$$\operatorname{div}_{\xi,\eta} \bar{F}_0 = 0 \quad (2.12a)$$

$$\bar{F}_0 = -D(x, y = 0, t) \nabla_{\xi,\eta} \bar{\rho}_1 \quad (2.12b)$$

Boundary condition (2.3c) becomes:

$$\frac{\bar{v}}{\sigma_0} \cdot (\bar{F}_0 + \tilde{F}_0) = S(\tilde{\rho}_0, x, y = 0, t)$$

where

$$\sigma_0 = \sqrt{1 + (\partial_\xi h)^2}$$

The goal is now to decouple the bars from the tildes, so there will be 2 separate problems, one for the outer solution and one for the inner solution. For this purpose the following 2 lemmas are necessary:

Lemma 2.1. *All solutions $\rho(x, \xi, \eta, t)$ of the diffusion equation*

$$\Delta_{\xi, \eta} \rho = 0$$

which are periodic with period 1 in the variable ξ and satisfy $\lim_{\eta \rightarrow \infty} \rho = 0$, are of the form

$$\rho(x, \xi, \eta, t) = \sum_{n \in \mathbb{Z}} g_n(x, t) \exp[2\pi i \xi - 2\pi \eta]$$

For the proof of Lemma 2.1, see [GR98].

Lemma 2.2. *If*

$$\int_0^1 d\xi f(x, \xi, t) = 0$$

holds for all values of x and t then

$$\nabla_{\xi, \eta} \rho(x, \xi, h(x, \xi), t) = f(x, \xi, t)$$

where $f(x, \xi, t)$ is periodic with period 1 in the variable ξ , has a solution of the form

$$\rho(x, \xi, h(x, \xi), t) = \sum_{n \in \mathbb{Z}} g_n(x, t) \exp[2\pi i \xi - 2\pi h(x, \xi)].$$

For the proof of Lemma 2.2, see [GR98].

Suppose equations (2.12a) and (2.12b) have some solution $\bar{\rho}_1$ found with the help of Lemma 2.1. Then the boundary condition will become

$$-\nabla_{\xi, \eta} \bar{\rho}_1(x, \xi, h(x, \xi), t) = k\sigma_0 \tilde{\rho}_0 - \bar{v} \cdot \tilde{F}_0 \quad (2.13)$$

Apply Lemma 2.2 to get

$$\int_0^1 d\xi (-\nabla_{\xi,\eta} \bar{\rho}_1(x, \xi, h(x, \xi), t)) = 0$$

Then the boundary condition (2.13) will become, after integrating over ξ :

$$\tilde{F}_0 = \left(\int_0^1 d\xi \sigma_0(x, \xi) \right) k \tilde{\rho}_0$$

So, now the solution of the following problem is the outer solution $(\tilde{\rho}_0, \tilde{F}_0)$:

$$\begin{aligned} \partial_t \tilde{\rho}_0 &= -\text{div}_{x,y} \tilde{F}_0 + R(\tilde{\rho}_0, x, y, t), \quad \tilde{F}_0 = -D(x, y, t) \nabla_{x,y} \tilde{\rho}_0 \\ \tilde{\rho}_0(x, y, t) &= \rho_b(x, y, t), \quad (x, y) \in \Gamma_t \\ \nu \cdot \tilde{F}_0(x, y, t) &= 0, \quad (x, y) \in \Gamma_w \\ \tilde{F}_0(x, y, t) &= \left(\int_0^1 d\xi \sigma_0(x, \xi) \right) k \tilde{\rho}_0, \quad (x, y) \in \Gamma_a \end{aligned} \quad (2.14)$$

The boundary layer correction given by the correction term $(\bar{\rho}_1, \bar{F}_0)$ is the solution the following problem:

$$\begin{aligned} \text{div}_{\xi,\eta} \bar{F}_0 &= 0, \quad \bar{F}_0 = -\nabla_{\xi,\eta} \bar{\rho}_1 \\ \frac{\bar{\nu}}{\sigma_0} \cdot (\bar{F}_0 + \tilde{F}_0) &= k \tilde{\rho}_0 \\ \lim_{\eta \rightarrow \infty} \bar{\rho}_j(x, \xi, \eta, t) &= 0, \quad \lim_{\eta \rightarrow \infty} \bar{F}_j(x, \xi, \eta, t) = 0 \quad \forall x, \xi, t, j \end{aligned}$$

and periodicity in the ξ variable of $\bar{\rho}_0$ and \bar{F}_0 .

It is possible to derive higher order terms in this expansion in the same way, these can be used for higher-order correction to the found solution.

2.2 Rigorous proof for Poisson equation

Suppose that the following equation holds for domain Ω_ϵ :

$$\left\{ \begin{array}{l} -\Delta u = f \text{ in } \Omega_\epsilon \\ -\nu \nabla u = k u \text{ on } \Gamma_\epsilon \\ -n u \nabla u = 0, \quad \text{on } \Gamma_{nf}, \\ u = 0, \quad \text{on } \Gamma_D. \end{array} \right. \quad (2.15)$$

Here, the subscript nf in Γ_{nf} refers to no-flux condition.

Theorem 2.1. *Suppose $\Omega \subset \Omega_\epsilon$ and u_0 is satisfying:*

$$\left\{ \begin{array}{l} -\Delta u_0 = f \text{ in } \Omega \\ -\nu \nabla u_0 = k u_0 \text{ on } \Gamma \\ -n u \nabla u_0 = 0, \quad \text{on } \Gamma_{nf}, \\ u_0 = 0, \quad \text{on } \Gamma_D. \end{array} \right. \quad (2.16)$$

Then u_0 can be extended to Ω_ϵ and furthermore difference $u_0 - u$ is small i.e.

$$\|u_0 - u\|_{H^1(\Omega_\epsilon)} \leq C\sqrt{\epsilon} \quad (2.17)$$

for some C that does not depend on ϵ .

For the proof of this theorem, we need the following two lemmas:

Lemma 2.3. *There exist constants C_1, C_2 such that for any $v \in H^1(\Omega_\epsilon, \Gamma_\epsilon)$ the following estimates hold*

$$\begin{aligned} \|v(x, \epsilon h(x, \frac{x}{\epsilon})) - v(x, 0)\|_{L_2(\Gamma_\epsilon)} &\leq C_1\sqrt{\epsilon}\|v\|_{H^1(\Omega_\epsilon)} \\ \|v\|_{L_2(\Omega_\epsilon \setminus \Omega)} &\leq C_2\sqrt{\epsilon}\|v\|_{H^1(\Omega_\epsilon)} \end{aligned}$$

hold.

For a proof, see [CFP99].

Lemma 2.4. *Let $h(x, \xi)$ be 1-periodic in ξ and Lipschitz such that*

$$\int_0^1 h(x, \xi) d\xi = 0$$

Then the following equality is satisfied (with C_4 depending only on the Lipschitz constant of h):

$$\left| \int_{\Gamma} h(x, \frac{x}{\epsilon}) u(x) v(x) dx \right| \leq C_4\sqrt{\epsilon} \|u\|_{H^{\frac{1}{2}}(\Gamma)} \|v\|_{H^{\frac{1}{2}}(\Gamma)} \quad (2.18)$$

For a proof, see [CFP99].

Proof of Theorem 2.1. The weak form for the equations read:

$$\int_{\Omega} \nabla u_0 \nabla v = \int_{\Omega} f v - \int_{\Gamma} k u v$$

for all $v \in H_{0,\Gamma_D}^1(\Omega)$.

$$\int_{\Omega^\epsilon} \nabla u \nabla v = \int_{\Omega^\epsilon} f v - \int_{\Gamma^\epsilon} k u v$$

for all $v \in H_{0,\Gamma_D}^1(\Omega^\epsilon)$.

Note that under the assumption that has been made here, namely, $\Omega \subset \Omega_\epsilon$, Equation (2.16) can be extended to Ω_ϵ by reflection (See [HJ91]), because of $u_0 \in H_{0,\Gamma_D}^1(\Omega)$ and the smoothness of the boundary $\partial\Omega$.

We obtain using the weak forms for the equations for u and u_0 :

$$\begin{aligned}
\int_{\Omega_\epsilon} \nabla(u_0 - u) \nabla v dx + \int_{\Gamma_\epsilon} k(u_0 - u)v &= - \int_{\Omega_\epsilon} f v dx + \int_{\Gamma_\epsilon} k u_0 v ds + \int_{\Omega_\epsilon} \nabla u_0 \nabla v dx \\
&= - \int_{\Omega_\epsilon} f v dx + \int_{\Gamma_\epsilon} k u_0 v ds + \int_{\Omega} \nabla u_0 \nabla v dx + \int_{\Omega_\epsilon \setminus \Omega} \nabla u_0 \nabla v dx \\
&= - \int_{\Omega_\epsilon} f v dx + \int_{\Gamma_\epsilon} k u_0 v ds + \int_{\Omega_\epsilon \setminus \Omega} \nabla u_0 \nabla v dx + \int_{\Omega} f v dx - \int_{\Gamma} \tilde{k} u_0 v dx \\
&= \int_{\Omega_\epsilon \setminus \Omega} \nabla u_0 \nabla v dx - \int_{\Omega_\epsilon \setminus \Omega} f v dx + \int_{\Gamma_\epsilon} k u_0 v ds - \int_{\Gamma} \tilde{k} u_0 v dx \quad (2.19)
\end{aligned}$$

The first integral of the right-hand side of (2.19) can be estimated as:

$$\begin{aligned}
\left| \int_{\Omega_\epsilon \setminus \Omega} \nabla u_0 \nabla v dx \right| &\leq \|\nabla u_0\|_{L^2(\Omega_\epsilon \setminus \Omega)} \|\nabla v\|_{L^2(\Omega_\epsilon \setminus \Omega)} \\
&\leq \|\nabla u_0\|_{L^2(\Omega_\epsilon \setminus \Omega)} \|v\|_{H^1(\Omega_\epsilon \setminus \Omega)} \\
&\leq \|\nabla u_0\|_{L^2(\Omega_\epsilon \setminus \Omega)} \|v\|_{H^1(\Omega_\epsilon)} \\
&\leq c\sqrt{\epsilon} \|\nabla u_0\|_{H^1(\Omega_\epsilon)} \|v\|_{H^1(\Omega_\epsilon)} \\
&\leq c\sqrt{\epsilon} \|u_0\|_{H^2(\Omega_\epsilon)} \|v\|_{H^1(\Omega_\epsilon)} \quad (2.20)
\end{aligned}$$

where Lemma 2.3 is used.

The second integral of the right-hand side of (2.19) can be estimated as:

$$\begin{aligned}
\left| \int_{\Omega_\epsilon \setminus \Omega} f v dx \right| &\leq \|f\|_{L^2(\Omega_\epsilon \setminus \Omega)} \|v\|_{L^2(\Omega_\epsilon \setminus \Omega)} \\
&\leq \|f\|_{L^2(\Omega_\epsilon)} \|v\|_{L^2(\Omega_\epsilon \setminus \Omega)} \\
&\leq c\sqrt{\epsilon} \|f\|_{L^2(\Omega_\epsilon)} \|v\|_{H^1(\Omega_\epsilon)} \quad (2.21)
\end{aligned}$$

where again Lemma 2.3 is used.

Now we estimate the last two integrals of the right-hand side of (2.19):

$$\left| \int_{\Gamma_\epsilon} k u_0 v ds - \int_{\Gamma} \tilde{k} u_0 v dx \right|.$$

Note that

$$\int_{\Gamma} \tilde{k} u_0(x, 0) v(x, 0) ds = \int_{\Gamma_\epsilon} k u_0(x, 0) v_0(x, 0) dx$$

using $ds = \sqrt{\{1 + (\partial_\xi h(x, \xi))^2\}} dx$ and definition of \tilde{k} . Next,

$$\int_{\Gamma_\epsilon} k u_0 v ds - \int_{\Gamma} \tilde{k} u_0 v dx$$

$$\begin{aligned}
&= \int_{\Gamma_\epsilon} k u_0(x, \epsilon h) v(x, \epsilon h) - \int_{\Gamma_\epsilon} k u_0(x, 0) v(x, \epsilon h) \\
&+ \int_{\Gamma_\epsilon} k u_0(x, 0) v(x, \epsilon h) - \int_{\Gamma_\epsilon} k u_0(x, 0) v(x, 0),
\end{aligned}$$

Now,

$$\begin{aligned}
&\left| \int_{\Gamma_\epsilon} k u_0(x, \epsilon h) v(x, \epsilon h) - \int_{\Gamma_\epsilon} k u_0(x, 0) v(x, \epsilon h) \right| \\
&\leq C \sqrt{\epsilon} \|u_0\|_{H^1(\Omega_\epsilon)} \|v\|_{H^1(\Omega_\epsilon)}
\end{aligned}$$

and

$$\begin{aligned}
&\left| \int_{\Gamma_\epsilon} k u_0(x, 0) v(x, \epsilon h) - \int_{\Gamma_\epsilon} k u_0(x, 0) v(x, 0) \right| \\
&\leq C \sqrt{\epsilon} \|u_0\|_{H^1(\Omega_\epsilon)} \|v\|_{H^1(\Omega_\epsilon)} \\
&\leq C \sqrt{\epsilon} \|v\|_{H^1(\Omega_\epsilon)}
\end{aligned}$$

where Lemma 2.4 and the trace theorem are used.

When combining (2.20), (2.21), and (2.2), it yields:

$$\left| \int_{\Omega_\epsilon} \nabla(u_0 - u) \nabla v dx + \int_{\Gamma_\epsilon} k(u_0 - u) v \right| \leq C \sqrt{\epsilon} \|v\|_{H^1(\Omega_\epsilon)}$$

Substituting $v = u_0 - u$ gives

$$\int_{\Omega_\epsilon} (\nabla(u_0 - u))^2 dx \leq c \sqrt{\epsilon} \|u_0 - u\|_{H^1(\Omega_\epsilon)}$$

Poincaré inequality gives us that:

$$\int_{\Omega_\epsilon} (u_0 - u)^2 dx \leq C \int_{\Omega_\epsilon} (\nabla(u_0 - u))^2 dx$$

Division by $\|u_0 - u\|_{H^1(\Omega_\epsilon)}$ shows that

$$\|u_0 - u\|_{H^1(\Omega_\epsilon)} \leq C \sqrt{\epsilon} \quad \square$$

□

2.3 Rigorous proof for heat equation

Suppose that the following equation holds for domain Ω_ϵ :

$$\begin{cases} u_t - \Delta u = f & \text{in } \Omega_\epsilon \\ -\nu \nabla u = k u & \text{on } \Gamma_\epsilon \end{cases} \quad (2.22)$$

Theorem 2.2. *Suppose u_0 is satisfying:*

$$\begin{cases} (u_0)_t - \Delta u_0 = f & \text{in } \Omega \\ -\nu \nabla u_0 = \tilde{k} u_0 & \text{on } \Gamma \end{cases} \quad (2.23)$$

Also assume that the initial data satisfies the estimate

$$\|u(x, 0) - u_0(x, 0)\|_{L^2(\Omega_\epsilon)}^2 = O(\epsilon),$$

then the difference $u_0 - u$ is small i.e.

$$\|u_0 - u\|_{L^2(0,T;H^1(\Omega_\epsilon))} \leq C\sqrt{\epsilon} \quad (2.24)$$

for some C that does not depend on ϵ .

Proof of Theorem 2.2.

We carry out the proof in the same spirit as in the elliptic case (2.1). What differs here is the treatment of the term:

$$\int_{\Omega_\epsilon} \frac{\partial}{\partial t} (u_0 - u)(u_0 - u) dx + \|\nabla(u_0 - u)\|_{\Omega_\epsilon}^2 \leq C\sqrt{\epsilon} \|u_0 - u\|_{H^1(\Omega_\epsilon)}$$

which implies after integrating over $t \in (0, T)$

$$\|\nabla(u_0 - u)\|_{L^2(0,T;L^2(\Omega_\epsilon))}^2 \leq C(T)\sqrt{\epsilon} \|u_0 - u\|_{L^2(0,T;H^1(\Omega_\epsilon))} + \|u_0 - u\|_{L^2(\Omega_\epsilon)}^2$$

and using Poincare inequality and bounds on the initial data, we obtain the assertion of the theorem. \square

3 Numerical results with COMSOL

In this section it is tried to identify results from the previous section in numerical experiments. For this goal, the program COMSOL Multiphysics is used. It allows the user to draw domains and define equations on the domain and its boundaries. The program uses finite element method to compute the numerical solutions.

3.1 Domains

The error caused by an oscillating boundary is calculated in the last chapter and its H^1 -norm is bounded by the $\sqrt{\epsilon}$ where ϵ represents the magnitude of the oscillation. We perform the numerical experiments for the domain with oscillating boundary and the corresponding effective equation in the domain with flat boundaries and compute the error involved in the upscaling process.

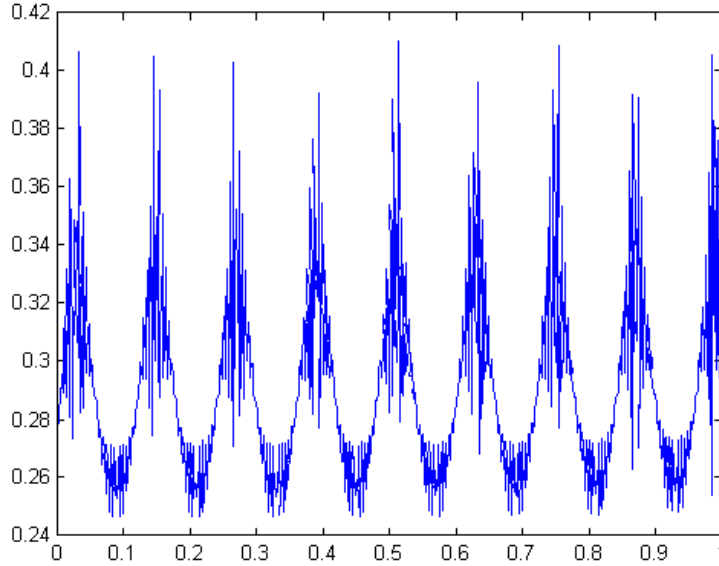


Figure 1: In an oscillating domain also the flux oscillates.

In order to be able to compute any error, first some domains have to be defined. Our reference domain will be the unit square (with $\epsilon = 0, (0, 1) \times (0, 1)$). All other domains will be an extension of this domain by changing the lower boundary $y = 0$ to:

$$y = h^\epsilon(x) = h\left(\frac{x}{\epsilon}\right) = \epsilon \left(-1.1 \cdot \sin\left(\pi \frac{x}{\epsilon}\right) \right) \quad (3.1)$$

The ϵ -values that are used in the numerical models are respectively 0 (flat boundary), 0.01, 0.0125, 0.025, 0.04, 0.05, 0.06, 0.075, 0.09 and 0.1.

Also, in oscillating domains the flux will oscillate. An example can be found in Figure 1. To get a good approximation for this flux, it is vital to discretize with enough elements in order to catch these oscillations.

3.2 Laplace equation

The first equation for which numerical results are achieved is the Laplace equation. Specifically, we consider the following equation defined in $\Omega_\epsilon := ((0, 1) \times (h^\epsilon(x), 1))$:

$$\begin{aligned} -\Delta u^\epsilon &= 0, & \text{in } \Omega_\epsilon, \\ -\nu \cdot \nabla u^\epsilon &= 0, & \text{on } x = 0 \cup x = 1, \\ -\nu \cdot \nabla u^\epsilon &= u^\epsilon, & \text{on } y = h^\epsilon(x), \\ u^\epsilon &= 1, & \text{on } y = 1. \end{aligned}$$

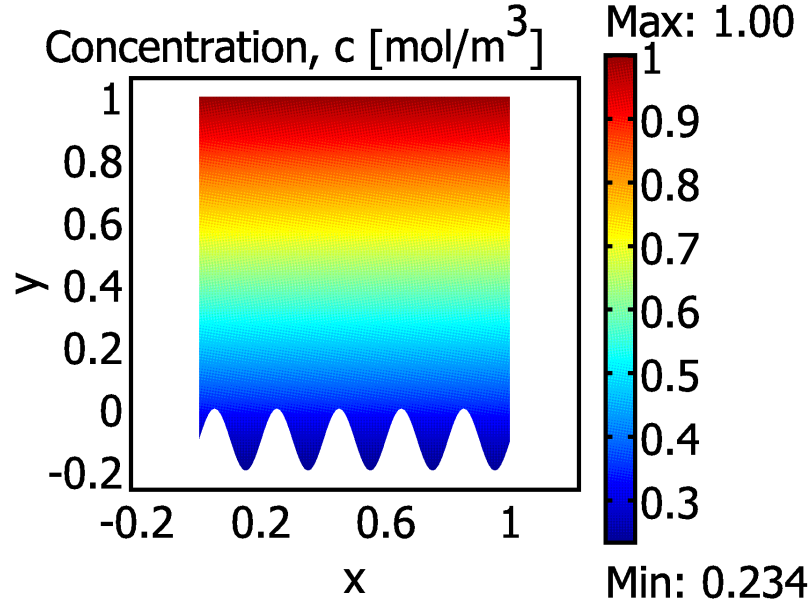


Figure 2: Solution u^ϵ for the Laplace equation for $\epsilon = 0.1$, relatively larger oscillations.

We compare the solution of u^ϵ with the solution u of the following equation defined in $\Omega := ((0, 1) \times (0, 1))$.

$$\begin{aligned}
 -\Delta u &= 0, & \text{in } \Omega, \\
 -\nu \cdot \nabla u &= 0, & \text{on } x = 0 \cup x = 1, \\
 -\nu \cdot \nabla u &= \left\{ \int_0^1 h(\xi) d\xi \right\} u, & \text{on } y = 0, \\
 u &= 1, & \text{on } y = 1.
 \end{aligned} \tag{3.2}$$

Note that the effective boundary condition for the flat boundary (3.2) contains the modification factor $\int_0^1 h(\xi) d\xi$, seen before in equation (2.14). Moreover, by construction we make sure that $\Omega \subset \Omega_\epsilon$. We compute $\|u^\epsilon - u\|_{L^2(\Omega)}$, $\|\nabla u^\epsilon - \nabla u\|_{L^2(\Omega)}$ and observe the variation of this error with respect to ϵ . We obtain the error matrix at the grid points uniformly spaced with discretization spacing 0.01. The finite element method provides the numerical solutions for u^ϵ and u . The L^2 error in the oscillations can be computed for every ϵ . To obtain the L^2 error we approximate the L^2 norm by the sum of the squares of error at the grid points multiplied by the inverse of square of discretization spacing. A plot of this error against the values of ϵ can be found in Figure 11.

The meshing of the different domains has been shown in Figures 3, 6 and 8. For finer oscillations note how fine discretization is needed to retrieve the oscillatory behaviour of the solution near the boundary. This provides a clear advantage in favor of the upscaling where such finer discretization is not required. In Figure 4 and 10 the solutions for the oscillating domains are shown for two cases. Figure 4 refers to the solution for the case of domain

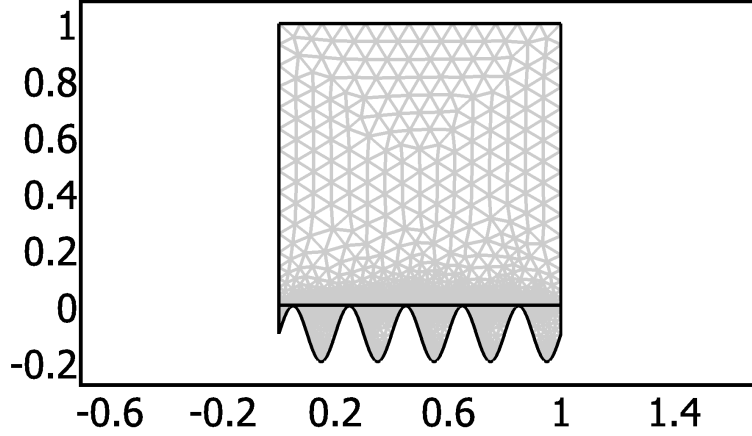


Figure 3: Mesh and discretization of Ω_ϵ for the Laplace equation for $\epsilon = 0.1$.

with oscillations with relatively larger amplitude. Notice that the relatively big error in the gradient in the concentration near the oscillatory boundary and that these oscillations decay pretty fast (see Figure 5). Away from the oscillatory regions, the solutions for the flat domain and the oscillatory domains are pretty close. This explains why the formal asymptotics work the way it has been constructed; namely that the solution near the oscillatory domain is a function of $\frac{x}{\epsilon}, \frac{y}{\epsilon}, x$. This is a crucial information to consider the formal asymptotics for different boundary conditions.

Also the H^1 error can be computed. A plot of this (again against ϵ) can be found in Figure 12.

As can be seen from these plots, the H^1 error is significantly higher than the L^2 error. This can be explained due to the high difference of the (y) -gradient close to the oscillating boundary (see Figure 5).

3.3 Heat equation

We consider the following equation defined in Ω_ϵ :

$$\begin{cases} \delta_t u^\epsilon - \Delta u^\epsilon & = 0, & \text{in } \Omega_\epsilon, \\ -\nu \cdot \nabla u^\epsilon & = 0, & \text{on } x = 0 \cup x = 1, \\ -\nu \cdot \nabla u^\epsilon & = u^\epsilon, & \text{on } y = h^\epsilon(x), \\ u^\epsilon & = 1, & \text{on } y = 1. \end{cases} \quad (3.3)$$

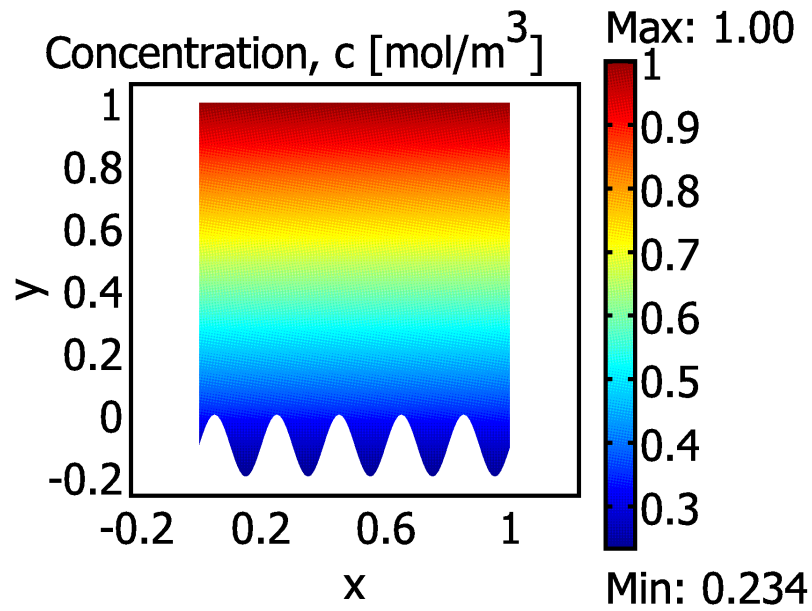


Figure 4: Solution u^ϵ for the Laplace equation defined in Ω_ϵ for $\epsilon = 0.1$.

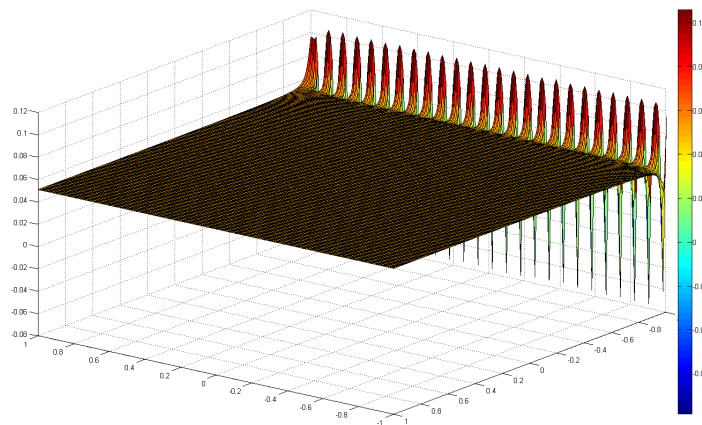


Figure 5: The error made in computing the gradient of the difference between u and u^ϵ .

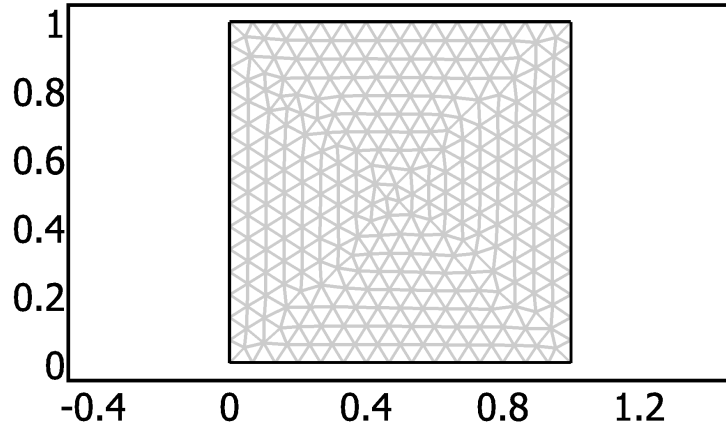


Figure 6: Mesh and discretization of Ω for the Laplace equation for $\epsilon = 0$, an unperturbed domain.

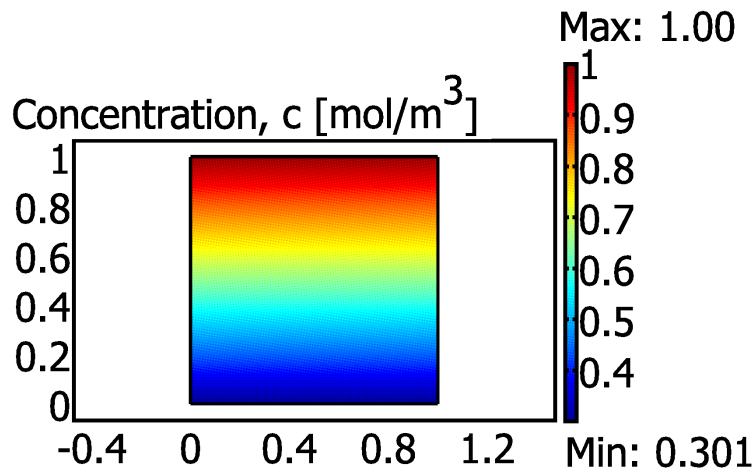


Figure 7: Solution u for the Laplace equation defined in Ω for $\epsilon = 0$, an unperturbed domain.

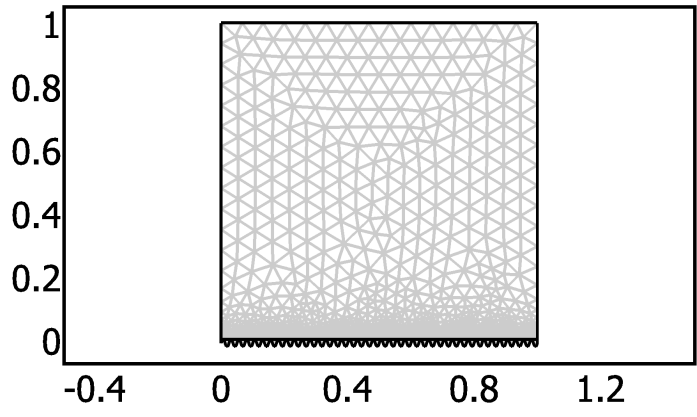


Figure 8: Mesh and discretization of Ω_ϵ for the Laplace equation for $\epsilon = 0.01$.

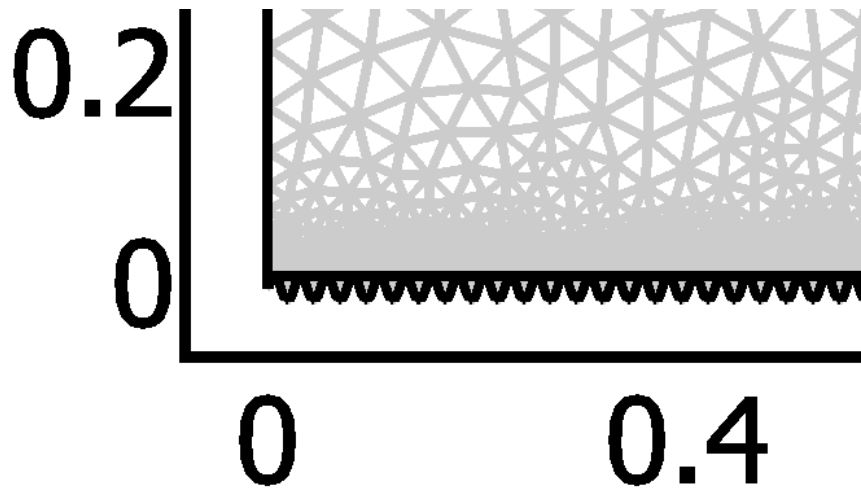


Figure 9: Mesh and discretization of Ω_ϵ for the Laplace equation for $\epsilon = 0.01$, zoomed in at the boundary.

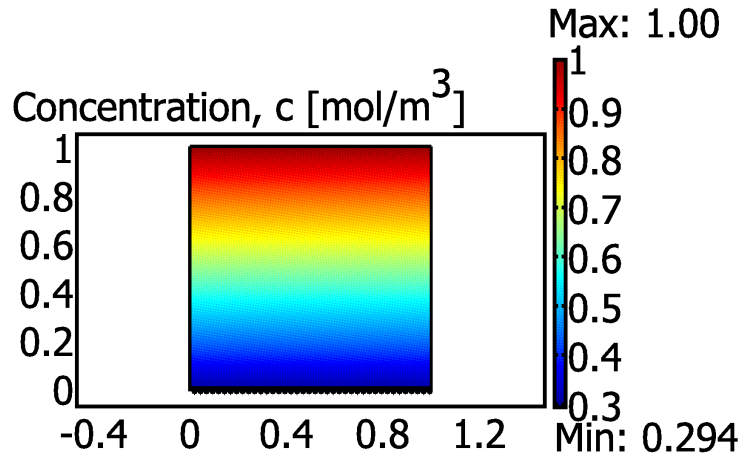


Figure 10: Solution u^ϵ for the Laplace equation for $\epsilon = 0.01$, fine oscillations.

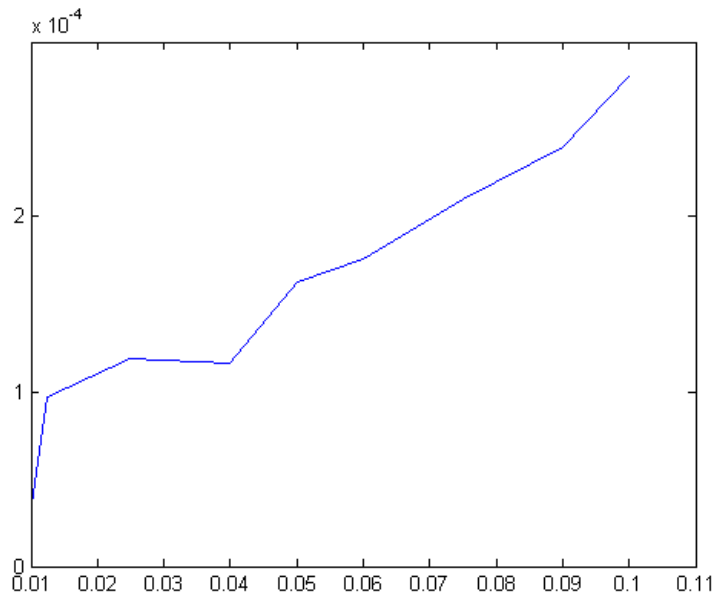


Figure 11: A plot of the L^2 error of the Laplace equation against values of ϵ .

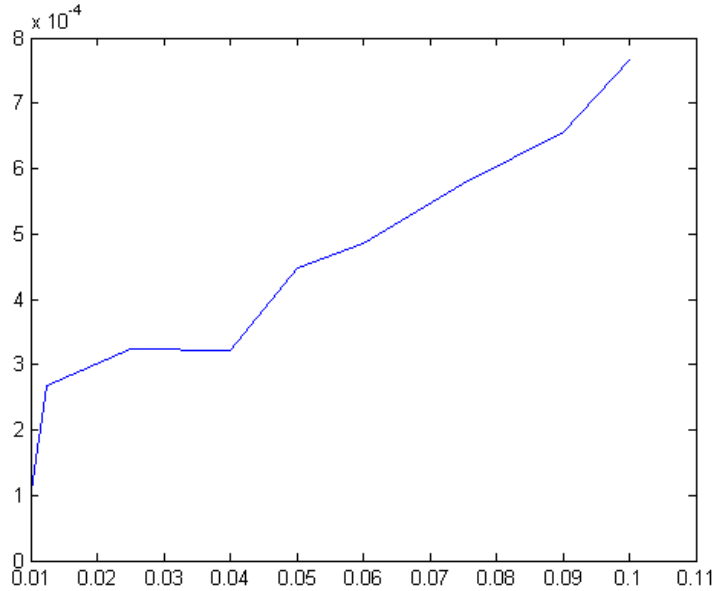


Figure 12: A plot of the H^1 error of the Laplace equation against values of ϵ .

We compare the solution of u^ϵ with the solution u of the following equation defined in Ω .

$$\begin{cases} \delta_t u - \Delta u & = 0, & \text{in } \Omega, \\ -\nu \cdot \nabla u & = 0, & \text{on } x = 0 \cup x = 1, \\ -\nu \cdot \nabla u & = \left\{ \int_0^1 h(\xi) d\xi \right\} u, & \text{on } y = 0, \\ u & = 1, & \text{on } y = 1. \end{cases} \quad (3.4)$$

The domains that are used for the heat equation are equal to the domains used for the Laplace equation in the paragraph before. Also, the meshing will be the same. However, the errors differ significantly from those of the Laplace equation.

In Figure 13 one can see that the L^2 error (which is computed exactly as before, but now summed over all timesteps, and then divided over the number of timesteps) of the heat equation on domains with an oscillating boundary with respect to domains with a flat boundary is very small. Smaller even than the L^2 error of the Laplace equation.

The H^1 error however, shown in Figure 14, even though relatively small, is a lot larger than in the case of the Laplace equation. Again, the difference of the (y)-gradient close to the oscillating boundary is causing this.

4 Scaling the domain

Splitting the solutions in an outer solution and an inner solution is only one of the possible techniques that can be used to solve the problem at hand. It is also possible to scale the

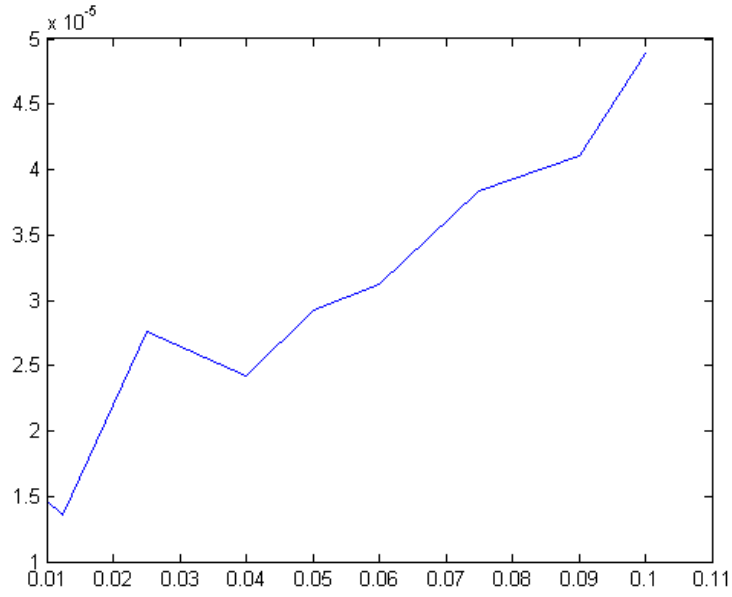


Figure 13: A plot of the L^2 error of the Heat equation against values of ε .

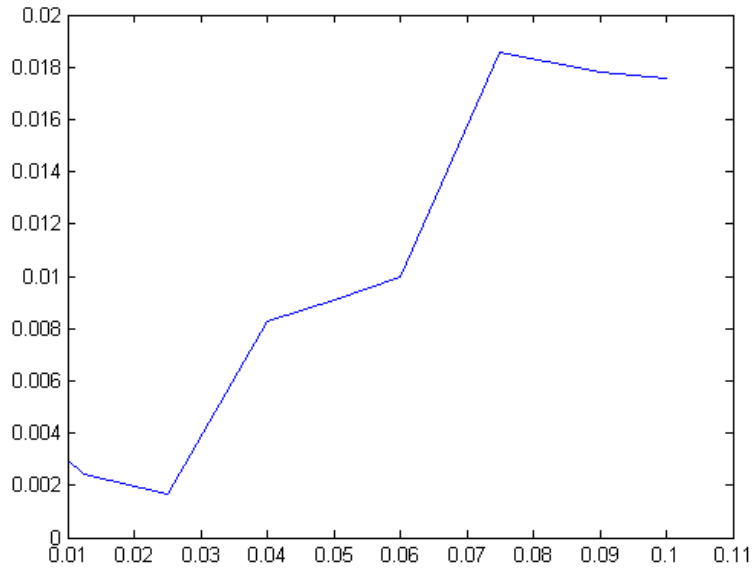


Figure 14: A plot of the H^1 error of the Heat equation against values of ε .

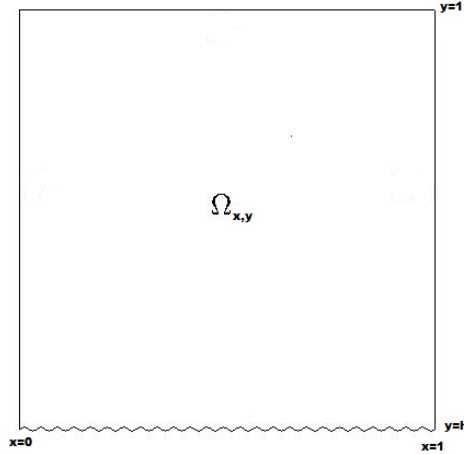


Figure 15: The original domain.

domain in such a way that the boundary is no longer oscillating and becomes flat. This can be done in a lot of ways, but from a practical point of view a few methods have been selected. The original domain is $\Omega_{x,y}$ given by Figure 15, on this domain define the Laplace equation:

$$\Delta_{x,y}u = 0 \quad (4.1)$$

4.1 Linear scaling

Since it is known that in the domain $\Omega_{x,y}$, $y \in [h, 1]$ and $x \in [0, 1]$, it is possible to define

$$\psi := \frac{y - h(x)}{1 - h(x)} \text{ and } \phi = x \quad (4.2)$$

When converting x, y to ϕ, ψ , the new domain $\Omega_{\phi,\psi}$ will have $\psi \in [0, 1]$ and $\phi \in [0, 1]$. By this construction, equation (4.1), defined in domain $\Omega_{x,y}$, will no longer hold and a new equation needs to be computed for $\Omega_{\phi,\psi}$.

In order to compute the laplacian in the new coordinate system, first the derivatives should be rewritten, using equation (4.2). The first derivative with respect to y becomes:

$$u_y = \frac{\partial u}{\partial y} = \frac{\partial u}{\partial \psi} \frac{\partial \psi}{\partial y} + \frac{\partial u}{\partial \phi} \frac{\partial \phi}{\partial y} = \frac{1}{1 - h(\phi)} u_\psi$$

The second derivative with respect to y :

$$u_{yy} = \frac{\partial u_y}{\partial y} = \frac{\partial u_y}{\partial \psi} \frac{\partial \psi}{\partial y} + \frac{\partial u_y}{\partial \phi} \frac{\partial \phi}{\partial y} = \frac{1}{(1 - h(\phi))^2} u_{\psi\psi}$$

The first derivative with respect to x :

$$u_x = \frac{\partial u}{\partial x} = \frac{\partial u}{\partial \psi} \frac{\partial \psi}{\partial x} + \frac{\partial u}{\partial \phi} \frac{\partial \phi}{\partial x} = \frac{(\psi - 1)h'(\phi)}{1 - h(\phi)} u_\psi + u_\phi$$

The second derivative with respect to x is computed in the following steps:

$$\begin{aligned}
\frac{\partial u_x}{\partial \psi} &= \frac{h'(\phi)}{1-h(\phi)}u_\psi + \frac{h'(\phi)(\psi-1)}{1-h(\phi)}u_{\psi\psi} + u_{\phi\psi} \\
\frac{\partial \psi}{\partial x} &= \frac{h'(\phi)(\psi-1)}{1-h(\phi)} \\
\frac{\partial u_x}{\partial \phi} &= \frac{(h''(\phi)(1-h(\phi)) + h'(\phi)^2)(\psi-1)}{(1-h(\phi))^2}u_\psi + \frac{h'(\phi)(\psi-1)}{1-h(\phi)}u_{\psi\phi} + u_{\phi\phi} \\
\frac{\partial \phi}{\partial x} &= 1 \\
u_{xx} &= \frac{\partial u_x}{\partial x} \\
&= \frac{\partial u_x}{\partial \psi} \frac{\partial \psi}{\partial x} + \frac{\partial u_x}{\partial \phi} \frac{\partial \phi}{\partial x}
\end{aligned}$$

So

$$u_{xx} = \left(\frac{h''(\phi)(1-h(\phi)) + 2h'(\phi)^2(\psi-1)}{(1-h(\phi))^2} \right) u_\psi + \left(\frac{h'(\phi)(\psi-1)}{1-h(\phi)} \right)^2 u_{\psi\psi} + \frac{2h'(\phi)(\psi-1)}{1-h(\phi)} u_{\psi\phi} + u_{\phi\phi}$$

So, equation (15) is now converted to:

$$\begin{aligned}
\Delta_{\phi,\psi} u &= \left(\frac{h''(\phi)(1-h(\phi)) + 2h'(\phi)^2(\psi-1)}{(1-h(\phi))^2} \right) u_\psi + \left(\frac{h'(\phi)(\psi-1) + 1}{1-h(\phi)} \right)^2 u_{\psi\psi} \\
&\quad + \frac{2h'(\phi)(\psi-1)}{1-h(\phi)} u_{\psi\phi} + u_{\phi\phi} \\
&= 0
\end{aligned}$$

When looking at this equation, it is clear that its extra (and complicated) terms do not provide a simplification of the problem.

4.2 Exponential scaling

In the domain $\Omega_{x,y}$, $y \in [h, 1]$ and $x \in [0, 1]$. Now define:

$$\psi = c_1 e^y + c_2 e^{-y} \text{ and } \phi = x \quad (4.3)$$

Because the desired result would be an $\Omega_{\phi,\psi}$ where $\phi \in [0, 1]$ and $\psi \in [0, 1]$, it is obvious that:

$$c_1 e^1 + c_2 e^{-1} = 1, \quad c_1 e^h + c_2 e^{-h} = 0$$

When solving these 2 equations, the result is:

$$c_1 = \frac{-1}{e^{2h-1} - e^1}, \quad c_2 = \frac{1}{e^{-1} - e^{1-2h}}$$

Now define $y = \ln(z)$. Then:

$$\begin{aligned} c_1 z + c_2 \frac{1}{z} &= \psi \\ c_1 z^2 - \psi z + c_2 &= 0 \end{aligned}$$

Using the ABC-formula and the fact that x can only be a positive number,

$$\begin{aligned} z &= \frac{\psi + \sqrt{\psi^2 + 4c_2}}{2c_1} \\ y &= \ln \left(\frac{\psi + \sqrt{\psi^2 + 4c_2}}{2c_1} \right) \end{aligned}$$

Now, again, it is possible to express equation 4.1 in terms of our new variables ϕ and ψ . For example:

$$u_y = \frac{\partial u}{\partial y} = \frac{\partial u}{\partial \psi} \frac{\partial \psi}{\partial y} + \frac{\partial u}{\partial \phi} \frac{\partial \phi}{\partial y} = \left(\frac{-1}{e^{2h-1} - e^1} e^y - \frac{1}{e^{-1} - e^{1-2h}} e^{-y} \right) u_\psi$$

This expression already has some complicated terms. Further calculations will not make matters better, so that is left for the reader.

5 Conclusion and future extensions

The work refers to upscaling of the rough boundaries. We derive effective equations that are posed in the domains having flat boundaries instead of oscillating boundaries. This leads to, among others, advantages in the numerical computations. We have considered the Laplace equation and the heat equation for the analysis and the numerical computations. Following conclusions can be derived from the work considered here.

1. The upscaled equation approximates the original equations in L^2 as well as H^1 norm. The formal asymptotics approach has been used to derive the effective boundary conditions. The equations inside the new domain retain the original form and only the boundary conditions are replaced.
2. The ideas from the proof of convergence between the effective equation and the original equations for the elliptic case can be extended to the heat equation and we derived the convergence proof for the heat equation using ideas from the elliptic case.
3. The numerical simulations suggest that the H^1 norm of the error is much larger than the L^2 error and this is understandable since near the boundaries the derivatives are much larger. More details are given in the section on numerical computations.

4. The mapping of the domain containing oscillating boundary to a domain having non-oscillating boundary is possible and the mapping is easy to define at least for 2-D case, however the resulting equations become much more complicated and the oscillations enter into the coefficients of the equations. This approach is found to be too complicated to handle.
5. The replacement of the oscillating boundary by a flat boundary in the way described above also ensures that the total fluxes are also approximated well. Moreover, the flux in the case of oscillating boundaries is oscillating. This means that we require much more elements for the discretization to capture these oscillations. For the flat boundary case, we do not need these many discretizations greatly simplifying the numerical computations.

One can use these techniques for a wide variety of problems. For now we have assumed the geometry to be fixed because of the reactions taking place at the boundaries, however we can use the same techniques to find the effective boundary conditions for the moving boundary situation. In this case, the effective boundary conditions become time dependent. Furthermore, it would be interesting to obtain rigorous proofs for the moving boundary case. Also, for an entirely different application of the coupling between the porous media and the free flow regions, the same techniques can be used.

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