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HOMOGENIZATION OF THE TRANSPORT EQUATION DESCRIBING CONVECTION-DIFFUSION PROCESSES IN A MATERIAL WITH FINE PERIODIC STRUCTURE

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Abstract: In the present contribution we discuss mathematical homogenization and numerical solution of the elliptic problem describing convection-diffusion processes in a material with fine periodic structure. Transport processes such as heat conduction or transport of contaminants through porous media are typically associated with convection-diffusion equations. It is well known that the application of the classical Galerkin finite element method is inappropriate in this case since the discrete solution is usually globally affected by spurious oscillations. Therefore, great care should be taken in developing stable numerical formulations. We describe a variational principle for the convection-diffusion problem with rapidly oscillating coefficients and formulate the corresponding homogenization results. Further, based on the variational principle, we derive a stable numerical scheme for the corresponding homogenized problem. A numerical example will be solved to illustrate the overall performance of the proposed method.

Keywords: variational principles, homogenization, Γ -convergence, convection-diffusion equation, optimal artificial diffusion

MSC: 35B27, 35B38, 70G75, 76R05

1. Introduction

Let Ω be a bounded domain in \mathbb{R}^d , $d = 1, 2, 3$. In particular, we assume that Ω is a domain with Lipschitz boundary $\partial\Omega$ (in case $d = 2, 3$). Further, Γ_D and Γ_N are open disjoint subsets of $\partial\Omega$ such that $\partial\Omega = \overline{\Gamma_D} \cup \overline{\Gamma_N}$, $\Gamma_D \neq \emptyset$. We use the standard function spaces $W^{1,2}(\Omega)$, $W^{1,\infty}(\Omega)$, $L^2(\Omega)$, $L^\infty(\Omega)$, $L^2(\Gamma_N)$. These function spaces we use are rather familiar and we omit the precise definitions, see e.g. [9] for details. Further, define the space V by $V := \{v \in W^{1,2}(\Omega); v = 0 \text{ on } \Gamma_D\}$ (more precisely,

$v = 0$ on Γ_D means that the trace of v is vanishing on Γ_D). We study the family of boundary-value problems

$$-\nabla \cdot \left(a \left(\frac{\mathbf{x}}{\varepsilon} \right) \nabla u^\varepsilon(\mathbf{x}) \right) + \mathbf{b} \left(\frac{\mathbf{x}}{\varepsilon} \right) \cdot \nabla u^\varepsilon(\mathbf{x}) = f(\mathbf{x}) \quad \text{in } \Omega, \quad (1)$$

$$u^\varepsilon(\mathbf{x}) = 0 \quad \text{on } \Gamma_D, \quad (2)$$

$$-\mathbf{n} \cdot a \left(\frac{\mathbf{x}}{\varepsilon} \right) \nabla u^\varepsilon(\mathbf{x}) = \alpha u^\varepsilon(\mathbf{x}) + \gamma_N(\mathbf{x}) \quad \text{on } \Gamma_N. \quad (3)$$

Here, \mathbf{n} denotes the unit exterior normal vector to the boundary $\partial\Omega$. We assume that the transport coefficients a and \mathbf{b} periodically depend on a fine scale \mathbf{x}/ε ($\varepsilon > 0$ being a small scalar parameter). We then let $\varepsilon \rightarrow 0_+$ and study the asymptotic behavior of the problem. In particular, our aim is to formulate a variational principle for (1)–(3). Note that, in general, (1) is not in a *divergence form*, however, under the assumptions below, there exists a functional \mathcal{I}^ε on V whose *minimizers* are solutions of (1)–(3). Then the Γ -convergence of \mathcal{I}^ε (as $\varepsilon \rightarrow 0_+$) is equivalent to the homogenization of (1)–(3).

The following assumptions will be needed throughout the paper.

- $\alpha > 0$ is a real positive parameter, fixed throughout the paper, $f \in L^2(\Omega)$ and $\gamma_N \in L^2(\Gamma_N)$.
- $a: \mathbb{R}^d \times \mathbb{R}$ is given by a strictly positive and bounded function, such that

$$0 < a_1 \leq a(\boldsymbol{\xi}) \leq a_2 < +\infty \quad \text{for all } \boldsymbol{\xi} \in \mathbb{R}^d \quad (a_1, a_2 = \text{const}).$$

- The coefficient functions are rapidly oscillating, i.e. of the form

$$a^\varepsilon(\mathbf{x}) := a \left(\frac{\mathbf{x}}{\varepsilon} \right),$$

$$\mathbf{b}^\varepsilon(\mathbf{x}) := \mathbf{b} \left(\frac{\mathbf{x}}{\varepsilon} \right)$$

for all $\mathbf{x} \in \Omega$, where the functions a, b_1, \dots, b_d are Y -periodic in \mathbb{R}^d with periodicity cell

$$Y = \{\mathbf{y} = (y_1, \dots, y_d) : 0 < y_i < 1 \text{ for } i = 1, \dots, d\}$$

and ε is a scale parameter.

- The coefficient functions are taken to be a gradient field in the sense that

$$-\nabla \varphi^\varepsilon(\mathbf{x}) = \frac{\mathbf{b}^\varepsilon(\mathbf{x})}{a^\varepsilon(\mathbf{x})}$$

with potential φ^ε .

- The potential φ^ε is a Lipschitz function, $\varphi^\varepsilon \in W^{1,\infty}(\Omega)$ such that

$$\varphi^\varepsilon(\mathbf{x}) = \mathbf{R}_0 \cdot \mathbf{x} + \varepsilon \psi\left(\frac{\mathbf{x}}{\varepsilon}\right)$$

with some $\mathbf{R}_0 \in \mathbb{R}^d$ and $\psi \in W^{1,\infty}(\Omega)$ Y -periodic in \mathbb{R}^d .

For smaller and smaller ε , the coefficients a^ε and \mathbf{b}^ε oscillate more and more rapidly and it is natural to study the limit of u^ε in (1)–(3) as $\varepsilon \rightarrow 0$.

2. Standard weighted residual method and the Galerkin formulation

A weak formulation of the problem is to find $u \in V$ satisfying

$$\begin{aligned} \int_{\Omega} a^\varepsilon(\mathbf{x}) \nabla u^\varepsilon \cdot \nabla v \, d\Omega + \int_{\Omega} \mathbf{b}^\varepsilon(\mathbf{x}) \cdot \nabla u^\varepsilon v \, d\Omega + \alpha \int_{\Gamma_N} u^\varepsilon v \, d\sigma \\ = \int_{\Omega} f v \, d\Omega + \int_{\Gamma_N} \gamma_N v \, d\sigma \end{aligned}$$

for all $v \in V$. Here $d\Omega$ denotes Lebesgue measure and $d\sigma$ is the surface area measure on the boundary $\partial\Omega$. By \mathcal{T}_h we denote an admissible partition of Ω with mesh size h with standard properties from the finite element theory (see e.g. [4]). Let $V_h \subset C(\overline{\Omega}) \cap V$ be the standard conforming linear finite element space over \mathcal{T}_h . A finite element formulation corresponding to the problem can be written as follows: find $u_h \in V_h$ satisfying

$$\begin{aligned} \int_{\Omega} a^\varepsilon(\mathbf{x}) \nabla u_h^\varepsilon \cdot \nabla v_h \, d\Omega + \int_{\Omega} \mathbf{b}^\varepsilon(\mathbf{x}) \cdot \nabla u_h^\varepsilon v_h \, d\Omega + \alpha \int_{\Gamma_N} u_h^\varepsilon v_h \, d\sigma \\ = \int_{\Omega} f v_h \, d\Omega + \int_{\Gamma_N} \gamma_N v_h \, d\sigma \quad (4) \end{aligned}$$

for all $v_h \in V_h$.

It is well-known that, as the convective term represents a nonsymmetric operator, the standard Galerkin finite element method loses the *best approximation property*. As a consequence, when the convective term is significant, the Galerkin formulation produces node-to-node spurious oscillations. One possible way is to choose a sufficiently fine grid such that the element Péclet number is less than one. However, this approach may not always be practical from the computational point of view. Therefore, several stabilized methods have been developed to avoid unphysical spurious oscillations on coarse grids, see e.g. [6] and the references given there. In particular, the authors in [11] have shown a variational basis for the *optimal artificial diffusion method*. Following this observation, we provide a variational principle for the problem (1)–(3) such that the solution u^ε minimizes a certain functional \mathcal{I}^ε over the appropriate solution space V . Using the theory of Γ -convergence, we identify the limit \mathcal{I}_{hom} of \mathcal{I}^ε as ε goes to 0, such that the minima of \mathcal{I}^ε converge to the

minimum of the homogenized functional \mathcal{I}_{hom} . Based on the variational structure of this problem, i.e. from the fact that the *homogenized solution* minimizes a certain *homogenized functional*, the finite element solution possesses the *best approximation property*. Namely, the finite element approximation of the homogenized solution (the solution of the problem with the constant *homogenized* coefficients) gives nodally exact solutions for 1D problems with constant coefficients.

3. A variational principle for the advection-diffusion problems

Define $\chi^\varepsilon(\mathbf{x}) := \exp[\varphi^\varepsilon(\mathbf{x})]$. Then $\chi^\varepsilon \in W^{1,\infty}(\Omega)$ and $\chi^\varepsilon(\mathbf{x}) \geq c > 0$ on $\overline{\Omega}$. The function χ^ε will be called a *multiplier* for this variational problem. It is easily verified that sufficiently smooth function u^ε solves (1) provided

$$-\nabla \cdot (\chi^\varepsilon(\mathbf{x}) a^\varepsilon(\mathbf{x}) \nabla u^\varepsilon) = \chi^\varepsilon(\mathbf{x}) f(\mathbf{x}) \quad \text{in } \Omega.$$

This equation is in divergence form so there is a variational principle for its solutions. Consider the problem of minimizing \mathcal{I}^ε on V , where $\mathcal{I}^\varepsilon: V \rightarrow \mathbb{R}$ is defined by, $w \in V$,

$$\mathcal{I}^\varepsilon(w) := \int_{\Omega} \chi^\varepsilon(\mathbf{x}) \left(\frac{a^\varepsilon(\mathbf{x})}{2} |\nabla w|^2 - f(\mathbf{x}) w \right) d\Omega + \int_{\Gamma_N} \chi^\varepsilon(\mathbf{x}) \left(\frac{\alpha}{2} w^2 - \gamma_N w \right) d\sigma. \quad (5)$$

Note that this functional involves the advection field solely through the multiplier $\chi^\varepsilon(\mathbf{x})$. Using the theory in [13], there will be a minimizer of \mathcal{I}^ε . When $v \in V \cap C(\overline{\Omega})$, the first variation of \mathcal{I}^ε at $u^\varepsilon \in V$,

$$\delta \mathcal{I}^\varepsilon(u^\varepsilon, v) = \lim_{t \rightarrow 0} \frac{1}{t} [\mathcal{I}^\varepsilon(u^\varepsilon + tv) - \mathcal{I}^\varepsilon(u^\varepsilon)],$$

exists and is given by

$$\begin{aligned} \delta \mathcal{I}^\varepsilon(u^\varepsilon, v) &= \int_{\Omega} \chi^\varepsilon(\mathbf{x}) (a^\varepsilon(\mathbf{x}) \nabla u^\varepsilon \cdot \nabla v - f(\mathbf{x}) v) d\Omega \\ &\quad + \int_{\Gamma_N} \chi^\varepsilon(\mathbf{x}) (\alpha u^\varepsilon v - \gamma_N u^\varepsilon v) d\sigma. \end{aligned} \quad (6)$$

At the minimizer $u^\varepsilon \in V$, (6) will be zero. Hence, we have

$$\begin{aligned} \int_{\Omega} \chi^\varepsilon(\mathbf{x}) a^\varepsilon(\mathbf{x}) \nabla u^\varepsilon \cdot \nabla v d\Omega + \int_{\Gamma_N} \chi^\varepsilon(\mathbf{x}) \alpha u^\varepsilon v d\sigma \\ = \int_{\Omega} \chi^\varepsilon(\mathbf{x}) f(\mathbf{x}) v d\Omega + \int_{\Gamma_N} \chi^\varepsilon(\mathbf{x}) \gamma_N u^\varepsilon v d\sigma \end{aligned} \quad (7)$$

for all $v \in V$. It is easy to see that (7) is the weak formulation for the boundary value problem

$$-\nabla \cdot (\chi^\varepsilon(\mathbf{x}) a^\varepsilon(\mathbf{x}) \nabla u^\varepsilon) = \chi^\varepsilon(\mathbf{x}) f(\mathbf{x}) \quad \text{in } \Omega, \quad (8)$$

$$u^\varepsilon(\mathbf{x}) = 0 \quad \text{on } \Gamma_D, \quad (9)$$

$$-\mathbf{n} \cdot a^\varepsilon(\mathbf{x}) \nabla u^\varepsilon(\mathbf{x}) = \alpha u^\varepsilon(\mathbf{x}) + \gamma_N(\mathbf{x}) \quad \text{on } \Gamma_N. \quad (10)$$

A corresponding finite element formulation for the problem (8)–(10) reads as follows: find $u_h \in V_h$ such that

$$\begin{aligned} \int_{\Omega} \chi^\varepsilon(\mathbf{x}) a^\varepsilon(\mathbf{x}) \nabla u_h^\varepsilon \cdot \nabla v_h \, d\Omega + \int_{\Gamma_N} \chi^\varepsilon(\mathbf{x}) \alpha u_h^\varepsilon v_h \, d\sigma \\ = \int_{\Omega} \chi^\varepsilon(\mathbf{x}) f(\mathbf{x}) v_h \, d\Omega + \int_{\Gamma_N} \chi^\varepsilon(\mathbf{x}) \gamma_N u_h^\varepsilon v_h \, d\sigma \end{aligned}$$

for all $v_h \in V_h$.

4. Γ -convergence

We now consider a family of functionals (5) depending on $w \in V$. Let \mathcal{I}_{hom} denote the homogenized functional defined by

$$\begin{aligned} \mathcal{I}_{\text{hom}}(w) := \int_{\Omega} \exp(\mathbf{R}_0 \cdot \mathbf{x}) (\mathcal{W}_{\text{hom}}(\nabla w(\mathbf{x})) - f(\mathbf{x})w(\mathbf{x})) \, d\Omega \\ + \int_{\Gamma_N} \exp(\mathbf{R}_0 \cdot \mathbf{x}) \left(\frac{\alpha}{2} w(\mathbf{x})^2 - \gamma_N(\mathbf{x})w(\mathbf{x}) \right) \, d\sigma, \quad (11) \end{aligned}$$

where the homogenized energy \mathcal{W}_{hom} is given by

$$\mathcal{W}_{\text{hom}}(\lambda) = \inf_{\xi \in W_{\text{per}}^{1,2}(Y)} \int_Y \frac{a(\mathbf{y})}{2} |\lambda + \nabla_{\mathbf{y}} \xi(\mathbf{y})|^2 \, dY, \quad (12)$$

where $W_{\text{per}}^{1,2}(Y)$ is the space of elements of $W^{1,2}(Y)$ having the same trace on opposite face of Y .

Applying [10, Theorem 1.5] (see also [3, 7]), the sequence \mathcal{I}^ε Γ -converges to \mathcal{I}_{hom} . This implies the following fact on the minimizers: for each value $\varepsilon > 0$, let $u^\varepsilon \in V$ be an minimizer of the functional \mathcal{I}^ε . Then, up to a subsequence, u^ε converges weakly in V to a limit u which is precisely a minimizer of the homogenized functional \mathcal{I}_{hom} , i.e.,

$$u^\varepsilon \rightharpoonup u \text{ weakly in } V$$

further

$$\mathcal{I}^\varepsilon(u^\varepsilon) \rightarrow \mathcal{I}(u), \quad \inf_{v \in V} \mathcal{I}^\varepsilon(v) \rightarrow \min_{v \in V} \mathcal{I}(v) \quad \text{and} \quad \mathcal{I}(u) = \min_{v \in V} \mathcal{I}(v).$$

Computing the infima in (12) and minimizers $u \in V$ of (11) yields the following homogenized problem,

$$\begin{aligned} \int_{\Omega} \exp(\mathbf{R}_0 \cdot \mathbf{x}) A^* \nabla u \cdot \nabla v \, d\Omega + \int_{\Gamma_N} \exp(\mathbf{R}_0 \cdot \mathbf{x}) \alpha u v \, d\sigma \\ = \int_{\Omega} \exp(\mathbf{R}_0 \cdot \mathbf{x}) f(\mathbf{x}) v \, d\Omega + \int_{\Gamma_N} \exp(\mathbf{R}_0 \cdot \mathbf{x}) \gamma_N u v \, d\sigma \quad (13) \end{aligned}$$

for all $v \in V$. The homogenized diffusion tensor is given by its entries

$$A_{ij} = \int_Y a(\mathbf{y}) (\mathbf{e}_i + \nabla_y w_i) (\mathbf{e}_j + \nabla_y w_j) dY, \quad (14)$$

where w_i are defined as the unique solutions in $W_{\text{per}}^{1,2}(Y)$ of the cell problems:

$$-\nabla_y \cdot (a(\mathbf{y})(\mathbf{e}_i + \nabla_y w_i)) = 0 \quad \text{in } Y \quad \text{and} \quad \int_Y w_i dY = 0, \quad i = 1, \dots, d. \quad (15)$$

5. Application to the 1D problem

We now study a convection-diffusion process in layered medium which is described by the following one-dimensional problem. Let $\Omega = (0, 1)$ be an interval in \mathbb{R} , $\varepsilon > 0$, and consider the problem

$$-\frac{du}{dx} \left(a^\varepsilon(x) \frac{du}{dx} \right) + b^\varepsilon(x) \frac{du}{dx} = 1 \quad \text{in } (0, 1) \quad (16)$$

$$u(x=0) = u(x=1) = 0. \quad (17)$$

Here, $a^\varepsilon(x) = a(x/\varepsilon)$ and $b^\varepsilon(x) = b(x/\varepsilon)$ and we assume that a and b are piecewise constant 1-periodic functions such that

$$a(y) = \begin{cases} a_1 & y \in (0, 1/2) \\ a_2 & y \in (1/2, 1) \end{cases} \quad b(y) = \begin{cases} b_1 & y \in (0, 1/2) \\ b_2 & y \in (1/2, 1) \end{cases} \quad (18)$$

where $a_1, a_2 \in \mathbb{R}_+$ and $b_1, b_2 \in \mathbb{R}$. In the one-dimensional case, analytical solutions to (14)–(15) are well known, see e.g. [5]. In particular, for (18) we have

$$A^* = \frac{2a_1a_2}{a_1 + a_2} \quad \text{and} \quad R_0 = -\frac{a_1b_2 + a_2b_1}{2a_1a_2}. \quad (19)$$

Given any positive integer N , let $\pi: 0 = x_0 < \dots < x_{N+1} = 1$ denote a uniform partition of the unit interval with nodes $x_i = ih$, $h = 1/(N+1)$, $0 \leq i \leq N+1$. Then V_h denotes the set of all continuous functions defined on $[0, 1]$ which are linear on each subinterval $[x_i, x_{i+1}]$, $0 \leq i \leq N$, and which vanish at the end points.

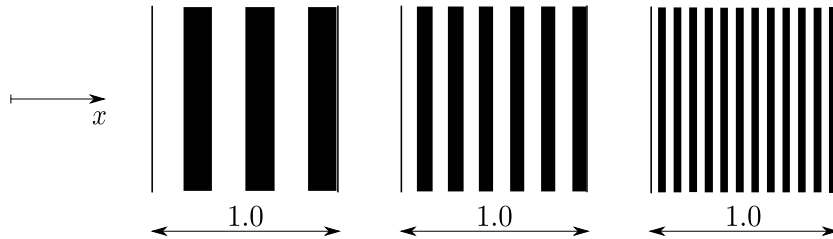


Figure 1: Layered medium.

A convenient basis on V_h can be constructed in a standard way as follows: let $v_i(x)$, $1 \leq i \leq N$, be the element in V_h which satisfies $v_i(x_j) = \delta_{ij}$, $1 \leq j \leq N$. Then the collection $\{v_i(x), 1 \leq i \leq N\}$ constitutes a basis in V_h : any function $v_h(x) \in V_h$ can be written as

$$v_h(x) = \sum_{i=1}^N \zeta_i v_i(x).$$

A finite element formulation corresponding to the problem (16)–(17) can be written as follows: find $u_h^\varepsilon \in V_h$, $u_h^\varepsilon(x) = \sum_{i=1}^N \xi_i v_i(x)$, such that ($1 \leq i \leq N$)

$$\sum_{j=1}^N \left\{ \int_0^1 a^\varepsilon(x) \frac{dv_i}{dx} \frac{dv_j}{dx} dx \right\} \xi_j + \sum_{j=1}^N \left\{ \int_0^1 b^\varepsilon(x) v_i \frac{dv_j}{dx} dx \right\} \xi_j = \int_0^1 v_i dx. \quad (20)$$

The results presented in this section are obtained using an in-house PYTHON code. Recall that the standard Galerkin formulation gives node-to-node spurious oscillations. In Figure 2, we compare the numerical solutions from the standard Galerkin formulation for various steps h . As one can see from the figure, the Galerkin formulation produces spurious node-to-node oscillations for high values of h (namely $h = 0.1$ and $h = 0.05$).

We now apply the new variational formulation to the 1D problem according to (13) (reformulated to the 1D case and Dirichlet boundary conditions). The corresponding finite element formulation reads as follows: find $u_h \in V_h$, $u_h(x) = \sum_{i=1}^N \eta_i v_i(x)$, such that

$$\sum_{j=1}^N \left\{ \int_0^1 \exp(R_0 x) A^* \frac{dv_i}{dx} \frac{dv_j}{dx} dx \right\} \eta_j = \int_0^1 \exp(R_0 x) v_i dx, \quad 1 \leq i \leq N. \quad (21)$$

According to a specific construction of the basis on V_h , it is easy to see that

$$u_h(x) = \eta_{j-1} g_{-1}(x) + \eta_j g_0(x) + \eta_{j+1} g_{+1}(x) \quad \text{on } \langle x_{j-1}, x_{j+1} \rangle,$$

where

$$\begin{aligned} g_{-1}(x) &= \begin{cases} -\frac{x-x_j}{h} & -h \leq x - x_j \leq 0 \\ 0 & 0 < x - x_j \leq +h \end{cases} \\ g_0(x) &= \begin{cases} \frac{x-x_j+h}{h} & -h \leq x - x_j \leq 0 \\ \frac{h-(x-x_j)}{h} & 0 < x - x_j \leq +h \end{cases} \\ g_{+1}(x) &= \begin{cases} 0 & -h \leq x - x_j \leq 0 \\ \frac{x-x_j}{h} & 0 < x - x_j \leq +h \end{cases} \end{aligned}$$

Hence, in view of (21), $(\eta_1, \eta_2, \dots, \eta_N)$ is a solution of the following system of equations

$$\eta_{i-1} \omega_{-1} + \eta_i \omega_0 + \eta_{i+1} \omega_{+1} = 1, \quad 1 \leq i \leq N, \quad \eta_0 = \eta_{N+1} = 0,$$

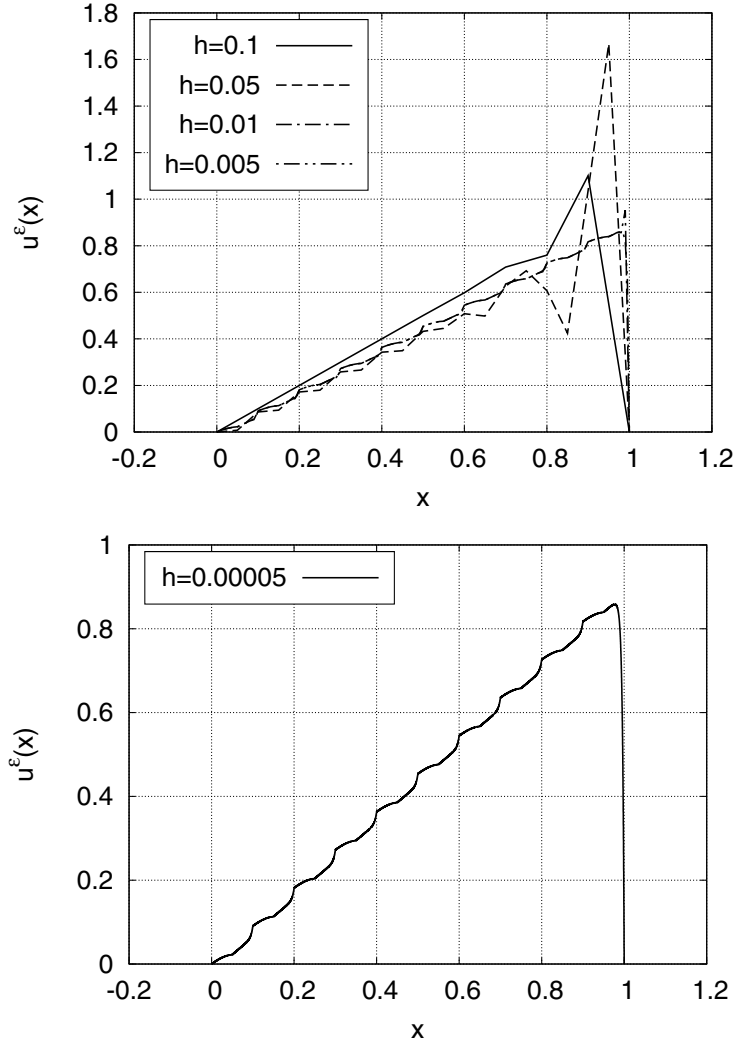


Figure 2: Comparison of Galerkin approximations for various steps h and fixed $\varepsilon = 0.1$. The following values have been chosen in this example: $a_1 = 0.05$, $a_2 = 0.005$, $b_1 = 0.8$ and $b_2 = 1.2$.

where

$$\begin{aligned}\omega_{-1} &= \frac{\int_{-h}^{+h} \exp(R_0 x) A^* g'_0(x) g'_{-1}(x) dx}{\int_{-h}^{+h} \exp(R_0 x) g_0(x) dx} = \frac{R_0 A^*}{2h} (1 - \coth(R_0 h/2)), \\ \omega_0 &= \frac{\int_{-h}^{+h} \exp(R_0 x) A^* g'_0(x) g'_0(x) dx}{\int_{-h}^{+h} \exp(R_0 x) g_0(x) dx} = \frac{R_0 A^*}{h} \coth(R_0 h/2), \\ \omega_{+1} &= \frac{\int_{-h}^{+h} \exp(R_0 x) A^* g'_0(x) g'_{+1}(x) dx}{\int_{-h}^{+h} \exp(R_0 x) g_0(x) dx} = \frac{-R_0 A^*}{2h} (1 + \coth(R_0 h/2)).\end{aligned}$$

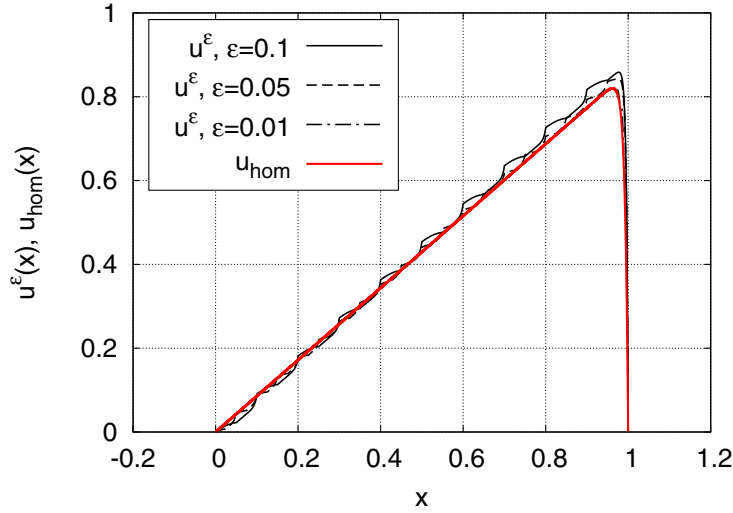


Figure 3: Comparison of the fine scale solutions and the homogenized results.

It is worth noting that the coefficients ω_{-1} , ω_0 and ω_{+1} are, respectively, the same as obtained using the optimal artificial diffusion method, c.f. [11]. In Figure 3, we compare the numerical solution u_{hom} of (21) obtained using the stable homogenized formulation with $h = 0.05$ (based on the variational principle, which gives nodally exact solutions) with the solutions of (20) using the standard Galerkin approximations with $h = 5.0 \times 10^{-5}$ and for various values of scale parameters of ε .

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