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A PENALTY METHOD FOR SOLVING PARTIAL DIFFERENTIAL EQUATIONS WITH PERIODIC BOUNDARY CONDITION: APPLICATION TO THE HOMOGENIZATION THEORY

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We present a numerical method, based on a penalization technique, for the solution of an elliptic problem with periodic boundary conditions. The convergence of the method is established and an error estimate is given. Numerical tests are performed on some problems from homogenization theory.

1. Introduction

Here we deal with the numerical solution of an elliptic problem with periodic boundary condition, by a finite element method. Such problems arise, in particular in homogenization theory.[10] Several methods are currently used. We refer to Charpentier and Maday's note[3] where two iterative methods, based on the domain decomposition technique, are presented. We refer also to Refs. 8 and 11 and the references therein.

In this study, we give a new solution method to this type of problem. It is a direct method of approximation which relies on a penalization technique.

The standard conforming finite element method consists of using shapes functions satisfying the boundary conditions. In comparison with this method, our approach has the following advantages:

(i) It is easily implementable.
(ii) It allows the use of the standard finite elements.
(iii) It is less memory consuming and presents a gain in CPU time solution.

The numerical tests are performed on some cellular problems considered by Cioranescu and Saint Jean Paulin.[5] The solutions obtained by this method are compared to those obtained, without penalization, by a standard finite element method.

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The present work was partly announced in Refs. 1 and 9.

2. Position of the Problem

We consider the typical problem studied in Ref. 3:

$$\begin{cases} \dfrac{\partial}{\partial y_i}\left(a_{ij}\dfrac{\partial u}{\partial y_j}\right) = f \quad \text{in } Y\,, \\ \left(a_{ij}\dfrac{\partial u}{\partial y_j}\right) n_i = 0 \qquad \text{on } \partial Y \backslash (\Gamma^0 \cup \Gamma^1)\,, \\ u_{|\Gamma^0} = u_{|\Gamma^1}\,, \\ \displaystyle\int_Y u\,dx = 0\,, \end{cases} \tag{1}$$

where Y is a domain of $]0,1[^2$, the boundary ∂Y is smooth enough. The opposite faces Γ^0 and Γ^1 are such that $|\Gamma^i| \neq 0$ and are defined by $\Gamma^i := \partial Y \cap \{y_2 = i\}$ $(i = 0, 1)$, (they have the same length and the same variation domain in y_1) (see Fig. 1). The a_{ij} coefficients are in $L^\infty(Y)$ and verify the standard hypothesis of coercivity. Finally f is an element of $L^2(Y)$.

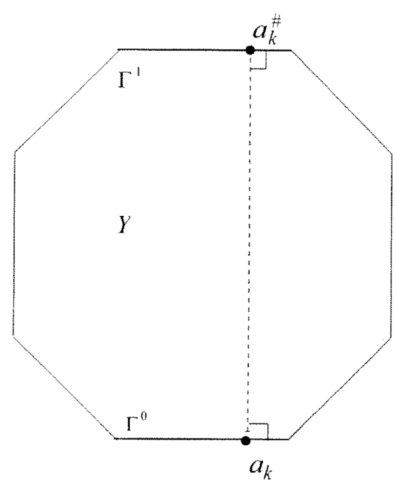

Fig. 1. An example of the domain Y. Γ^0 and Γ^1 are the opposite faces. a_k and $a_k^{\#}$ are the opposite points.

The weak formulation of Problem (1) is given by

$$\begin{cases} \text{Find } u \in Z^{\#} \text{ such that} \\ a(u,v) = (f,v) \text{ for all } v \in Z^{\#}\,, \end{cases} \tag{2}$$

where

$$Z^{\#} := \{v \in Z,\ v_{|\Gamma^0} = v_{|\Gamma^1}\}\,,$$

$$Z := \left\{v \in H^1(Y),\ \int_Y v\,dx = 0\right\}$$

and

$$a(u,v) := \int_Y a_{ij} \frac{\partial u}{\partial y_j}\frac{\partial v}{\partial y_i} dx\,, \quad (f,v) := \int_Y f v\,dx\,.$$

The sets Z and $Z^{\#}$ are Hilbert spaces for the usual norm of $H^1(Y)$ denoted $\|\cdot\|_{1,Y}$. By application of the Lax–Milgram theorem, Problem (2) has a unique solution.

3. Notations and Preliminaries

We introduce some notations and preliminaries which will be used in the sequel. We denote by h a parameter which tends to zero and by $\mathcal{T}_h := \{\mathcal{K}\}$ a uniformly regular triangulation of Y in the sense of Ref. 4. The set $\mathcal{T}_h$ is composed of triangles which have a diameter less than h. Using the P_1-conforming finite element method, we construct a finite-dimensional space Z_h such that:

$$Z_h := \{v \in Z :\ v_{|\mathcal{K}} \in P_1 \text{ for all } \mathcal{K} \in \mathcal{T}_h\}\,. \tag{3}$$

In order to simplify the presentation of the method, we assume that the trace of the triangulation on the side Γ^0 is symmetrical to the one on Γ^1 (see Fig. 2). Consider the following space:

$$Z_h^{\#} := \{v_h \in Z_h,\ v_{h_{|\Gamma^0}} = v_{h_{|\Gamma^1}}\}\,.$$

We verify, by the classical finite element theory, that for all $v \in Z^{\#}$ there is a sequence $v_h \in Z_h^{\#}$, such that:

$$\lim_{h\to 0} \|v - v_h\|_{1,Y} = 0\,. \tag{4}$$

In this study, we denote by $\{a_k\}$ the set of the vertices of triangulation and by $\{\phi_k\}$ the set of the associated basis functions satisfying: $\phi_i(a_j) = \delta_{ij}$, δ is the Kronecker's symbol.

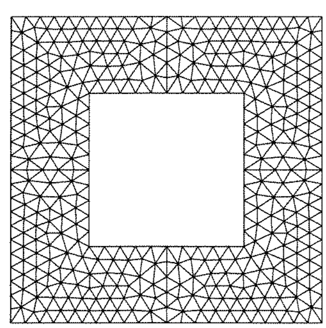

Fig. 2. The triangulation of the domain.

Let Γ be the part of ∂Y such that

$$\Gamma := \Gamma^0 \cup \Gamma^1 .$$

For all a_k located on the boundary Γ, we denote by $a_k^{\#}$ the vertex on Γ, opposite to a_k (see Fig. 1). And for all $v_h \in Z_h$ we denote by $v_h^{\#}$, the unique function in Z_h, defined by:

$$v_h^{\#}(a_k) = \begin{cases} v_h(a_k^{\#}) & \text{if } a_k \in \Gamma , \\ v_h(a_k) & \text{otherwise.} \end{cases}$$

Thus, a function $v_h \in Z_h$ is in $Z_h^{\#}$, if and only if $v_h^{\#} = v_h$. Moreover, we have the following identities:

$$a_k^{\#^{\#}} = a_k$$

and

$$v_h^{\#^{\#}} = v_h .$$

In order to take into account the periodicity conditions, we introduce the following form:

$$e_h(u_h, v_h) = \frac{1}{2} \sum_{a_k \in \Gamma} ((u_h - u_h^{\#})(v_h - v_h^{\#}))(a_k) \tag{5}$$

and the bilinear form defined on Z_h by:

$$b_h(u_h, v_h) = a(u_h, v_h) + \lambda e_h(u_h, v_h) , \tag{6}$$

where λ is the positive parameter of penalization.

4. Solution of the Approximate Problem

We approximate Problem (2) by the following:

$$\begin{cases} \text{Find } u_h^{\lambda} \in Z_h \text{ such that} \\ b_h(u_h^{\lambda}, v_h) = (f, v_h) \text{ for all } v_h \in Z_h . \end{cases} \tag{7}$$

Note that this formulation is meaningless in Z. However, it is obvious that this problem has a unique solution u_h^{λ}.

The components of the associated stiffness matrix $K := (K_{i,j})$ are given by:

$$\begin{cases} K_{i,i} = a(\phi_i, \phi_i) + \lambda & \text{if } a_i \in \Gamma , \\ K_{i,j} = a(\phi_j, \phi_i) - \lambda & \text{if } a_i,\ a_j \in \Gamma \text{ and opposite,} \\ K_{i,j} = a(\phi_j, \phi_i) & \text{otherwise.} \end{cases} \tag{8}$$

In order to study the sequence $\{u_h^{\lambda}\}$, we establish the following two lemmas:

Lemma 1. *For every $v_h \in Z_h$, we have*:

$$\alpha \left(h \sum_{a_k \in \Gamma} v_h^2(a_k) \right)^{1/2} \le |v_h|_{0,\Gamma} \le \beta \left(h \sum_{a_k \in \Gamma} v_h^2(a_k) \right)^{1/2} , \tag{9}$$

where α and β are two positive constants which are independent of h, $|\cdot|_{0,\Gamma}$ is the usual norm in $L^2(\Gamma)$.

Proof. Let v_h be an element of Z_h,

$$\begin{aligned}|v_h|_{0,\Gamma}^2 &= \int_\Gamma \left(\sum_{a_k\in\Gamma} v_h(a_k)\phi_k \right)^2 ds \\ &\leq 2 \sum_{a_k\in\Gamma} \int_\Gamma [v_h(a_k)\phi_k]^2\, ds \\ &\leq 2 \sum_{a_k\in\Gamma} v_h^2(a_k) \int_\Gamma (\phi_k)^2\, ds \\ &\leq \beta^2 \left[h \sum_{a_k\in\Gamma} v_h^2(a_k) \right] .\end{aligned}$$

The second inequality is obtained by application of Simpson's integration formula. □

Lemma 2. *For every $v_h \in Z_h$, the following inequalities hold:*

$$\|v_h - v_h^{\#}\|_{0,Y} \leq ch^{1/2} |v_h - v_h^{\#}|_{0,\Gamma} , \tag{10}$$

$$\|v_h - v_h^{\#}\|_{1,Y} \leq ch^{-1/2} |v_h - v_h^{\#}|_{0,\Gamma} , \tag{11}$$

where $\|\cdot\|_{0,Y}$ is the usual norm in $L^2(Y), c$ is a generic positive constant which is independent of h.

Proof. Let v_h be an element of Z_h, we have:

$$v_h - v_h^{\#} = \sum_{a_k\in\Gamma} (v_h - v_h^{\#})(a_k)\phi_k .$$

Using the triangular inequality and the fact that the elements $\mathcal{K}$ of $\mathcal{T}_h$ are such that $|\mathcal{K}| \leq ch^2$, we verify:

$$\|v_h - v_h^{\#}\|_{0,Y}^2 \leq ch^2 \sum_{a_k\in\Gamma} |(v_h - v_h^{\#})(a_k)|^2 . \tag{12}$$

By Lemma 1, we obtain the estimate (10).

Using inequality (10) and the following inverse inequality:

$$\|v_h\|_{1,Y} \leq ch^{-1} \|v_h\|_{0,Y} \text{ for all } v_h \in Z_h \tag{13}$$

we get (11). □

We give first a convergence result.

Theorem 1. *Let u and u_h^λ be the respective solutions of the problems* (2) *and* (7). *We have*:

$$\lim_{h\to 0}\lim_{\lambda\to\infty}\|u-u_h^\lambda\|_{1,Y}=0\,. \tag{14}$$

Proof. First, we prove that the limit $\lim_{\lambda\to\infty} u_h^\lambda$ exists and belongs to $Z_h^\#$.

Choose $v_h = u_h^\lambda$ in (7), using Cauchy–Schwarz's and Poincaré–Wirtinger's inequalities, we obtain the following estimates:

$$\|u_h^\lambda\|_{1,Y}\le c\,, \tag{15}$$

$$\lambda\sum_{a_k\in\Gamma}(u_h^\lambda-u_h^{\lambda^\#})^2(a_k)\le c\,, \tag{16}$$

where c is a constant independent of h and λ.

From inequality (15), we deduce the existence of a subsequence (u_h^λ) which converges weakly toward a functional u_h in $H^1(Y)$ as $\lambda\to\infty$.

Using Lemma 1 and inequality (16), we get:

$$|u_h^\lambda-u_h^{\lambda^\#}|_{0,\Gamma}\le c\left(\frac{h}{\lambda}\right)^{1/2}\,. \tag{17}$$

Moreover, we have

$$|u_h-u_h^\#|_{0,\Gamma}\le|u_h-u_h^\lambda|_{0,\Gamma}+|u_h^\lambda-u_h^{\lambda^\#}|_{0,\Gamma}+|u_h^{\lambda^\#}-u_h^\#|_{0,\Gamma}\,.$$

Using trace continuity and inequality (17), it follows that the right-hand side of the inequality above converges to 0 as $\lambda\to\infty$. Consequently, we have

$$u_h\in Z_h^\#\,.$$

Secondly, we prove that u_h is the solution of the discrete problem associated to (2).

If we choose $v_h\in Z_h^\#$ in (7), we get:

$$a(u_h^\lambda,v_h)=(f,v_h)\,,$$

and then, letting $\lambda\to\infty$, we deduce that u_h is the unique solution of the following problem:

$$a(u_h,v_h)=(f,v_h)\text{ for all }v_h\in Z_h^\#\,. \tag{18}$$

According to the classical theory of conforming finite elements, to (2) and to (18), we have:

$$\lim_{h\to 0}\|u_h-u\|_{1,Y}=0\,.$$

Lastly, (14) follows from the triangle inequality:

$$\|u_h^\lambda-u\|_{1,Y}\le\|u_h^\lambda-u_h\|_{1,Y}+\|u_h-u\|_{1,Y}$$

as λ tends to ∞ and h tends to 0. $\square$

The following theorem provides us with error estimates:

Theorem 2. *Let u and u_h^λ be the solutions of problems* (2) *and* (7), *respectively. Assume that*:

$$\lambda \text{ is of order } h^{-p}. \tag{19}$$

Then

$$\|u - u_h^\lambda\|_{1,Y} \leq c\left\{\inf_{v_h \in Z_h^\#} \|u - v_h\|_{1,Y} + h^{p/2}\right\} \tag{20}$$

and

$$\lim_{h\to 0} \|u - u_h^\lambda\|_{1,Y} = 0 \quad \text{for all } p \geq 0. \tag{21}$$

Proof. Note that

$$a(u - u_h^\lambda, v_h) = 0 \quad \text{for all } v_h \in Z_h^\#.$$

In particular

$$a\left(u - u_h^\lambda, \frac{u_h^\lambda + u_h^{\lambda^\#}}{2}\right) = 0,$$

and then, for all $v_h \in Z_h^\#$,

$$a(u_h^\lambda - u, u_h^\lambda - u) = a\left(u_h^\lambda - u, u_h^\lambda - \frac{u_h^\lambda + u_h^{\lambda^\#}}{2}\right) + a(u_h^\lambda - u, v_h - u)$$

$$= \frac{1}{2}a(u_h^\lambda - u, u_h^\lambda - u_h^{\lambda^\#}) + a(u_h^\lambda - u, v_h - u).$$

Using the coercivity and continuity properties of $a(.,.)$, we get:

$$c\|u_h^\lambda - u\|_{1,Y}^2 \leq \|u_h^\lambda - u\|_{1,Y}\|u_h^\lambda - u_h^{\lambda^\#}\|_{1,Y} + \|u_h^\lambda - u\|_{1,Y}\|v_h - u\|_{1,Y},$$

thus

$$\|u_h^\lambda - u\|_{1,Y} \leq c\left\{\inf_{v_h \in Z_h^\#} \|v_h - u\|_{1,Y} + \|u_h^\lambda - u_h^{\lambda^\#}\|_{1,Y}\right\}. \tag{22}$$

From (17) and (19) we get

$$|u_h^\lambda - u_h^{\lambda^\#}|_{0,\Gamma} \leq ch^{(p+1)/2}. \tag{23}$$

And, using Lemma 2

$$\|u_h^\lambda - u_h^{\lambda^\#}\|_{1,Y} \leq ch^{p/2}. \tag{24}$$

Consequently, inequality (20) is obtained from relationships (22) and (24).

In order to establish (21), it is sufficient to prove it for $p = 0$.

Let δ_h be the function defined by:

$$\delta_h = \frac{1}{2}(u_h^\lambda - u_h^{\lambda^\#}),$$

from (10), (11) and (23) we obtain

$$\delta_h \text{ weakly converges to } 0 \text{ in } Z \text{ as } h \to 0. \tag{25}$$

Let w_h be the function in $Z^{\#}$ given by

$$w_h := \frac{1}{2}(u_h^\lambda + u_h^{\lambda^{\#}}). \tag{26}$$

This function splits as

$$w_h = u_h^\lambda - \delta_h ,$$

and then

$$a(w_h, v_h) = (f, v_h) - a(\delta_h, v_h) \text{ for all } v_h \in Z_h^{\#} .$$

Using (15), (24) and (25), we deduce the existence of a subsequence of (w_h) and afterwards a subsequence of (u_h^λ) which converges weakly to the solution u of problem (2) as $h \to 0$.

The strong convergence is obtained by using the inequality

$$a(u_h^\lambda - u, u_h^\lambda - u) \leq (f, u_h^\lambda) - a(u_h^\lambda, u) - a(u, u_h^\lambda) + (f, u)$$

as h tends to 0. □

Remarks.

1. For $p = 2$, the method is of first-order.
2. The extension of the method to three dimensions and to other types of finite elements can be obtained by similar techniques.
3. In order to reduce the bandwidth of the stiffness matrix, we considered the penalization term of the form (5). However, the results in Theorems 1 and 2 remain true if we consider the following form:

$$e_h(u, v) = \frac{1}{h}\int_\Gamma ((u_h - u_h^{\#})(v_h - v_h^{\#}))(s)\, ds .$$

4. This mathematical study can be used to justify the solution technique in Ref. 8.

5. Application

Let Ω be an open set of $\mathbb{R}^2$ and Ω_ε^* be the part of Ω which is occupied by a porous material having a periodic structure (we denote by ε the size of the pores) and let Y be the representative cell

$$Y =]0, 1[\times]0, 1[.$$

We denote by Y^* the part of Y occupied by the material and we assume that the hole T does not intercept the boundary ∂Y.

Consider the following problem[5]:

$$\begin{aligned} -\frac{\partial}{\partial x_i}\left(a_{ij}\left(\frac{x}{\varepsilon}\right)\frac{\partial u^\varepsilon}{\partial x_j}\right) &= f \quad \text{in } \Omega_\varepsilon^* , \\ u^\varepsilon &= 0 \quad \text{on } \partial\Omega , \\ a_{ij}\left(\frac{x}{\varepsilon}\right)\frac{\partial u^\varepsilon}{\partial x_j} n_i &= 0 \quad \text{on the boundary of the pores.} \end{aligned} \tag{27}$$

It is known[5] that the homogenized problem associated to (27) is given by:

$$-\frac{\partial}{\partial x_i}\left(q_{ij}\frac{\partial u}{\partial x_j}\right) = \frac{|Y^*|}{|Y|}f \quad \text{in } \Omega\,,$$
$$u = 0 \qquad \text{on } \partial\Omega\,,$$

where the homogenized coefficients q_{ij} are given by

$$q_{ij} = \frac{1}{|Y|}\int_{Y^*}\left(a_{ij} - a_{kj}\frac{\partial \chi^i}{\partial y_k}\right)dy\,, \tag{28}$$

and the functions χ^1 and χ^2 are solutions of the following problems

$$\begin{cases} -\dfrac{\partial}{\partial y_l}\left(a_{kl}\dfrac{\partial(\chi^i - y_i)}{\partial y_k}\right) = 0 & \text{in } Y^*\,, \\ a_{kl}\dfrac{\partial(\chi^i - y_i)}{\partial y_k}n_l = 0 & \text{on } \partial T\,, \qquad i = 1,2 \\ \chi^i Y\text{-periodic.} \end{cases} \tag{29}$$

A function $u \in H^1(Y)$ is Y-periodic if its traces are equal on each pair of the opposite faces of Y. Note that the above problems are of the same type as problem (1).

We apply the penalty method to solve the problems (29). The solutions will be compared with the non-penalized ones obtained by a standard finite element method FEM (MODULEF library[2]).

In this order, we consider the case where $(a_{ij}) = (\delta_{ij})$ in Y^* and where the porosity is 25% (see Fig. 2). Note that, in this case, the homogenized coefficients of conductivity q_{ij} are such that $q_{ij} = q\delta_{ij}$.

The used mesh consists of 728 triangles with three nodes for the interpolation of the functions (Fig. 2).

The parameter of penalization is $\lambda = 30$. In this numerical process, we use Gibbs's algorithm[6,7] to renumber the nodes, the storage of the matrices is in the skyline mode.

Let $Er_{\%}$ be the relative error in maximum norm $Er_{\%} = 100 \times \frac{\max_i |u_i^p - u_i^m|}{\max_i |u_i^m|}$, where u_i^p is the penalized solution and u_i^m is the solution obtained by the standard finite element method (MODULEF library[2]).

The homogenized coefficient of conductivity q, with nine significant digits, obtained by both methods is:

Penalization	$q = 0.624\ 177\ 583$
Standard FEM	$q = 0.624\ 101\ 099\,.$

6. Concluding Remarks

1. Table 1 shows a relative gain of memory of about 36%. But it is clear that this percentage increases with the number of nodes of the mesh (Fig. 3).

Table 1. The characteristics of the matrices of the two methods.

	Penalization	Standard FEM
Number of necessary words to the storage of the matrix	7636	11980
Maximal difference between two nodes by element	43	196

Table 2. Relative error between penalized and non-penalized solution for the test problems.

	χ^1	χ^2
$Er_{\%}$	0.121326872	0.120717589

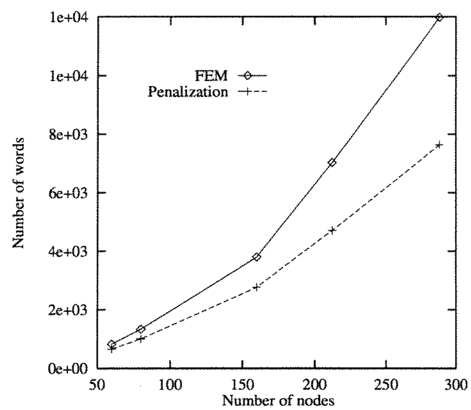

Fig. 3. Number of words, which are necessary for the matrix storage, as a function of the mesh size. The figure shows that the gain linked to the method of penalization increases with the number of nodes.

2. The penalized and non-penalized solutions do not present any significant differences (less than 0.4%) (Fig. 4).
3. This method leads to an economical CPU time of solution (about 10%) (Fig. 5).
4. Figure 6 presents the homogenized coefficients sensitivity, given by (28), as a function of the penalization parameter.
5. For the numerical processing of this method we suggest the following technique: For every opposite points $(a_k, a_k^{\#})$, we add to the topology of the elements the "fictitious" quadrangle $(a_k, a_k^{\#}, a_k, a_k^{\#})$ which has the following elementary

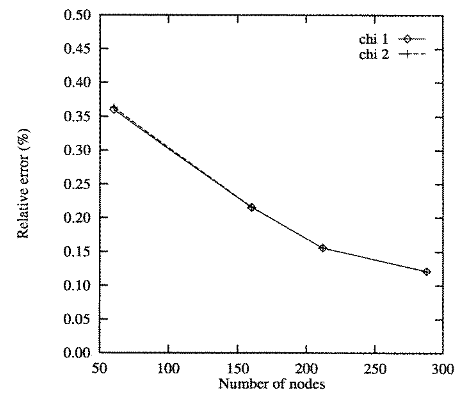

Fig. 4. Comparison between the penalized and non-penalized solutions of the test problems for several value of gridpoints.

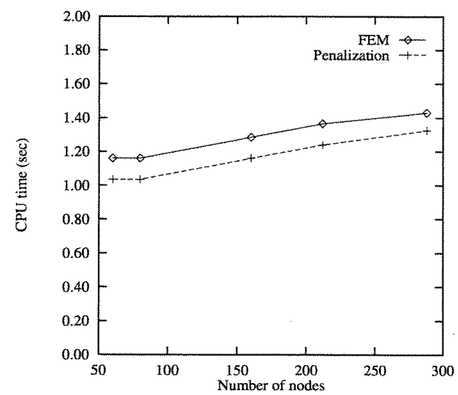

Fig. 5. Comparison of CPU time in the two approaches for several values of gridpoints.

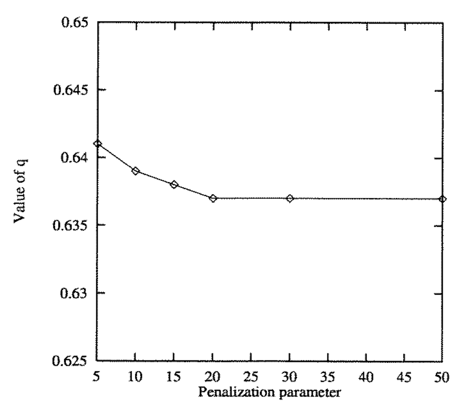

Fig. 6. Variation of the homogenized coefficient q as a function of the penalization parameter. After several numerical tests, we have observed that the value of penalization parameter which gives the desired is of order $30 \times \max(a_{ij})$, where a_{ij} are the domain characteristics.

associated matrix:

$$\begin{pmatrix} \lambda & -\lambda & 0 & 0 \\ -\lambda & \lambda & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Thus, at the time of the assembling stage, we get the contribution of the form $\lambda e_h(.,.)$ to the global matrix.

Acknowledgments

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