# An error bound for statistically invariant fields in stochastic PDEs

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## Abstract

A methodology to compute the error due to homogenization of an heterogeneous stochastic problem is presented. The method is developed for the heat equation, and in order to be applicable, it is required that the conductivity is statistically invariant over the domain. Examples illustrate the behaviour of the bounds.

## 1 Introduction

In this paper a methodology to compute the error due to homogenization of an heterogeneous stochastic problem is presented. By bounding the error, we mean to bound the difference between the expectation of a quantity dependent of the solution that is defined by the analyst and its estimation from the homogenized problem. The computation of the bound is purely deterministic, however, it involves the solution of another problem, called the dual problem.

All the theory regarding the bound is presented for a Poisson problem (heat equation), though this method can be extended to much wider that fulfill some characteristics listed in this work.

The main features of the bound are its simplicity and low computational cost. On the other hand, under some circumstances, the interval defined by the bound can be very wide. An example is shown and an explanation to this behaviour is given in the Appendix.

The paper is organized as follows. In section 2, the problem is defined and the required notation is introduced. In section 3, the bounds are derived. The following section, presents a couple of simplifications which make the computation of the error bound very efficient. Section 5 presents two test cases to validate the presented bounds.

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## 2 Problem and notation

### 2.1 Stochastic problem

The problem is defined on a domain $\Omega \times \Theta$, where $\Omega \subseteq \mathbb{R}^2$ is the spatial domain and $\Theta$ is the stochastic domain. The boundary of $\Omega$ is denoted by $\Gamma$, which can be further divided in two subsets $\Gamma_D$ and $\Gamma_N$. Deterministic Dirichlet boundary conditions (temperatures) are prescribed on $\Gamma_D$, while deterministic Neumann boundary conditions (fluxes) are prescribed on $\Gamma_N$. The conductivity $k$ depends on the spatial coordinate and also on the realization; however, it is statistically invariant,

$$\int_\Theta k = \frac{1}{|\Omega|} \int_\Omega k. \tag{1}$$

With that notation, the partial differential equation reads,

$$\begin{aligned} -\nabla \cdot (k \nabla u) &= f(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \Omega \times \Theta \\ -k \nabla u \cdot \boldsymbol{n} &= g(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \Gamma_N \times \Theta \\ u &= h(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \Gamma_D \times \Theta \end{aligned}$$

where, $f, g$ and $h$ are known deterministic functions.

Through Green's lemma, the problem can be rewritten in its weak form:

Find $u \in H^1$

$$\int_{\Omega \times \Theta} k \nabla u \cdot \nabla v = \int_{\Omega \times \Theta} f v - \int_{\Gamma_N \times \theta} v g \qquad \forall \boldsymbol{v} \in H_0^1 \tag{2}$$

where

$$H^1 = \left\{ u \in L^2(\Omega \times \Theta) | u = h(\boldsymbol{x}) \text{ on } \Gamma_D \times \Omega \text{ and } \frac{\partial u}{\partial x_i} \in L^2(\Omega \times \Theta) \right\}$$

and

$$H_0^1 = \left\{ u \in L^2(\Omega \times \Theta) | u = 0 \text{ on } \Gamma_D \times \Omega \text{ and } \frac{\partial u}{\partial x_i} \in L^2(\Omega \times \Theta) \right\}$$

We conclude this section introducing more notation. The left hand side of (2) is a bilinear form, that will be denoted by

$$a(u, v) = \int_{\Omega \times \Theta} k \nabla u \cdot \nabla v$$

and its induced norm (since it defines an inner product)

$$\|v\|_a = \sqrt{a(u, u)}$$

; while the right hand side will be denoted by

$$L(v) = \int_{\Omega \times \Theta} f v - \int_{\Gamma_N \times \theta} v g$$

## 2.2 Quantity of interest

The quantity of interest is the result of applying a certain functional to the solution field. This functional must be expressed as the integral of a linear operator $J$ over a subset of $\Omega$, therefore, the average temperature on a square or the average flux on part of the boundary are examples of quantity of interest. Due to the stochastic nature of the model, this paper is concerned with the expectation of the quantity of interest. The quantity of interest will be denoted by

$$q_\theta(u) = \int_{\Omega'} J(u)$$

and its expectation will be denoted by

$$q(u) = E[q(u)] = \int_\Theta \int_{\Omega'} J(u)$$

Now, we proceed to introduce the adjoint problem,

Find $\phi \in H_0^1$

$$\int_{\Omega\times\Theta} k\nabla\phi \cdot \nabla v = q(v) \qquad \forall \boldsymbol{v} \in H_0^1 \tag{3}$$

Its relevance will be made clear in the following sections.

## 2.3 Homogenized problems

In this section, we proceed to introduce two more problems. Both problems are deterministic since $k$ is substituted by $\bar{k}$ obtained through homogenization. Since the following problems are easier to solve, their solution is going to be used to compute the quantity of interest and the error due to the substitution will be bounded. The problem reads

Find $\bar{u} \in \bar{H}^1$

$$\int_\Omega \bar{k}\nabla u \cdot \nabla v = \int_\Omega fv - \int_{\Gamma_N} vg \qquad \forall \boldsymbol{v} \in \bar{H}_0^1 \tag{4}$$

where

$$\bar{H}^1 = \left\{ u \in L^2(\Omega) | u = h(\boldsymbol{x}) \text{ on } \Gamma_D \text{ and } \frac{\partial u}{\partial x_i} \in L^2(\Omega) \right\}$$

and

$$\bar{H}_0^1 = \left\{ u \in L^2(\Omega) | u = 0 \text{ on } \Gamma_D \text{ and } \frac{\partial u}{\partial x_i} \in L^2(\Omega) \right\}$$

We will denote the approximation of the solution of this problem (obtained by finite elements, for instance) by $u^h$. And the error field, $u - u^h$ will be denoted by $e$. The second problem reads:

Find $\bar{\phi} \in \bar{H}_0^1$

$$\int_\Omega \bar{k} \nabla \bar{\phi} \cdot \nabla v = q(v) \qquad \forall \boldsymbol{v} \in \bar{H}_0^1 \tag{5}$$

The approximation of its solution will be denoted by $\phi^h$, while its associated error field, $\phi - \phi^h$, will be denoted by $e_\phi$.

# 3 Derivation of the error bounds

In this section, we proceed to bound the following quantity,

$$q(u) - q(u^h)$$

with an upper and lower bound. The computation of those bounds will not involve the solution of a stochastic problem.

We start by using using equation (3) and the fact that $a$ is linear with respect to its second argument,

$$q(u) - q(u^h) = a(\phi, e)$$

To this expression, we add and subtract $a(\phi^h, e)$ to obtain

$$q(u) - q(u^h) = a(e_\phi, e) + a(\phi^h, e) \tag{6}$$

Now, we make use of the following result related to the residue,

$$R(v) = L(v) - a(u^h, v) = L(v) + [a(u, v) - a(u, v)] - a(u^h, v) = a(e, v)$$

which allows us to rewrite (6)

$$q(u) - q(u^h) = R(\phi^h) + a(e_\phi, e)$$

It is relevant to emphasize that $R(\phi^h)$ is a deterministic quantity, since

$$R(\phi^h) = \underbrace{L(\phi^h)}_{\text{deterministic}} - \int_\Omega \int_\Theta k \nabla u^h \cdot \nabla \phi^h = L(\phi^h) - \underbrace{E[k] \int_\Omega \nabla u^h \cdot \nabla \phi^h}_{\text{deterministic}}$$

since $k$ is statistically invariant.

Since the bilinear form $a(\cdot, \cdot)$ defines an inner product, we can use the Cauchy-Schwarz inequality to obtain,

$$R(\phi^h) - \|e_\phi\|_a \|e\|_a \leq q(u) - q(u^h) \leq R(\phi^h) + \|e_\phi\|_a \|e\|_a$$

Now, we proceed to bound the norms of the errors since they are not computable. In order to do that, we introduce an inner product, its induced norm,

$$< u, v >_{k^{-1}} = \int_{\Omega \times \Theta} k^{-1} uv \qquad \|u\|_{k^{-1}} = \sqrt{< u, u >_{k^{-1}}}$$

and a vectorial field $\hat{\boldsymbol{Q}}$ that fulfills,

$$\begin{aligned} \nabla \cdot \hat{\boldsymbol{Q}} &= f(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \Omega \\ \hat{\boldsymbol{Q}} &= g(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \Gamma_N \end{aligned}$$

In other words, a flux field that fulfills the prescribed flux boundary conditions. Notice that all the terms in those two equations are deterministic. In [1] several techniques to compute a field with such characteristics are compared.

The aim is to prove that,

$$\|e\|_a \leq \|\hat{\boldsymbol{Q}} + k\nabla u^h\|_{k^{-1}} = \eta \tag{7}$$

Firstly, we turn our attention to the following equalities,

$$-\int_{\Omega\times\Theta} \hat{\boldsymbol{Q}} \cdot \nabla v = L(v) \qquad \forall v \in H_0^1$$
$$\int_{\Omega\times\Theta} k\nabla u \cdot \nabla v = L(v) \qquad \forall v \in H_0^1$$

and to their difference,

$$0 = \int_{\Omega\times\Theta} (\hat{\boldsymbol{Q}} + k\nabla u) \cdot \nabla v \qquad \forall v \in H_0^1$$

Setting $v = -u + u^h$, we obtain that

$$< \hat{\boldsymbol{Q}} + k\nabla u, -k\nabla u + k\nabla u^h >_{k^{-1}} = 0$$

in other words, $\hat{\boldsymbol{Q}}+k\nabla u$ is orthogonal to $-k\nabla u+k\nabla u^h$ in the $k^{-1}$-inner product. This allows us to use the Pythagoras theorem to obtain the desired result

$$\|\hat{\boldsymbol{Q}} + k\nabla u^h\|^2_{k^{-1}} = \|\hat{\boldsymbol{Q}} + k\nabla u - k\nabla u + k\nabla u^h\|^2_{k^{-1}} =$$
$$= \|\hat{\boldsymbol{Q}} + k\nabla u\|^2_{k^{-1}} + \| - k\nabla u + k\nabla u^h\|^2_{k^{-1}} = \|\hat{\boldsymbol{Q}} + k\nabla u\|^2_{k^{-1}} + \|e\|^2_a \geq \|e\|^2_a$$

In a similar manner, the result can be extended to $\|e_\phi\|_{k-1}$. The bounds can be summarized in the following equation

$$\zeta_l = R(\phi^h) - \eta\eta_\phi \leq q(u) - q(u^h) \leq R(\phi^h) + \eta\eta_\phi = \zeta_u$$

Finally, we show that $\eta$ is a also deterministic quantity. By expanding its square,

$$\begin{aligned}\|\hat{\boldsymbol{Q}} + k\nabla u^h\|^2_{k^{-1}} &= \int_{\Omega\times\Theta} k^{-1}\hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{Q}} + \int_{\Omega\times\Theta} k\nabla u^h \cdot \nabla u^h + 2\int_{\Omega\times\Theta} \hat{\boldsymbol{Q}} \cdot \nabla u^h \\ &= E[k^{-1}]\int_\Omega \hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{Q}} + E[k]\int_\Omega \nabla u^h \cdot \nabla u^h + 2\int_\Omega \hat{\boldsymbol{Q}} \cdot \nabla u^h \end{aligned} \tag{8}$$

it becomes explicit that it is only a sum of integrals over the spatial domain.

Before concluding this section, it is worth to mention this error bound can be extended to other problems, such as linear elasticity. The results required that the bilinear form to define an inner product, in order to be able to use the Cauchy-Schwarz inequality.

## 3.1 Deterministic heterogeneous problem

We would like to emphasize that the derivations exposed in the previous could be session could be repeated to compare the solution of an heterogeneous deterministic problem and the solution of it homogenized counterpart. However, in this case, an integral would have to be performed over the heterogeneous domain which may involve the generation of an integration mesh, while for stochastic problem, since the material properties are statistically invariant, the integral is performed over an homogeneous domain, which greatly reduces the computational costs.

# 4 Simplifications

In this section, we intend to show how under some assumptions, it becomes very efficient to compute the error bound proposed. Our first assumption considers that the homogenized problems were solved through the finite element method with a mesh that is fine enough to assume $\hat{\boldsymbol{Q}} = -\bar{k}\nabla u^h$. We will be also assuming that the Dirichlet boundary conditions are homogeneous. Given that, the finite element method would produce the following two system of equations, for the primal and the dual problem:

$$[\boldsymbol{A}][\boldsymbol{u}] = [\boldsymbol{l}]$$
$$[\boldsymbol{A}][\boldsymbol{\phi}] = [\boldsymbol{q}]$$

Now, the computation of $R(\phi^h)$ reduces to

$$R(\phi^h) = [\boldsymbol{l}]^T[\boldsymbol{\phi^h}] - \frac{E[k]}{\bar{k}}[\boldsymbol{u}]^{\boldsymbol{T}}[\boldsymbol{A}][\boldsymbol{\phi^h}]$$

and the three integrals that define $\eta^2$ are reduced to,

$$E[k^{-1}]\bar{k}[\boldsymbol{u}]^{\boldsymbol{T}}[\boldsymbol{A}][\boldsymbol{u}] + \frac{E[k]}{\bar{k}}[\boldsymbol{u}]^{\boldsymbol{T}}[\boldsymbol{A}][\boldsymbol{u}] - 2[\boldsymbol{u}]^{\boldsymbol{T}}[\boldsymbol{A}][\boldsymbol{u}]$$

# 5 Numerical results

In this section, two numerical examples are presented to illustrate the behaviour of the bound.

## 5.1 Low conductivity contrast

The domain of consideration is a L-shape (figure 5.1) made of matrix of conductivity $k_m = 1$ and filled with 75 circular particles of radius 0.05 and conductivity $k_i = 0.6$, resulting in approximate volume fraction of 0.196. The centers of the particles follow an uniform random variable inside, thus, the particles are not allowed to intersect with each other or with the boundaries of the domain. The functions $f, g$ and $h$ are defined as follows,

$$f(\boldsymbol{x}) = 0 \qquad \forall \boldsymbol{x} \in \Omega$$
$$g(\boldsymbol{x}) = \begin{cases} -10(y+1) & \forall \boldsymbol{x} \in \{1\} \times [-1,1] \\ -10(x+1) & \forall \boldsymbol{x} \in [-1,1] \times \{1\} \\ 0 & \forall \boldsymbol{x} \in \{-1\} \times [0,1] \cup [0,1] \times \{-1\} \end{cases}$$
$$h(\boldsymbol{x}) = 0 \qquad \forall \boldsymbol{x} \in [-1,0] \times \{0\} \cup \{0\} \times [-1,0]$$

On the other hand, an approximation of the solution is obtained in a domain with an homogeneous conductivity. The homogeneous conductivity $\bar{k}$ is obtained through the rule of mixture (which in this case, is the same as the $E[k]$) which gives a value of We define our quantity of interest to be the average temperature on $\omega = \{1\} \times [-1,1] \cup [-1,1] \times \{1\}$,

$$q_\theta(u) = \frac{1}{|\omega|}\int_\omega u$$

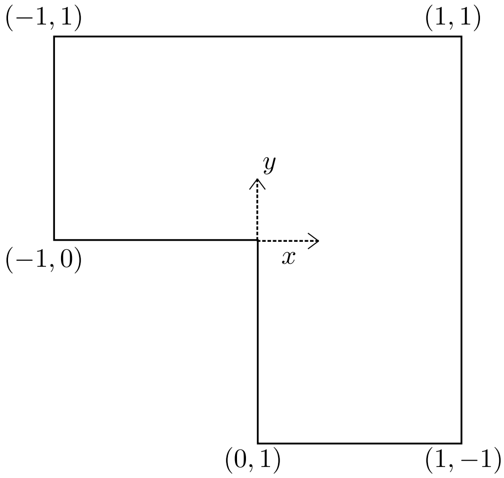


Figure 1: Domain

To validate the bounds a reference quantity of interest will be computed through Monte Carlo using 64 realizations.

Figure 5.1 and 5.1 show the temperature and the gradient field for the homogenized domain and for a random realization.

The following table summarizes the results

| $q(u^h)$ | $\zeta_l \leq$ | $q(u) - q(u^h)$ | $\leq \zeta_u$ | $\zeta_l + q(u^h) \leq$ | $q(u)$ | $\leq \zeta_u + q(u^h)$ |
|---|---|---|---|---|---|---|
| 22.10 | -1.20 | 0.46 | 1.20 | 20.90 | 22.56 | 23.30 |

It can be observed that the bounds for $q(u) - q(u^h)$ are symmetric, since $\phi^h$ belongs to the test space of the $u^h$.

### 5.2 High conductivity contrast

In this section, we are going to repeat the previous numerical example with a high contrast between the conductivity of the matrix and the inclusion. The conductivity of the matrix remains the same $k_m = 1$, however, the conductivity of the inclusion is set to $k_i = 0.1$. The following table summarizes the results:

| $q(u^h)$ | $\zeta_l \leq$ | $q(u) - q(u^h)$ | $\leq \zeta_u$ | $\zeta_l + q(u^h) \leq$ | $q(u)$ | $\leq \zeta_u + q(u^h)$ |
|---|---|---|---|---|---|---|
| 25.88 | -42.71 | 5.33 | 42.71 | -16.83 | 31.22 | 68.59 |

The purpose of this numerical example was to show that the interval described by the bounds grows in length very fast when there is a high contrast between the material conductivities, making it unusable. In the appendix an explanation for this behaviour is given.

## 6 Conclusions

An bound on the error due to homogenization of an heterogeneous stochastic problem was presented in this paper. The bounds can help to asses the validity

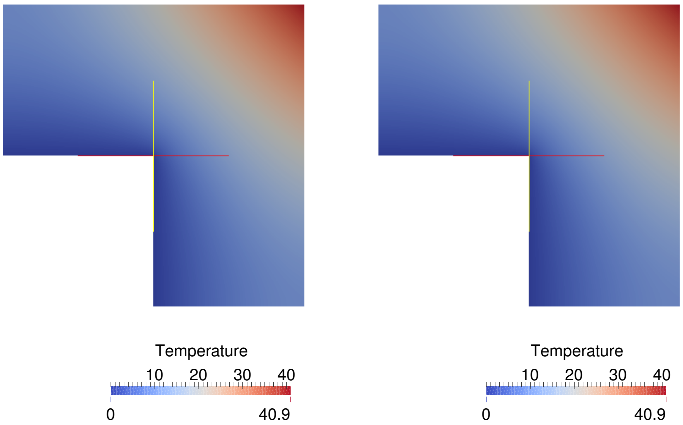


Figure 2: Left: Temperature field for a realization Right: Temperature field for the homogenized field

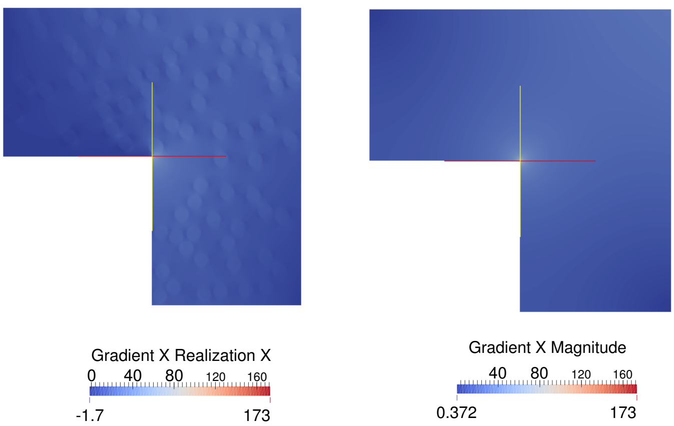


Figure 3: Left: Gradient in the X direction for a realization Right: Gradient in the X direction the homogenized field

of the approach. The computational cost, in some circumstances, is very low, specially, when compared to the deterministic approach, since it only involves an integral over an homogeneous domain.

On the other hand, the numerical examples have highlighted one of the limitations of this work. The error bounds do not behave well, when there exists a huge contrast between the conductivities of the several materials. This will be explored in future works.

That is not the only limitation of this work. The bounds presented are only valid for the expectation. For some analysis, the analyst might also be interested on how the quantities are spread around the expectation. Also, the bound does not take into account the effect of the shape of the particles. The authors have extended the present work to deal with the last two limitations, a bound on the variance, and a bound on the expectation that takes into account the particle shapes. Both ideas will be the object of upcoming publications.

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# APPENDIX

In this section, we intend to explain the behaviour shown in section (5.2). In order to do so, we start by finding the homogenized conductivity that minimizes $\eta$ and $\eta_\phi$ under the following considerations:

- The Dirichlet boundary conditions are homogeneous.
- $\bar{u}$ is the solution of the homogenized problem for a conductivity $\bar{k}$
- $\hat{\boldsymbol{Q}}$ is chosen to be the flux of $\bar{u}$, in short, $\hat{\boldsymbol{Q}} = -\bar{k}\nabla\bar{u}$

Under those considerations, if the conductivity is changed to $\bar{k}'$, the solution field becomes $\frac{\bar{k}}{\bar{k}'}u$. Applying the assumptions to eq. (8) gives

$$\left[\frac{E(k)}{\bar{k}'^2} - \frac{2}{\bar{k}'} + E(k^{-1})\right]\bar{k}^2\int_\Omega \nabla\bar{u}^2$$

an expression that can be minimized with respect of $\bar{k}'$. By taking its derivative with respect to $\bar{k}'$, we find that this expression reaches a minimum for $\bar{k}' = E(k)$, which means that the best bound is obtained, under the stated assumptions, when rule of mixture is applied. Substituting this value in the previous expression

$$\left[E(k^{-1}) - \frac{1}{E(k)}\right] \bar{k}^2 \int_\Omega \nabla \bar{u}^2 \tag{9}$$

If the expectation of the conductivity has the following form,

$$E(k) = \sum_{i=1}^{N} \alpha_i k_i \qquad \text{where} \qquad \sum_{i=1}^{N} \alpha_i = 1$$

then, the expectation of its reciprocal is

$$E(k^{-1}) = \sum_{i=1}^{N} \frac{\alpha_i}{k_i}$$

Bringing this into the expression inside brackets of equation (9), we obtain

$$E(k^{-1}) - \frac{1}{E(k)} = \sum_{i=1}^{N} \frac{\alpha_i}{k_i} - \frac{1}{\sum_{i=1}^{N} \alpha_i k_i}$$

which is the difference between the reciprocal of the weighted harmonic mean and the reciprocal of the weighted arithmetic mean of $k_i$ ($i = 1...N$). By the generalized mean inequality, it is known that this term will be always equal or greater than 0, having the equality only when $k_1 = k_2 = ... = k_N$. The greater the contrast between the conductivities, the further the expression is from 0. Figure 4 represents the difference between reciprocal of the means for $N = 2$.

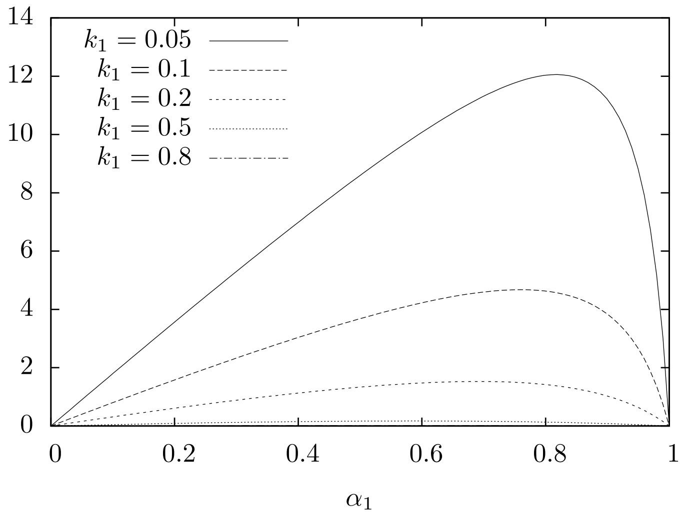


Figure 4: Difference between the reciprocals of the harmonic and the arithmetic mean for $k_2 = 1$ and $N = 2$.