Advances in error estimation for homogenisation

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Motivation

**Problem:** Analysis of an heterogeneous materials. Vague information available. The position of the particles is not available.
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**Solution:** Homogenisation.
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**Problem:** Analysis of an heterogeneous materials. Vague information available. The position of the particles is not available.

**Solution:** Homogenisation.

**New problem:**
Assess the validity of the homogenisation.
Key ideas

Exact model

- To estimate error, we need a reference to compare our solution
- **Reference**: solution of a stochastic PDE
  - Able to take into account the vague description of the domain

Error estimation

- **Objective**: Compare the solution of the two models (without solving the SPDE)
- Adapt classic a posteriori error bounds to this specific problem
Exact model
Idea: Understand the original problem as an SPDE (the center of particles is a random variable) and bound the distance between both models
**Proposed solution**

**SPDE:** Stochastic partial differential equation.
Collection of parametric problems + probability density function
**QoI:** Quantity of interest. The output. Scalar that depends of the solution.

\[ q(u) = \int_\Omega \int_\Theta \gamma(x) \cdot u(x, \theta) \quad \text{(linear)} \]
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q(u) = \int_{\Omega} \int_{\Theta} \gamma(x) \cdot u(x, \theta) \quad \text{(linear)}
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Problem statement

Heat equation

Heterogeneous problem

\[
 a(u, v) = \int_{\Omega} \int_{\Theta} k(\theta, x) \nabla u \cdot \nabla v \\
 l(v) = \int_{\Omega} \int_{\Theta} f v - \int_{\partial \Omega} \int_{\Theta} g v \\
 a(u, v) = l(v) \quad \forall v \in V
\]
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Homogeneous problem

\[ a_0(\bar{u}, v) = \int_\Omega \bar{k}(x) \nabla \bar{u} \cdot \nabla v \]

\[ a_0(\bar{u}, v) = l(v) \quad \forall v \in V_0 \]

\[ a_0(\bar{u}^h, v) = l(v) \quad \forall v \in V_0^h \subseteq V_0 \]
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**Aim**: Bound

\[
q(u) - q(\bar{u}^h)
\]

The computation of the bound must be deterministic.
Hypothesis

Deterministic boundary conditions
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Deterministic boundary conditions

Knowledge of the probability of being inside particle for every point of the domain.

\[ E[k(x, \theta)] = \int_{\Theta} k(x, \theta) \quad \text{E}[k(x, \theta)^{-1}] \]
Hypothesis

Deterministic boundary conditions

Knowledge of the probability of being inside particle for every point of the domain.

\[ E[k(x, \theta)] = \int_{\Omega} k(x, \theta) \quad E[k(x, \theta)^{-1}] \]

If not known, it can be assumed to be a constant equal to the volume fraction.
Error estimation
Error estimation

- **Objective:** Compare the solution of the two models (without solving the SPDE)

- To estimate the error, an equilibrated flux field is needed

- With an equilibrated flux field, we can estimate the error in energy norm

  \[ \|u - \bar{u}^h\| \leq \eta \]

- And with an estimator for the error in energy norm, we can estimate the error in the QoI

  \[ q(u) - q(\bar{u}^h) \leq \gamma \]
An equilibrated flux field fulfills

\[ \nabla \cdot \hat{Q} = f \quad x \in \Omega \]

\[ \hat{Q} \cdot n = g \quad x \in \partial\Omega_N \]

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In contrast, in “temperature” FE, the temperature is the unknown and

\[ \tilde{u}^h = h \quad x \in \partial\Omega_D \]

is fulfilled strongly.
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In contrast, in “temperature” FE, the temperature is the unknown and

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is fulfilled strongly.

In order to derive bounds, we will use flux FE to compute an homogenised equilibrated field \( \hat{Q} \).
Rewriting the problem in terms of the flux and the temperature

\[ \nabla \cdot Q = f \quad \forall x \in \Omega \times \Theta \]

\[ Q \cdot n = g \quad \forall x \in \partial \Omega_N \times \Theta \]

\[ u = h \quad \forall x \in \partial \Omega_D \times \Theta \]

\[ Q + k \nabla u = 0 \quad \forall x \in \Omega \times \Theta \]
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\( \hat{Q} \) will fulfill exactly the first 2 equations.
Error in the energy norm

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\( u^h \) will fulfill exactly the 3\textsuperscript{rd} equation.
Error in the energy norm

Rewriting the problem in terms of the flux and the temperature:

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\( \hat{Q} \) will fulfill exactly the first 2 equations.

\( u^h \) will fulfill exactly the 3rd equation.

In general, \( \hat{Q} + k \nabla u^h \neq 0 \)  Discrepancy = measure of the error.
Error in the energy norm

Formalizing this idea, it can be shown that

$$
\|e\|^2 = \|u - u^h\|^2 \leq \|u - u^h\|^2 + \underbrace{\| - k \nabla u - Q \|_{k-1}^2}_{\text{Controls effectivity}} = \underbrace{\| \hat{Q} + k \nabla u^h \|_{k-1}}_{\text{Computable}} =: \eta^2
$$
Error in the energy norm

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Expanding $\eta^2$

$$\eta^2 = \int_\Omega \int_\Theta k^{-1}\hat{Q} \cdot \hat{Q} + \int_\Omega \int_\Theta k\nabla u^h \cdot \nabla u^h + 2 \int_\Omega \int_\Theta \hat{Q} \cdot \nabla u^h$$
$$= \int_\Omega E[k^{-1}]\hat{Q} \cdot \hat{Q} + \int_\Omega E[k]\nabla u^h \cdot \nabla u^h + 2 \int_\Omega \hat{Q} \cdot \nabla u^h$$
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Expanding \( \eta^2 \)

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\[ = \int\int E[k^{-1}] \hat{Q} \cdot \hat{Q} + \int\int E[k] \nabla u^h \cdot \nabla u^h + 2 \int\int \hat{Q} \cdot \nabla u^h \]
Error in the energy norm

Formalizing this idea, it can be shown that

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\| e \|^2 = \| u - u^h \|^2 \leq \| u - u^h \|^2 + \| -k \nabla u - \hat{Q} \|_{k-1}^2 = \| \hat{Q} + k \nabla u^h \|_{k-1} =: \eta^2
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Expanding $\eta^2$

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\eta^2 = \int_{\Omega} \int_{\Theta} k^{-1} \hat{Q} \cdot \hat{Q} + \int_{\Omega} \int_{\Theta} k \nabla u^h \cdot \nabla u^h + 2 \int_{\Omega} \int_{\Theta} \hat{Q} \cdot \nabla u^h
$$

$$
= \int_{\Omega} E[k^{-1}] \hat{Q} \cdot \hat{Q} + \int_{\Omega} E[k] \nabla u^h \cdot \nabla u^h + 2 \int_{\Omega} \hat{Q} \cdot \nabla u^h
$$

$$
\sum \int_{\Theta} \int_{\Omega} \quad \quad \quad \quad \int_{\Omega} \int_{\Theta}
$$
Goal oriented error estimation

The error in energy norm is not always relevant.

**Goal:** Bound for the quantity of interest \( q(u) \)
The error in energy norm is not always relevant.

**Goal:** Bound for the quantity of interest \( q(u) \)

Dual problem

\[
a(\phi, v) = q(v) \quad \forall v \in V \quad a_0(\phi^h, v) = q(v) \quad \forall v \in V^h \subseteq V_0
\]
The error in energy norm is not always relevant.

**Goal:** Bound for the quantity of interest $q(u)$

Dual problem

$$a(\phi, v) = q(v) \quad \forall v \in V$$

$$a_0(\phi^h, v) = q(v) \quad \forall v \in V^h \subseteq V_0$$

$$q(u) - q(u^h) = R(\phi^h) + a(u - u^h, \phi - \phi^h) = R(\phi^h) + a(e, e_\phi)$$
The error in energy norm is not always relevant.

**Goal:** Bound for the quantity of interest \( q(u) \)

Dual problem

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a(\phi, v) = q(v) \quad \forall v \in V \\
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Cauchy-Schwarz inequality

\[
|a(e_\phi, e)| \leq ||e_\phi|| ||e||
\]
Goal oriented error estimation

The error in energy norm is not always relevant.

**Goal:** Bound for the quantity of interest \( q(u) \)

Dual problem

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a(\phi, v) = q(v) \quad \forall v \in V \quad a_0(\phi^h, v) = q(v) \quad \forall v \in V^h \subseteq V_0
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Cauchy-Schwarz inequality

\[
|a(e_\phi, e)| \leq \|e_\phi\| \|e\|
\]

Use the bound in the energy norm,

\[
R(\phi^h) - \eta\eta_\phi \leq q(u) - q(u^h) \leq R(\phi^h) + \eta\eta_\phi
\]
More bounds

It is possible to lower bound the error in energy norm

\[ \frac{|R(v)|}{||v||} \leq ||e|| \quad \forall v \in V_0 \]

Sharper bounds for the quantity of interest can be obtained through the use of polarisation identity

\[ q(u) - q(\bar{u}^h) = R(\phi^h) + a(e, e_\phi) = R(\phi^h) + \frac{1}{4}||se + s^{-1}e_\phi||^2 - \frac{1}{4}||se - s^{-1}e_\phi||^2 \]

It is tedious, but a bound for the second moment of the QoI can be obtained

\[ \int_\Theta q_\theta(u)^2 \leq f(E[k(x)], E[1/k(x)], \text{Cov}[k(x), k(y)]) \]
Numerical example
Validation

The quantity of the interest is the average temperature in the exterior faces.

The “exact” quantity of interest is computed with 512 MC realisations.
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The “exact” quantity of interest is computed with 512 MC realisations.
Validation

Studied in a domain homogenised through rule of mixture.

\[ Q = -20x \]

\[ v_f = 0.196 \]
\[ k_l = 0.5 \]
\[ k_M = 1 \]
\[ R_l = 0.05 \]
Studied in a domain homogenised through rule of mixture.

Dual problem

\[ a_0(\phi^h, v) = q(v) \]
Validation

Studied in a domain homogenised through rule of mixture.

Dual problem
\[ a_0(\phi^h, v) = q(v) \]

Two problems solved twice:
- Using “temperature” FE \( u^h, \phi^h \)
- Using “flux” FE \( \hat{Q}, \hat{Q}_\phi \)
Validation

<table>
<thead>
<tr>
<th>$q(u^h)$</th>
<th>$\zeta_l$</th>
<th>$q(u) - q(u^h)$</th>
<th>$\leq \zeta_u$</th>
<th>$\zeta_l + q(u^h) \leq$</th>
<th>$q(u)$</th>
<th>$\leq \zeta_u + q(u^h)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>21.92</td>
<td>-0.048</td>
<td>0.63</td>
<td>1.794</td>
<td>21.87</td>
<td>22.55</td>
<td>23.71</td>
</tr>
</tbody>
</table>
What if the bounds are not tight enough?

This is usually the case when the contrast is very high.

Two possible solutions

- **Adaptivity**: solve in a certain subdomain the heterogeneous problem

- **Enrichment**: solve an RVE and enrich the solution with its information
**Idea:** Solve RVEs, filter their solution

\[ u^RVE_x(x, \theta) \]

\[ u^RVE_y(x, \theta) \]

\[
    u^h(x, \theta) = \sum N_i(x)u_i + u^RVE_x(x, \theta) \sum N_i(x)a_i + u^RVE_y(x, \theta) \sum N_i(x)b_i
\]
Assembling the system of equations, 3 types of terms appear

\[ a(N_i, N_j) = \int_\Omega E[k] \nabla N_i \nabla N_j \]

\[ a(N_i, N_j u_d^{RVE}) = \int_\Omega E[k u_d^{RVE}] \nabla N_i \nabla N_j + \int_\Omega E[k \nabla u_d^{RVE}] \nabla N_i N_j \]

\[ a(N_i u_d^{RVE}, N_j u_d^{RVE}) = \int_\Omega E[k u_d^{RVE} u_d^{RVE}] \nabla N_i \nabla N_j + \int_\Omega [k \nabla u_d^{RVE} \nabla u_d^{RVE}] N_i N_j + \ldots \]

**Idea:** We do not need to solve the RVE for all particle layouts, we only need to compute

\[ E[k], E[k u_d^{RVE}], E[k u_d^{RVE} u_d^{RVE}], E[k \nabla u_d^{RVE} \nabla u_d^{RVE}], \ldots \]
**Enriched approximation**

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\[ E[k], \ E[k u_d^{RVE}], \ E[k u_d^{RVE} u_d'^{RVE}], \ E[k \nabla u_d^{RVE} \nabla u_d'^{RVE}], ... \]

**Remarks:**

- We choose a filter to remove space dependence of these terms
- A single realization gives a good approximation of those constants
- The computation of error bounds is straightforward
Enriched approximation

Preliminary results

\[ \|e\| \leq 1.37 \quad \text{(without enrichment)} \]
\[ \|e\| \leq 1.246 \quad \text{(with enrichment)} \]

10% reduction
Further improvement expected by enriching the equilibrated flux field
Summary

- A method to estimate error in homogenisation was presented
  - Represent the heterogeneous problem through an SPDE
  - A posteriori error estimation tools used to compute the error
  - The computation of the bound is deterministic
  - The second moment of the quantity of interest can be bounded

- On going work: Making the bounds sharper
  - Through adaptivity
  - Enriching the homogenised solution with the solution of an RVE
References

- **P Ladeveze, D Leguillon.** Error estimate procedure in the finite element method and applications. SIAM Journal on Numerical Analysis, 1983

