Efficient modelling of random heterogeneous materials with a uniform probability density function

Daniel Alves Paladim[1]

Pierre Kerfriden[1]

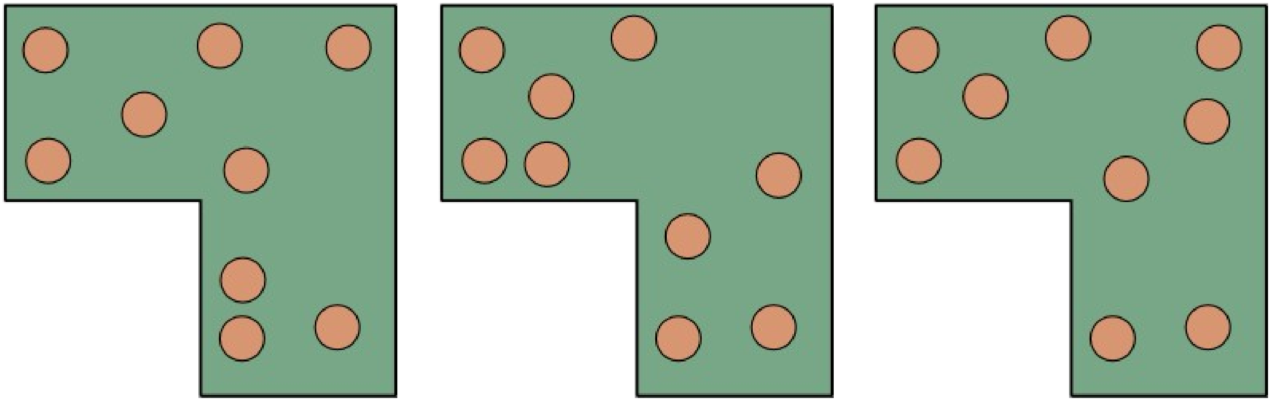
José Moitinho de Almeida[2]

Stéphane P. A. Bordas[1,3]

[1]School of Engineering, Cardiff University
[2]Instituto Superior Técnico, Universidade de Lisboa
[3]Faculté des Sciences, Université du Luxembourg

Motivation

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



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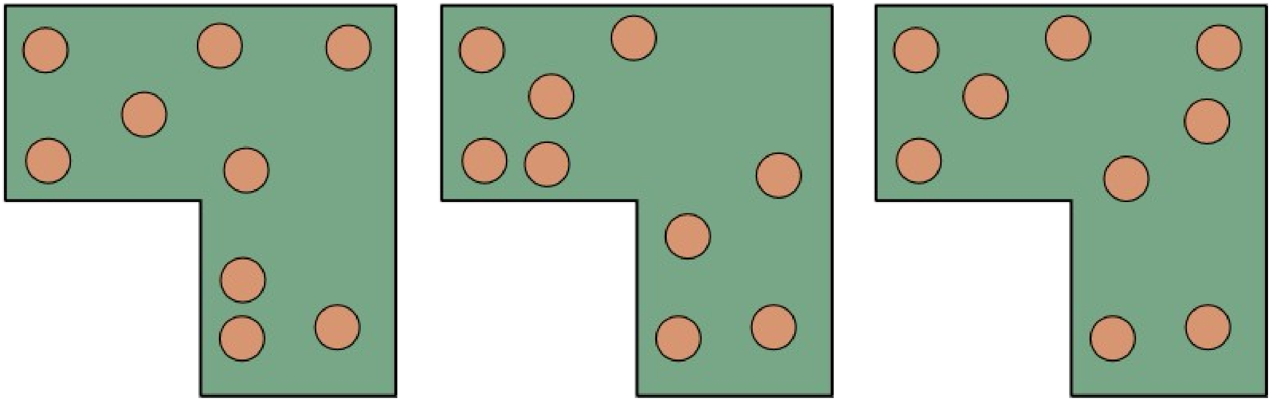
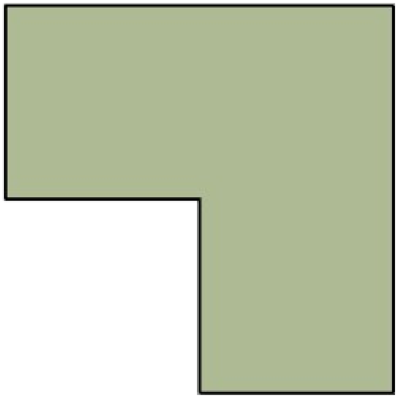


Solution: Homogenisation.



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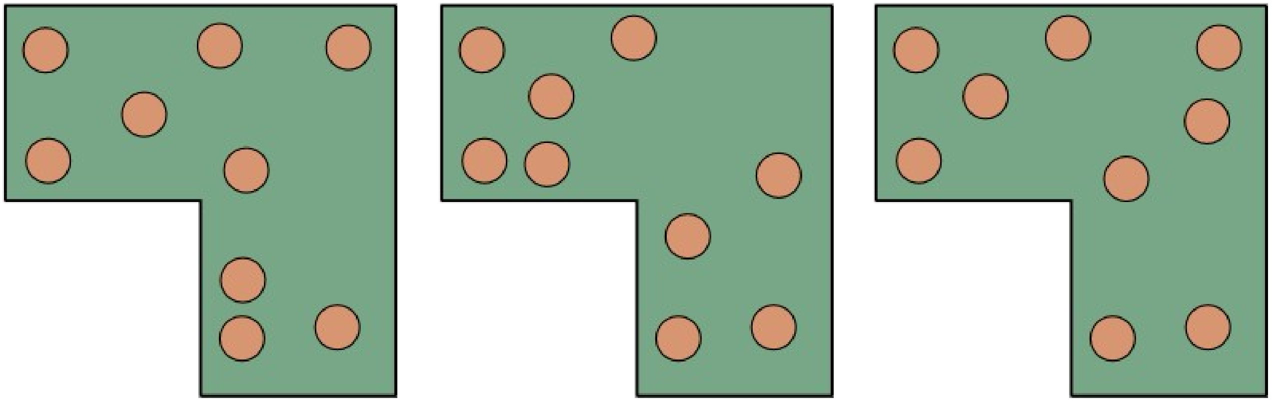

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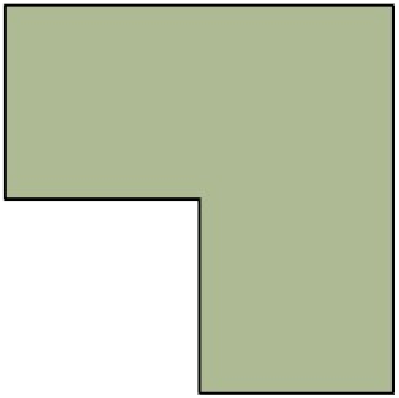
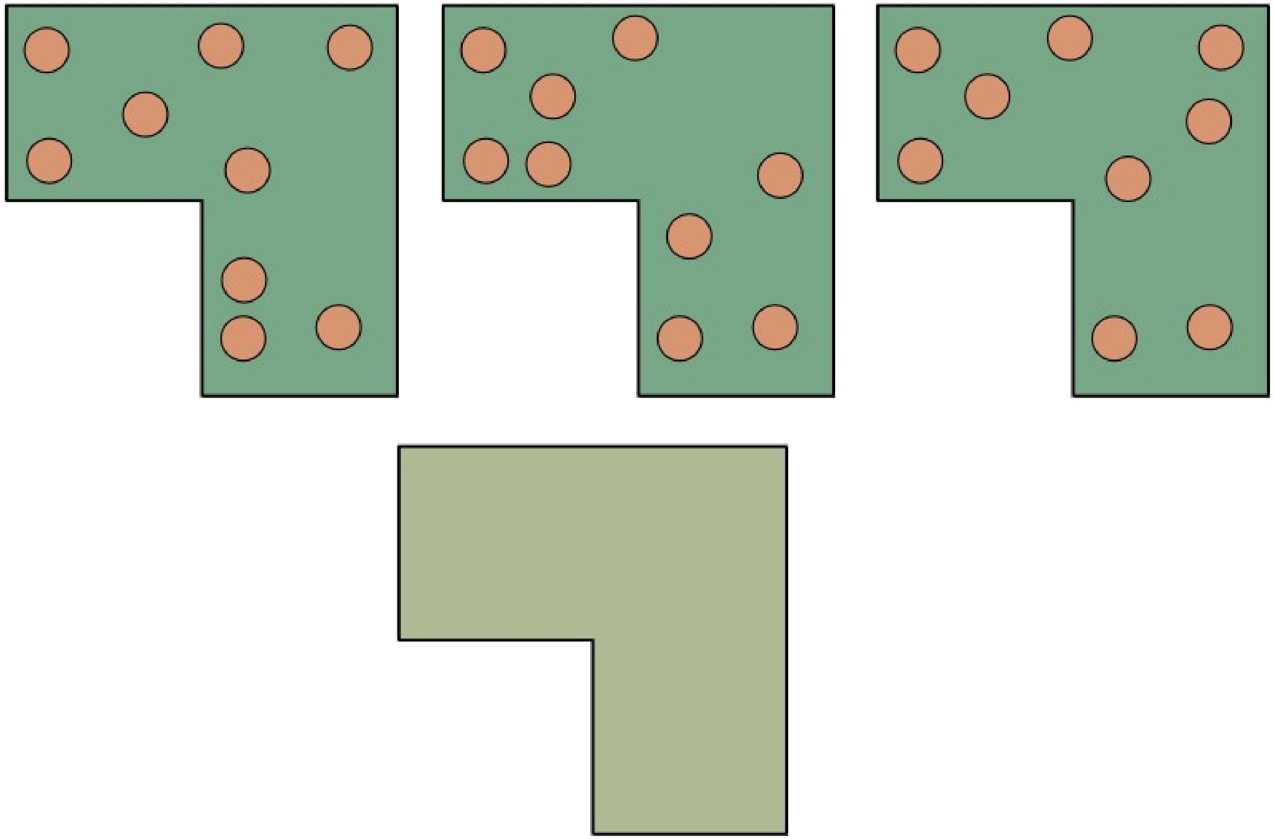


New problem:
Asses the validity of the homogenisation.

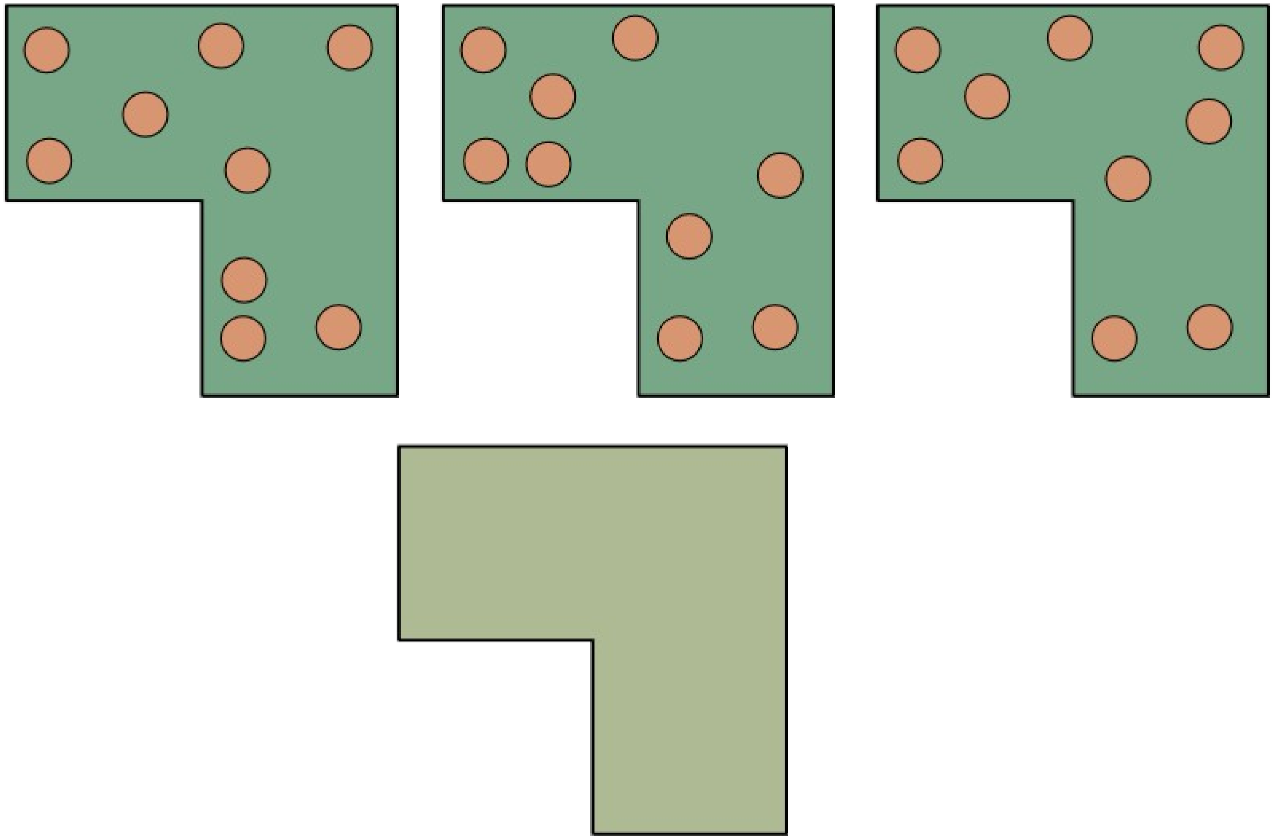
Proposed solution

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

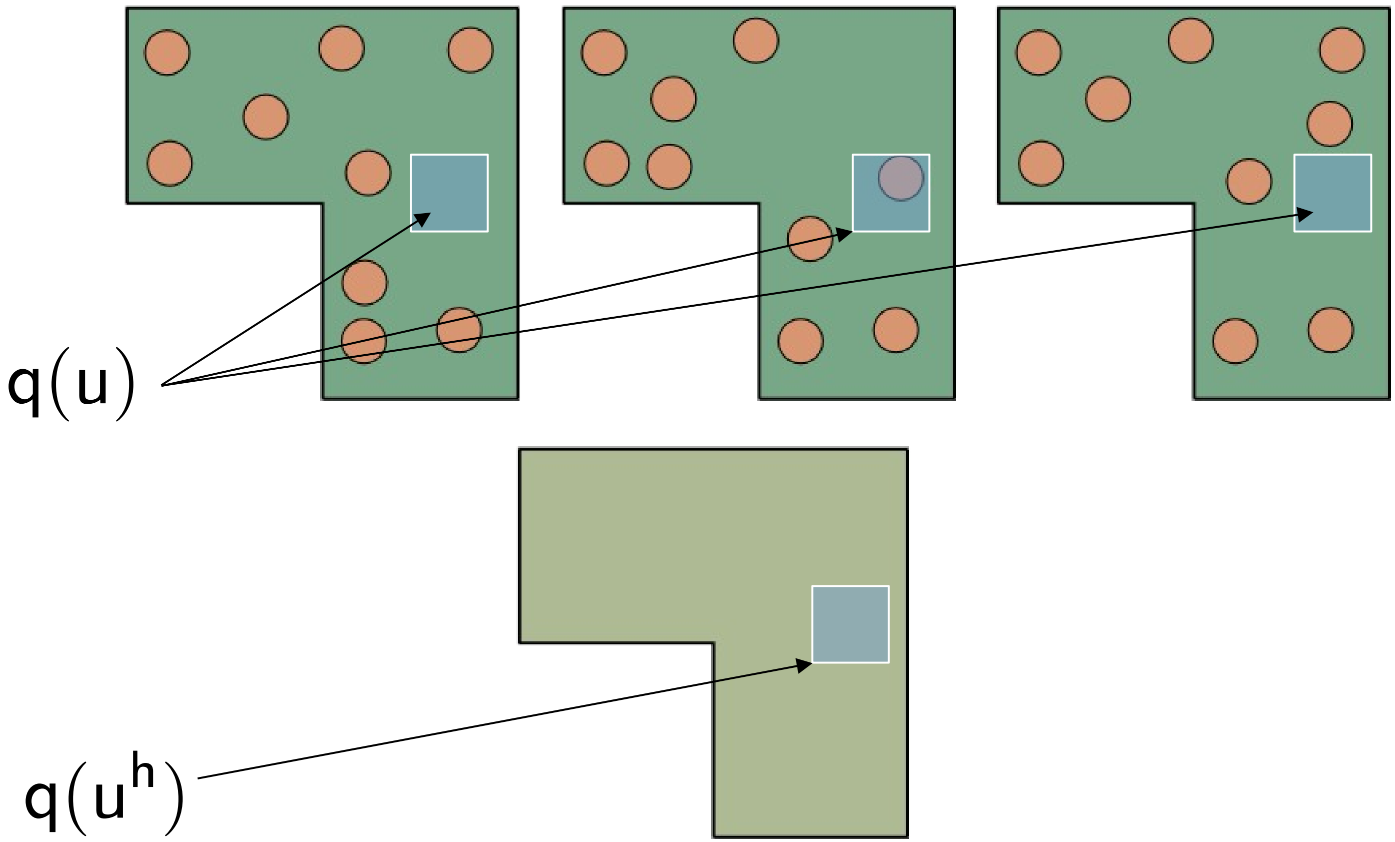
SPDE: Stochastic partial differential equation.
Collection of parametric problems + probability density function



Proposed solution

QoI: Quantity of interest. The output. Scalar that depends of the solution.

$$q(u) = \int_{\Omega} \int_{\Theta} \gamma(x) \cdot u(x, \theta) \quad \text{(linear)}$$



Remark: The quantity of interest is an expectation.

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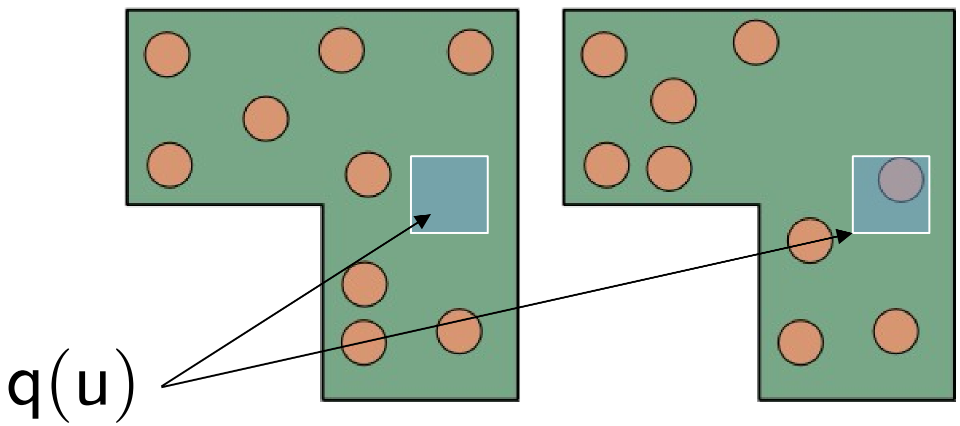

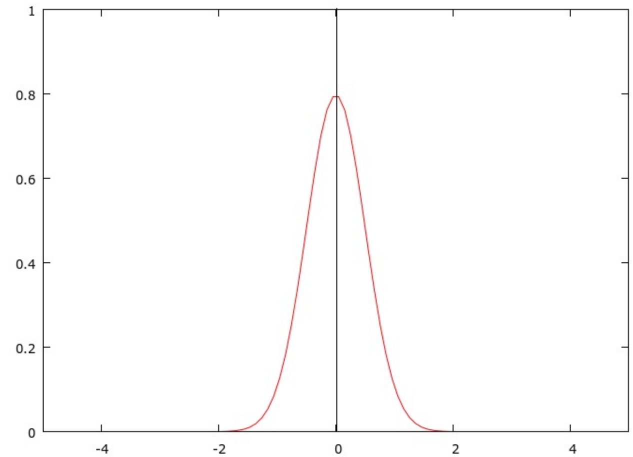

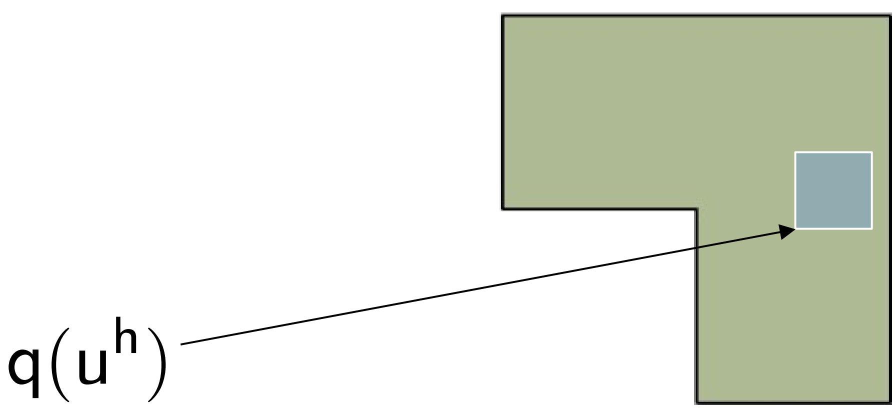

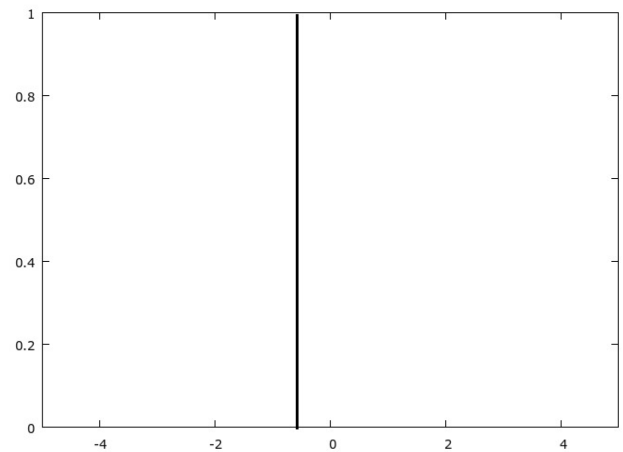

Notation

Heat equation

Boundary value problem

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

$$l(v) = \int_\Theta \int_\Omega fv - \int_{\partial\Omega} gv$$

$$a(u,v) = l(v) \quad \forall v \in V$$

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Homogenised boundary value problem

$$a_0(u_0,v) = \int_\Omega k_0 \nabla u \cdot \nabla v$$

$$a_0(u_0,v) = l(v) \quad \forall v \in V_0$$

$$a_0(u^h,v) = l(v) \quad \forall v \in V_0^h$$

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Aim: Bound

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

The computation of the bound must be purely deterministic.

Derivation

Hypothesis

Deterministic boundary conditions

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Deterministic boundary conditions

Constant volume fraction

$$\int_{\Omega} \mathsf{k}(\mathsf{x}, \theta) = \alpha_{\mathsf{I}} \mathsf{k}_{\mathsf{I}} + (1 - \alpha_{\mathsf{I}}) \mathsf{k}_{\mathsf{M}} \quad \forall \theta \in \Theta$$

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Constant PDF over the domain

$$\underbrace{\int_{\Theta} \mathsf{k}(\mathsf{x}, \theta)}_{\mathsf{E}[\mathsf{k}]} = \alpha_{\mathsf{I}} \mathsf{k}_{\mathsf{I}} + (1 - \alpha_{\mathsf{I}}) \mathsf{k}_{\mathsf{M}} \quad \forall \mathsf{x} \in \Omega$$

Derivation

1) Adjoint problem

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

Ladevèze et al. (1983) *Error estimate procedures in the finite element method and applications*

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

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$$|a(e_\phi, e)| \leq \|e_\phi\| \|e\|$$

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$$\langle r, s \rangle_{k^{-1}} := \int_\Omega \int_\Theta k^{-1} r \cdot s$$

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$$\langle r, s \rangle_{k^{-1}} := \int_\Omega \int_\Theta k^{-1} r \cdot s$$

Use that $\langle \hat{Q} + k\nabla u, -k\nabla u + \nabla u^h \rangle_{k^{-1}} = 0$

Flux field such that

$$\nabla \cdot \hat{Q} = f$$

and that fulfill flux Bcs.
“Stress FE”

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Use that $\langle \hat{Q} + k\nabla u, -k\nabla u + \nabla u^h \rangle_{k^{-1}} = 0$

to conclude through Pythagoras that

$$\underbrace{\|\hat{Q} + k\nabla u^h\|^2_{k^{-1}}}_{\text{Computable}} = \underbrace{\|\hat{Q} + k\nabla u\|^2_{k^{-1}}}_{\text{Controls effectivity}} + \|e\|^2 \geq \|e\|^2$$

Ladevèze et al. (1983) *Error estimate procedures in the finite element method and applications*

Derivation

Combining all the results

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

$$\eta = \|\hat{Q} + k\nabla u^h\|_{k^{-1}}$$

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Expanding

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

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

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Deterministic quantity (similar for the residue)

Derivation

How do we choose k_0?

$$\|\hat{Q} + k\nabla u^h\|_{k^{-1}}^2 = \|\hat{Q} + k\nabla u\|_{k^{-1}}^2 + \underbrace{\|e\|^2}_{\text{Minimized } k_0 = E[k]}$$

Derivation

How do we choose k_0?

$$\|\hat{Q} + k\nabla u^h\|^2_{k^{-1}} = \underbrace{\|\hat{Q} + k\nabla u\|^2_{k^{-1}}}_{\text{Minimized } k_0 = 1/E[k^{-1}]} + \|e\|^2$$

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"Usual" FE $u^h, \phi^h \Rightarrow k_0 = E[k]$

"Stress" FE $\hat{Q}, \hat{Q}_\phi \Rightarrow k_0 = \frac{1}{E[k^{-1}]}$

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$$\eta^2 = \left(E[k^{-1}]k_0 + \frac{E[k]}{k_0} - 2 \right) [u^h]^T [A][u^h]$$

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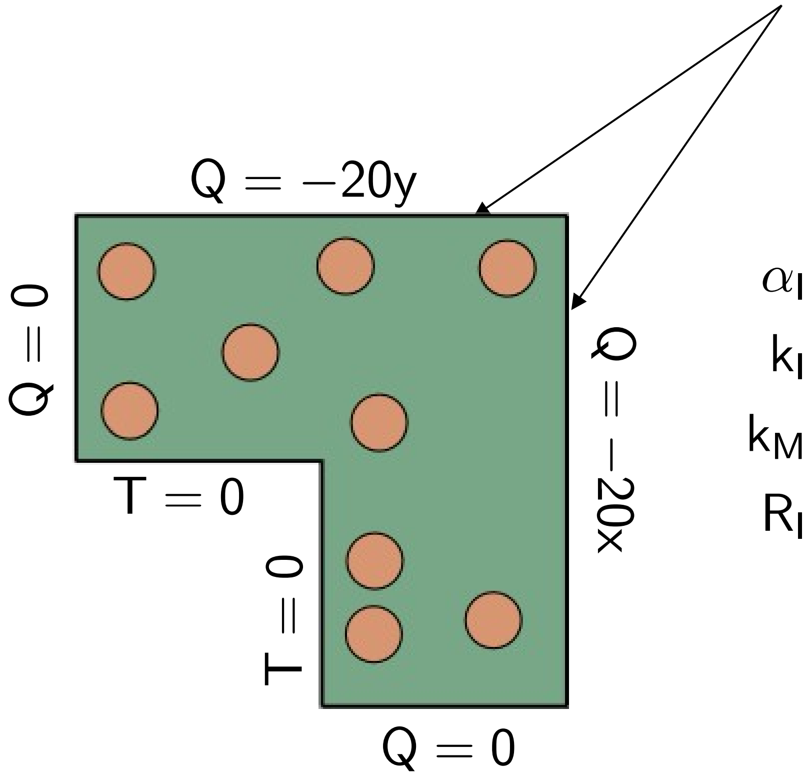
There is always a minimum for $k_0 \in \left[\frac{1}{E[k^{-1}]}, E[k] \right]$

Validation

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



$$\alpha_I = 0.2$$
$$k_I = 0.6$$
$$k_M = 1$$
$$R_I = 0.05$$

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

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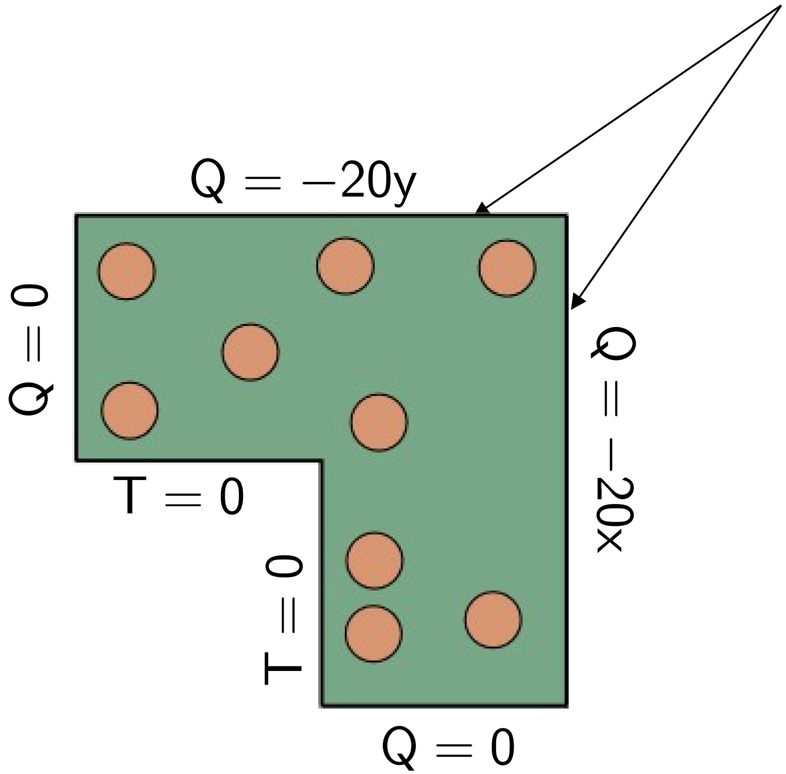

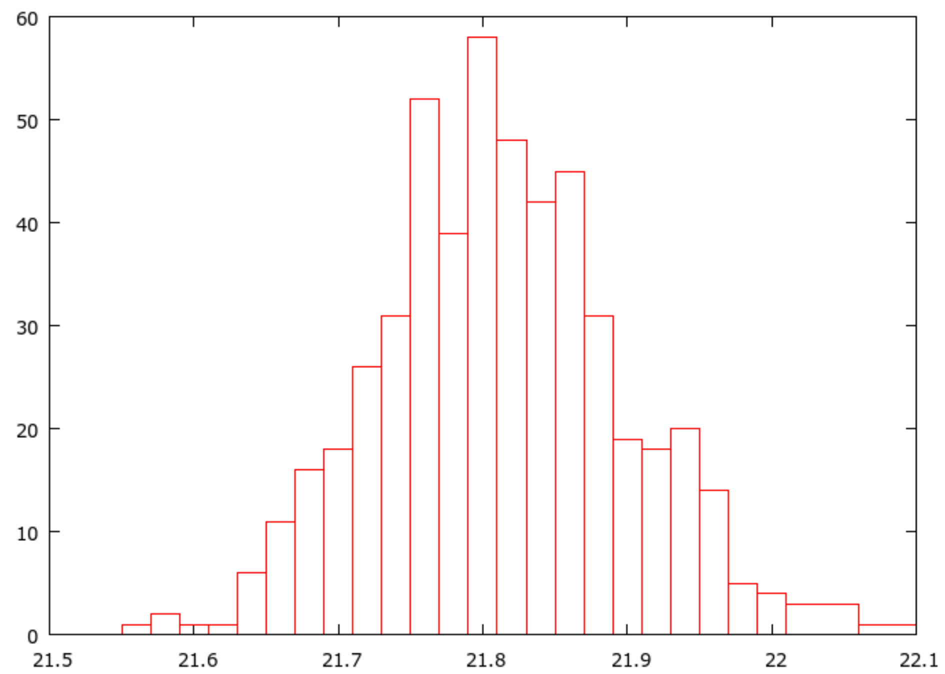

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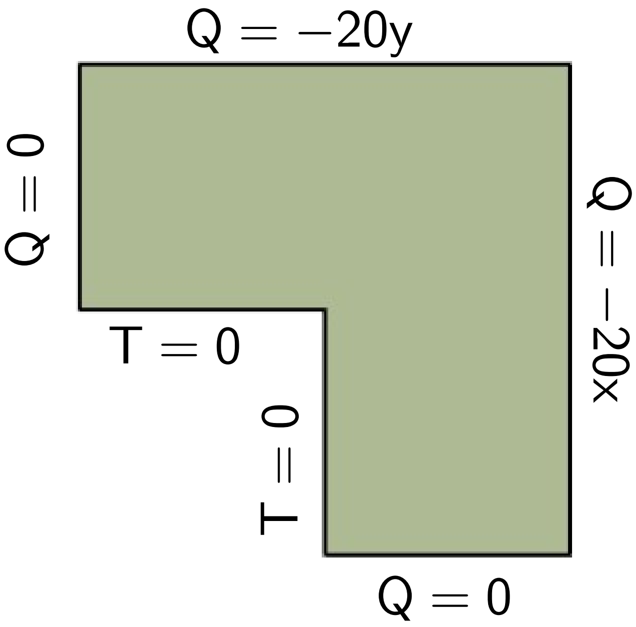
Studied in a domain homogenised through rule of mixture.



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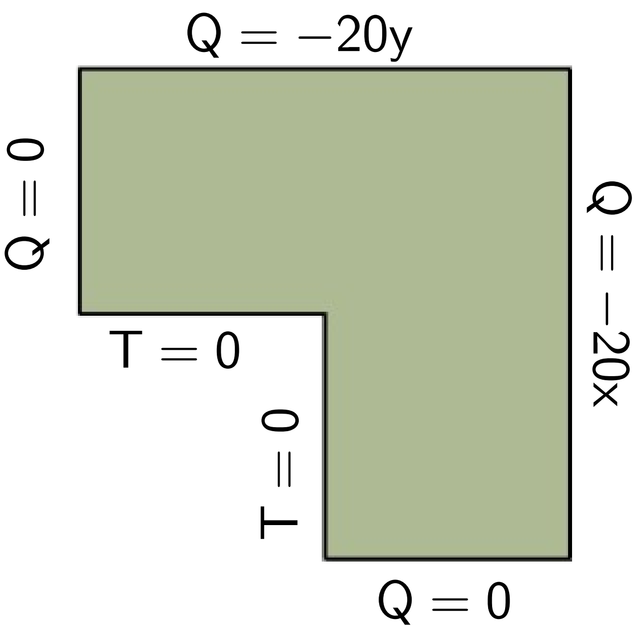

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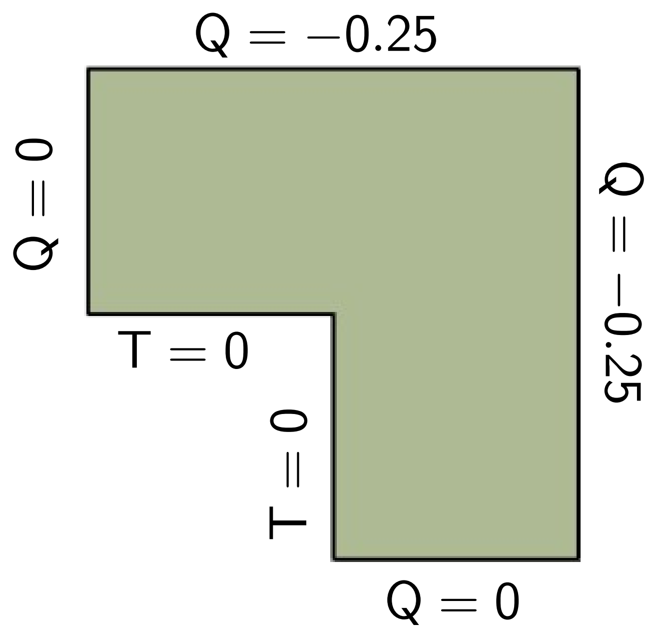
Dual problem

$$a_0(\phi^h, v) = q(v)$$



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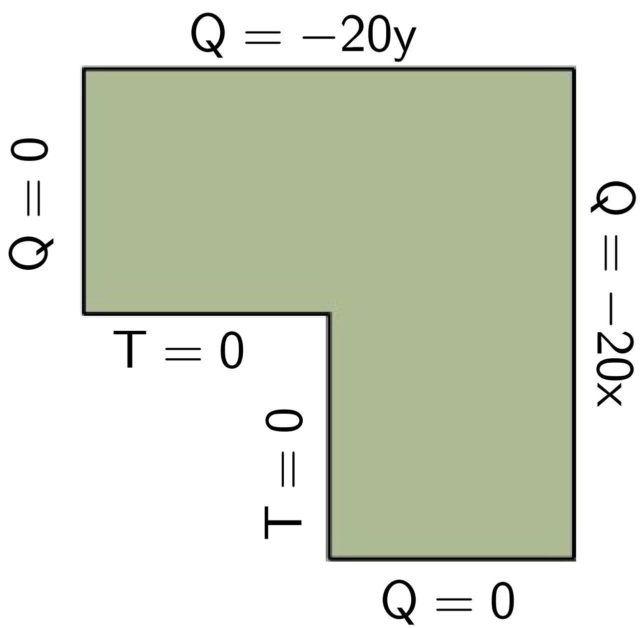

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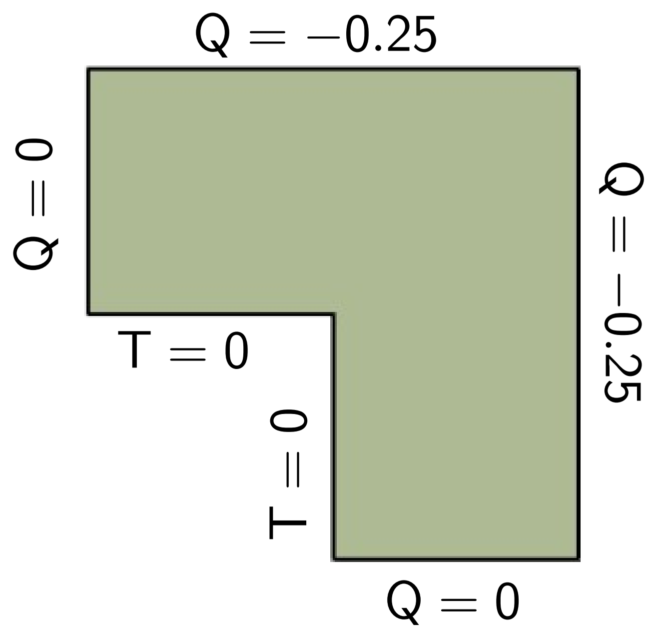
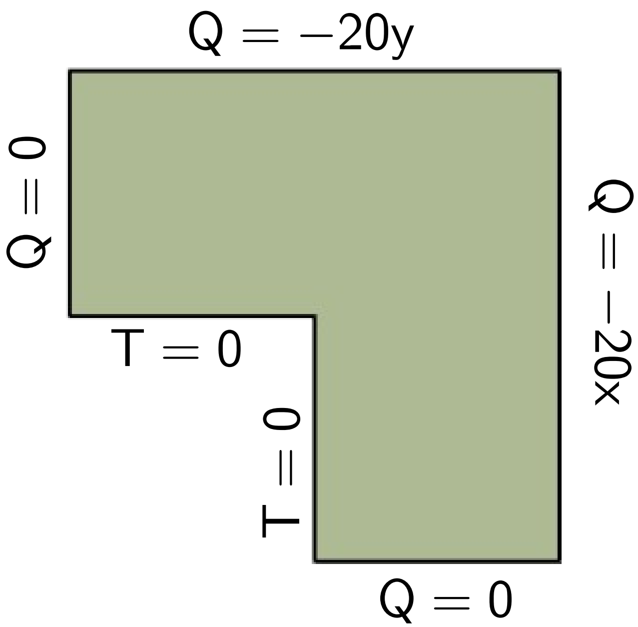


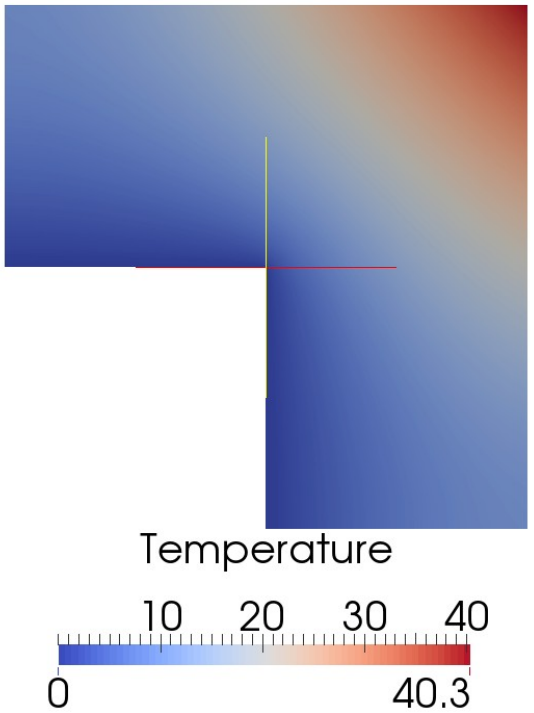
Two problems solved twice:

- Using "usual" FE u^h, ϕ^h
- Using "equilibrated" FE $\hat{Q}, \hat{Q}_\phi$

Validation

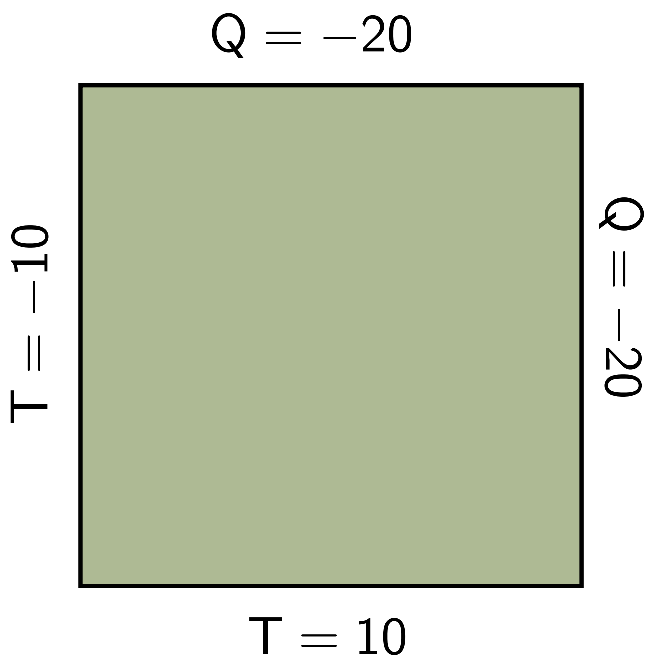


$$\alpha_l = 0.2$$
$$k_l = 0.6$$
$$k_M = 1$$
$$R_l = 0.05$$



$q(u^h)$	$\zeta_l \leq$	$q(u) - q(u^h)$	$\leq \zeta_u$	$\zeta_l + q(u^h) \leq$	$q(u)$	$\leq \zeta_u + q(u^h)$
21.46	− 0.97	0.34	0.97	20.49	21.80	22.42

Numerical example



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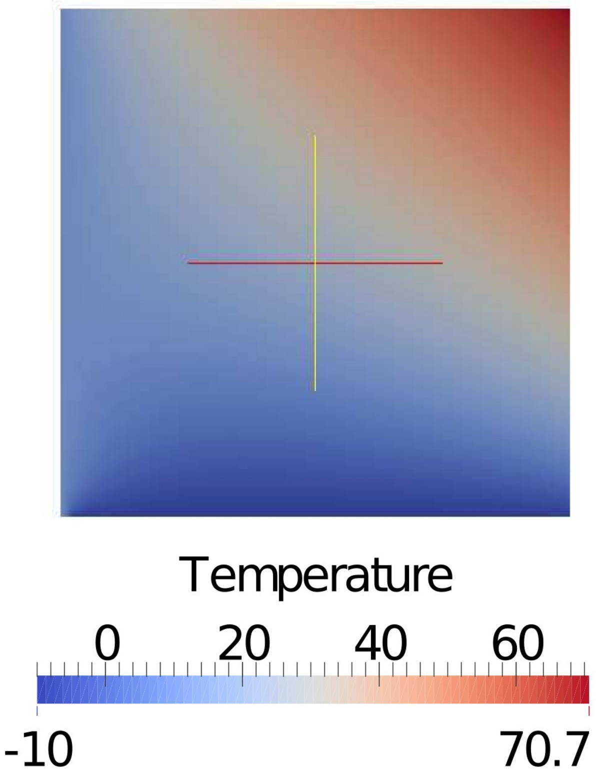
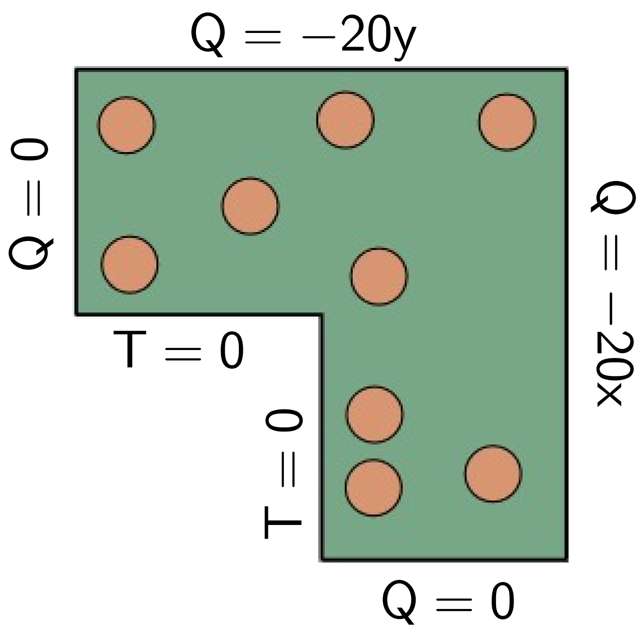


$q(u^h)$	$\zeta_l \leq$	$q(u) - q(u^h)$	$\leq \zeta_u$	$\zeta_l + q(u^h) \leq$	$q(u)$	$\leq \zeta_u + q(u^h)$
41.57	-5.00	-	5.00	36.57	-	46.57

Numerical example

First problem, different material properties.



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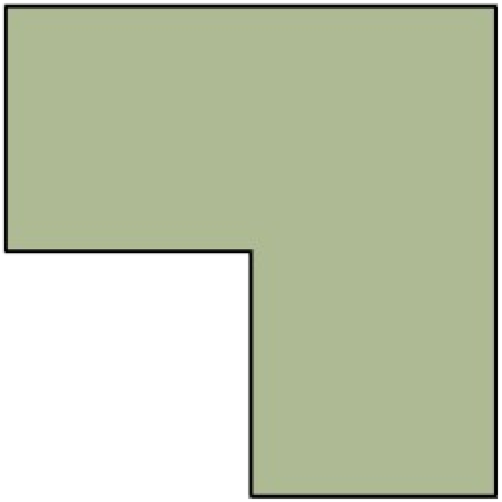

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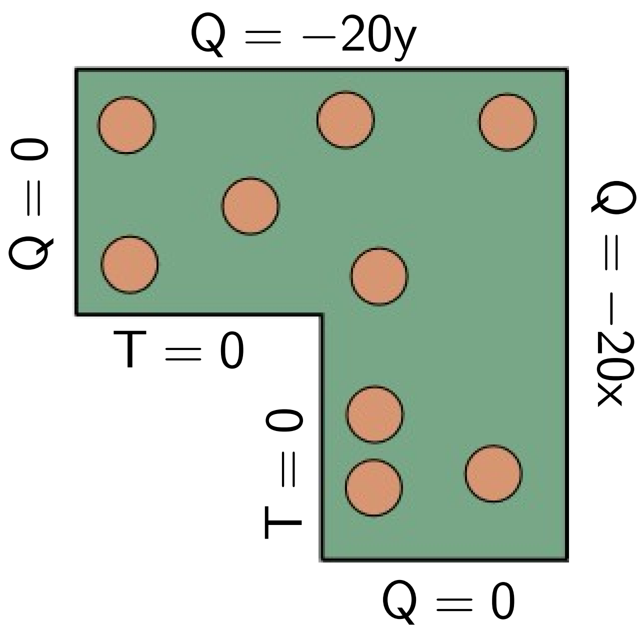

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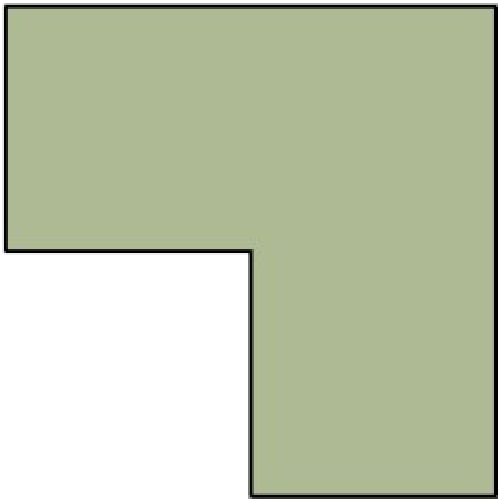

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25.88	− 42.71	5.33	42.71	− 16.83	31.22	68.59

Numerical example

For this problem, it is possible to write the error bound as a function of the homogenised conductivity.

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$$\eta(\mathsf{E}[\mathsf{k}]) \propto \left(\mathsf{E}[\mathsf{k}^{-1}] - \frac{1}{\mathsf{E}[\mathsf{k}]} \right)$$

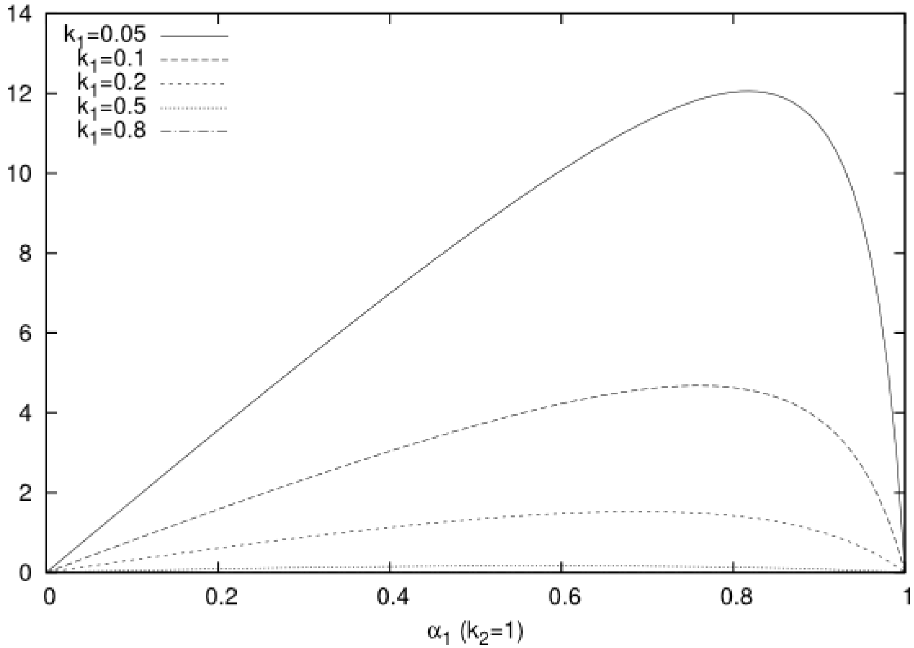
which is a form of the inequality between the harmonic and the arithmetic mean.

Numerical example

For this problem, it is possible to write the error bound as a function of the homogenised conductivity.

$$\eta(\mathsf{E}[\mathsf{k}]) \propto \left(\mathsf{E}[\mathsf{k}^{-1}] - \frac{1}{\mathsf{E}[\mathsf{k}]} \right)$$

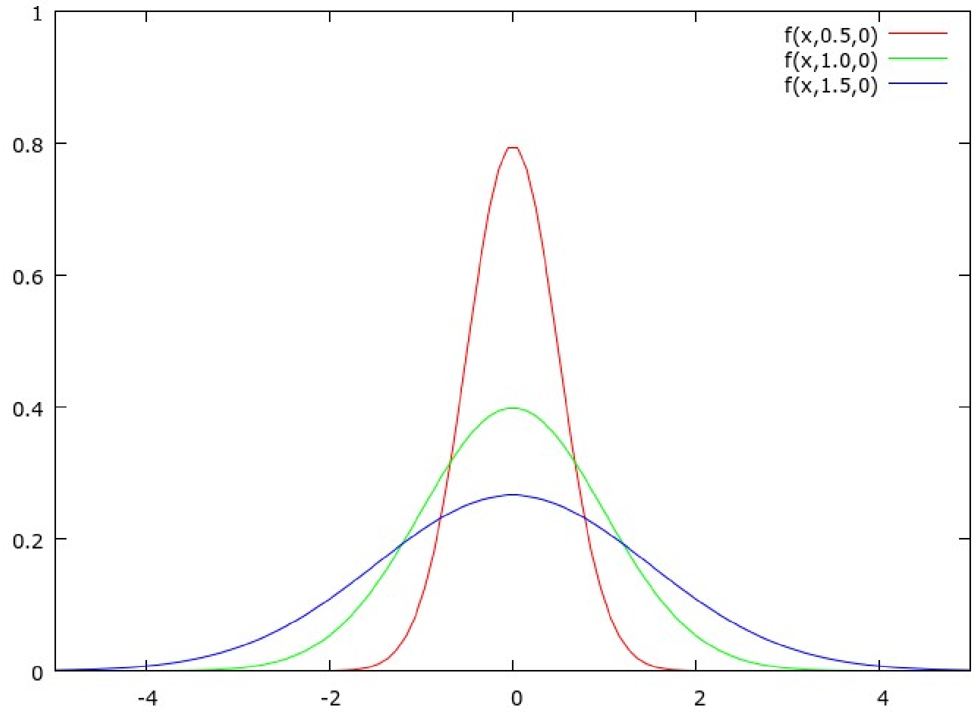
Only equal to 0 if $\mathsf{k}_1 = \mathsf{k}_2 = \ldots = \mathsf{k}_\mathsf{N}$



In summary, the interval grows as we increase the contrast between the material properties.

Work in progress

How representative is the expectation? Are the QoIs concentrated around one point?



Work in progress

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Solution: Bound the variance

$$\int_{\Omega}\int_{\Theta}[\gamma(\mathrm{x})\cdot\mathrm{u}(\mathrm{x},\theta)-\mathrm{q}(\mathrm{u})]^2$$

Characteristics of the bound

- Purely deterministic
- Depends on the shape of the particle (covariance).

$$\mathrm{E}[\mathrm{k}(\mathrm{x})\mathrm{k}(\mathrm{y})]$$

No numerical examples available at the moment.

Work in progress

– Improve the bounds.
  - Averaged solution of the Prager-Synge hypercircle.

$$\frac{1}{2}(\hat{Q} - k\nabla u^h)$$

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- Adapt the bound presented in “Multi-scale goal-oriented adaptive modelling of random heterogeneous materials” by Romkes, Oden and Prudhomme.

Summary

- A bound was presented for heterogenous problems that are homogenised.
- The computation of the bound is purely deterministic.
- The error estimate, should be used with care when there is a high contrast between the materials.

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Summary

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- The computation of the bound is purely deterministic.
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Thank you for your attention.