Advances in error estimation for homogenisation

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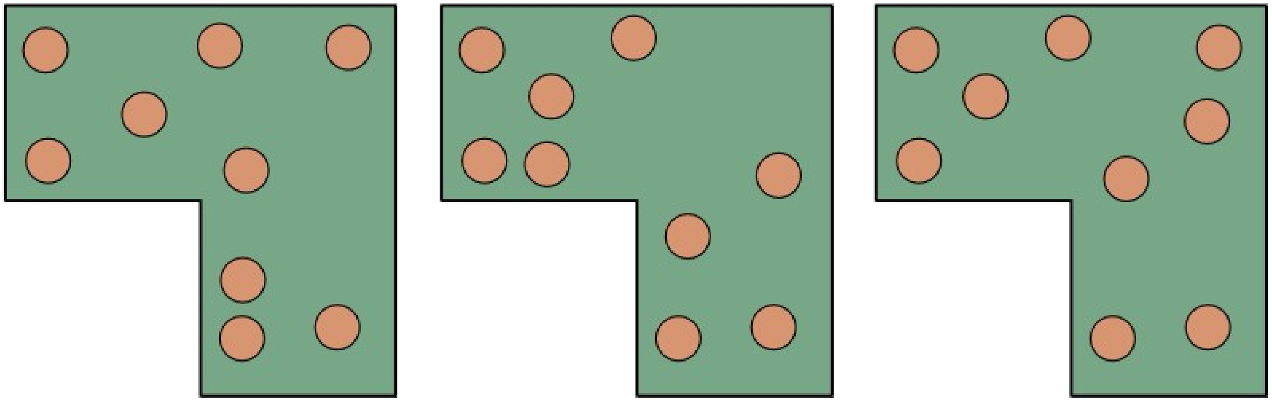
Motivation

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



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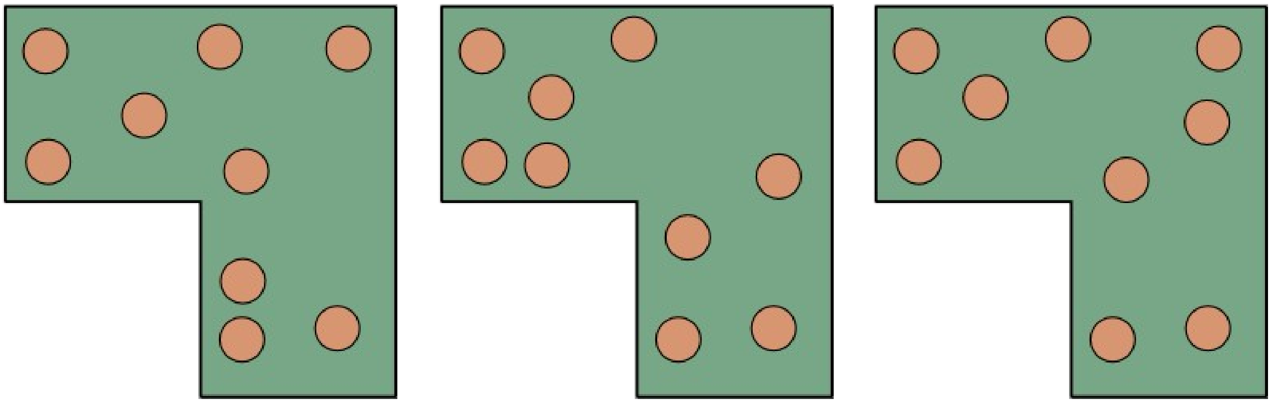
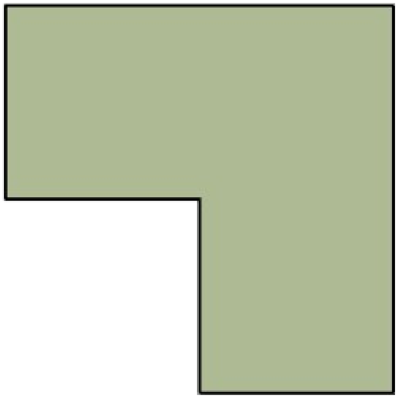


Solution: Homogenisation.



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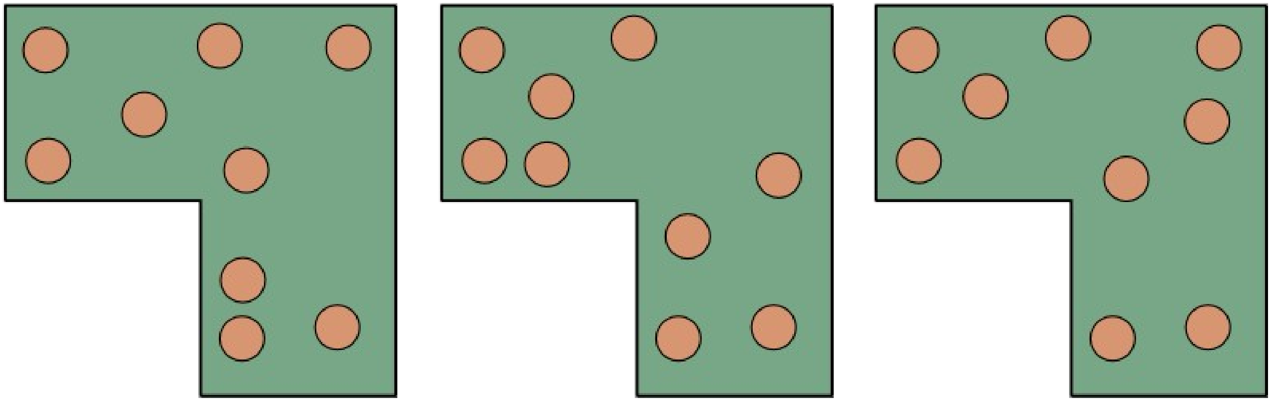

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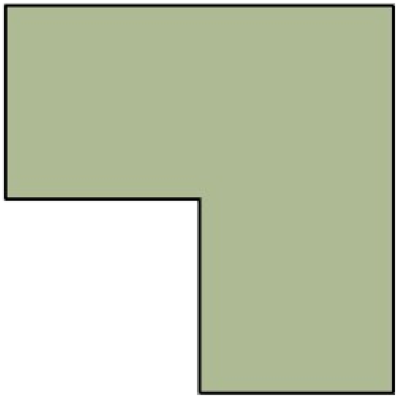


New problem:
Assess the validity of the homogenisation.

Key ideas

Exact model

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

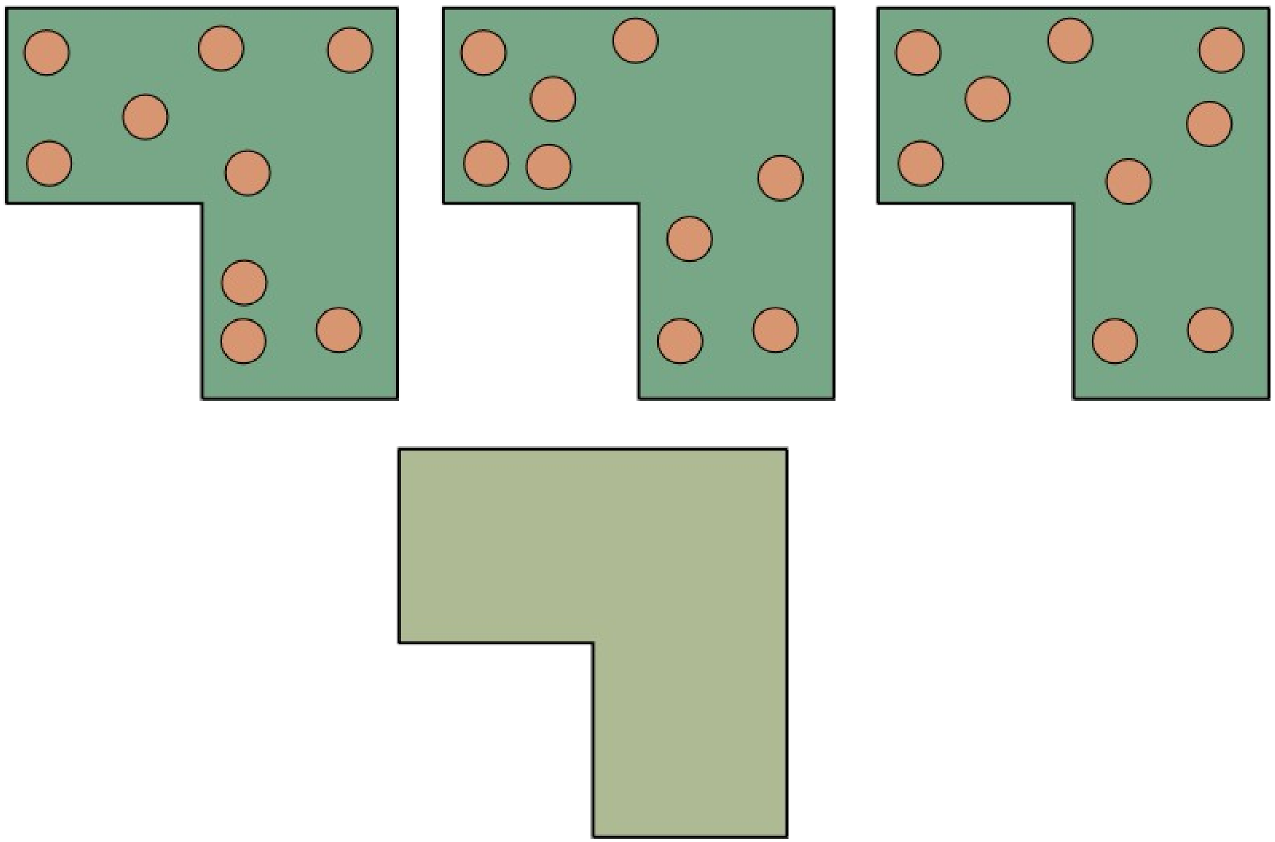
Error estimation

- **Objective:** Compare the solution of the two models (without solving the SPDE)
- Adapt classic a posteriori error bounds to this specific problem

Exact model

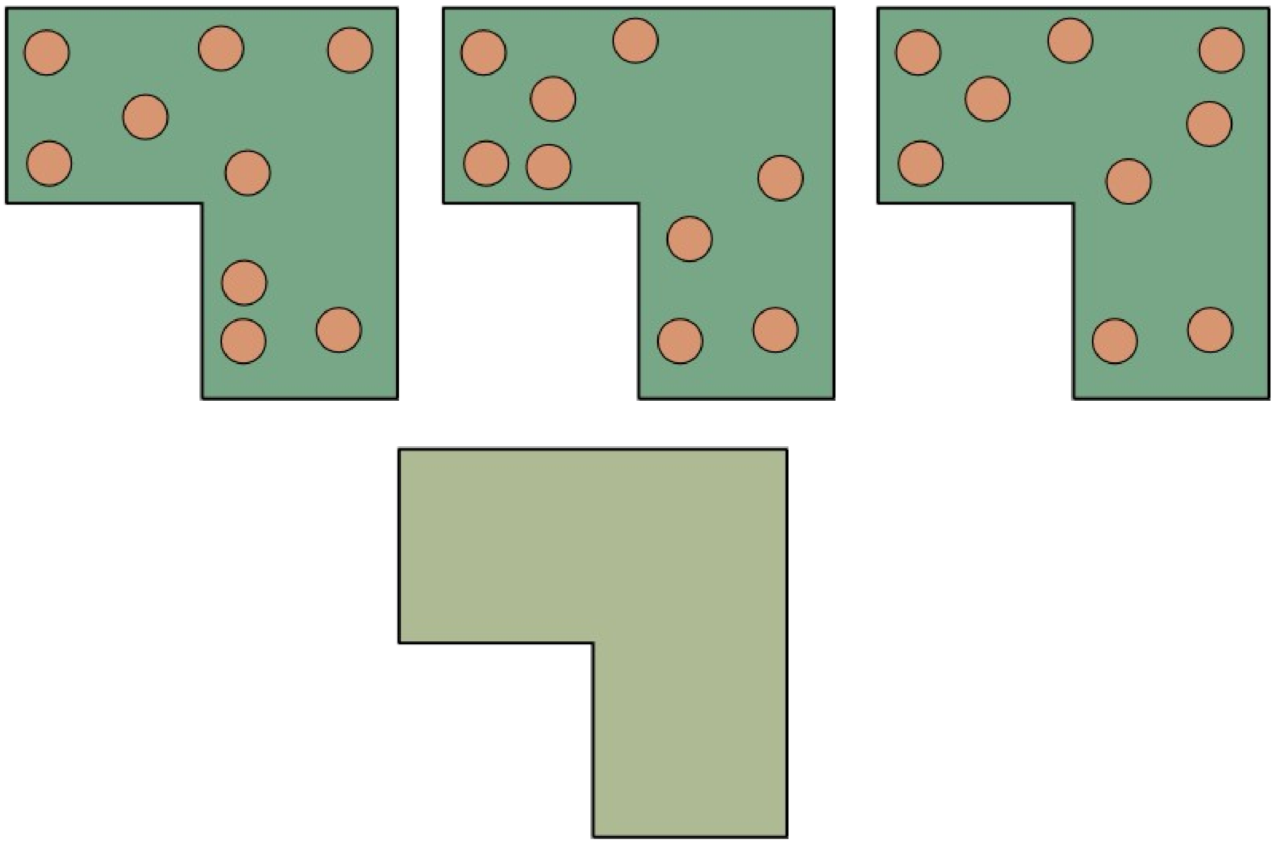
Proposed solution

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

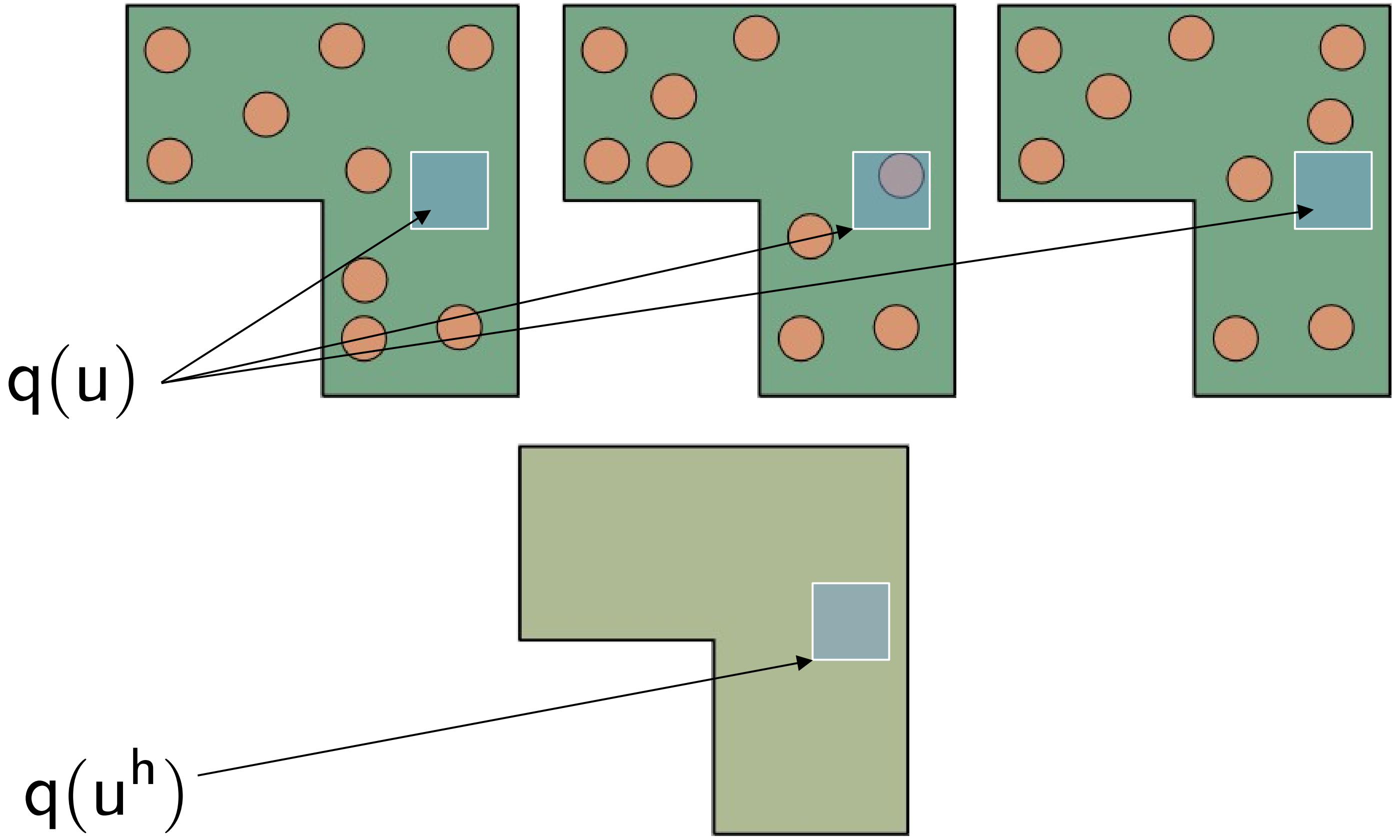
SPDE: Stochastic partial differential equation.
Collection of parametric problems + probability density function



Proposed solution

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

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



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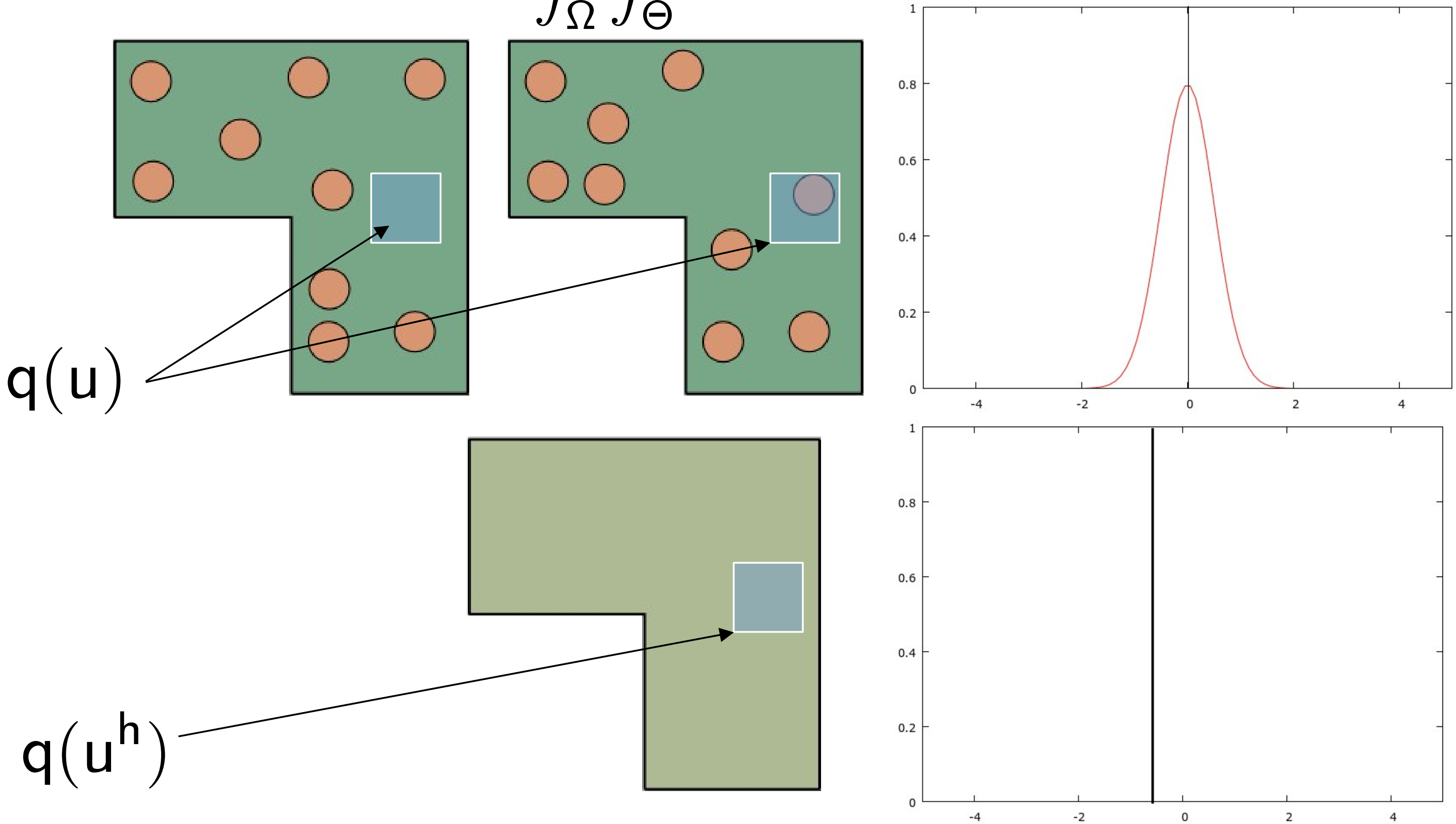

Heat equation

Heterogeneous problem

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

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

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

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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.

$$\mathsf{E}[\mathsf{k}(\mathsf{x},\theta)] = \int_{\Theta} \mathsf{k}(\mathsf{x},\theta) \qquad\qquad \mathsf{E}[\mathsf{k}(\mathsf{x},\theta)^{-1}]$$

Hypothesis

Deterministic boundary conditions

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

$$E[k(x,\theta)] = \int_{\Theta} k(x,\theta) \qquad\qquad E[k(x,\theta)^{-1}]$$

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

$$\|\mathrm{u} - \bar{\mathrm{u}}^{\mathrm{h}}\| \leq \eta$$

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

$$\mathrm{q}(\mathrm{u}) - \mathrm{q}(\bar{\mathrm{u}}^{\mathrm{h}}) \leq \gamma$$

Equilibrated flux field

An equilibrated flux field fulfills

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

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

strongly.

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In order to derive bounds, we will use flux FE to compute an homogenised equilibrated field $\hat{Q}$

Error in the energy norm

Rewriting the problem in terms of the flux and the temperature

$$
\begin{aligned}
\nabla \cdot Q &= f \quad \forall x \in \Omega \times \Theta \\
Q \cdot n &= g \quad \forall x \in \partial\Omega_N \times \Theta \\
u &= h \quad \forall x \in \partial\Omega_D \times \Theta \\
Q + k\nabla u &= 0 \quad \forall x \in \Omega \times \Theta
\end{aligned}
$$

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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

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

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Expanding η^2

$$\begin{aligned}\eta^2 &= \int_\Omega \int_\Theta k^{-1}\hat{Q}\cdot\hat{Q} + \int_\Omega \int_\Theta k\nabla u^h \cdot \nabla u^h + 2\int_\Omega \int_\Theta \hat{Q}\cdot\nabla u^h \\ &= \int_\Omega E[k^{-1}]\hat{Q}\cdot\hat{Q} + \int_\Omega E[k]\nabla u^h\cdot\nabla u^h + 2\int_\Omega \hat{Q}\cdot\nabla u^h\end{aligned}$$

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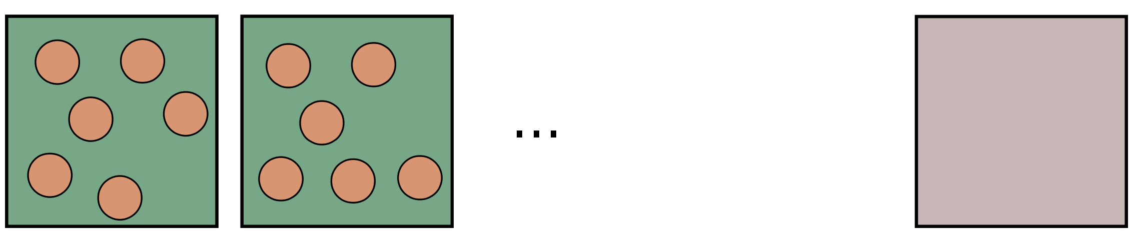
$$\int_\Theta\int_\Omega \qquad\qquad \int_\Omega\int_\Theta$$

$\sum$



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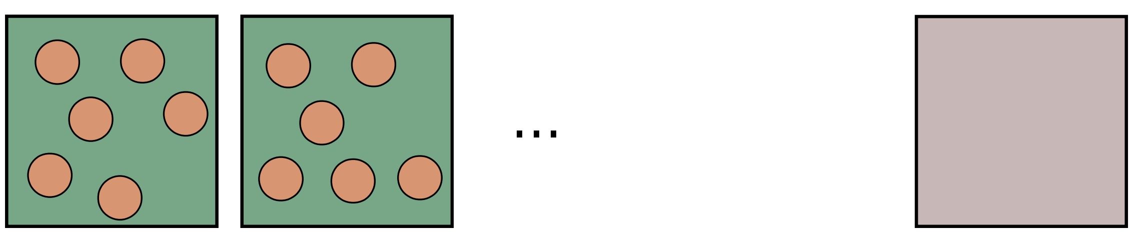

Goal oriented error estimation

The error in energy norm is not always relevant.

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Cauchy-Schwarz inequality

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

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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

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

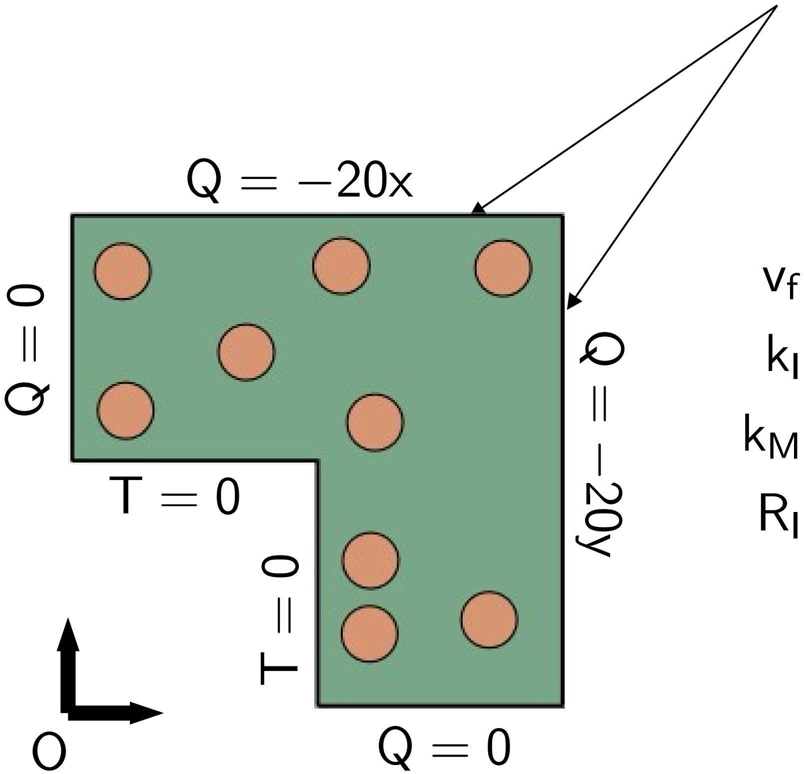
It is tedious, but a bound for the second moment of the QoI can be obtained

$$\int_\Theta q_\theta(u)^2 \leq f(E[k(x)], E[1/k(x)], Cov[k(x), k(y)])$$

Numerical example

Validation

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



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$$k_M = 1$$
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The “exact” quantity of interest is computed with 512 MC realisations.

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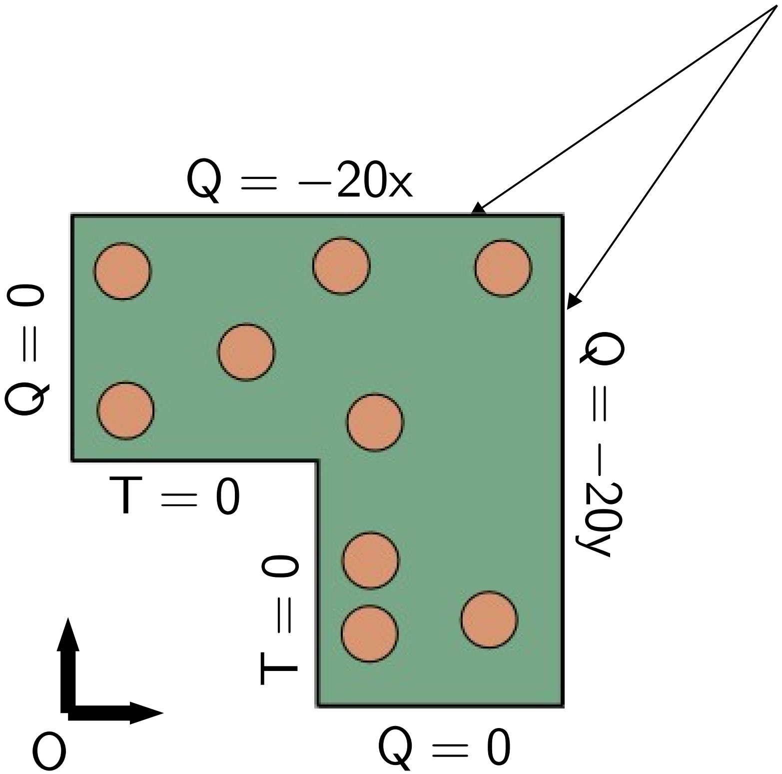

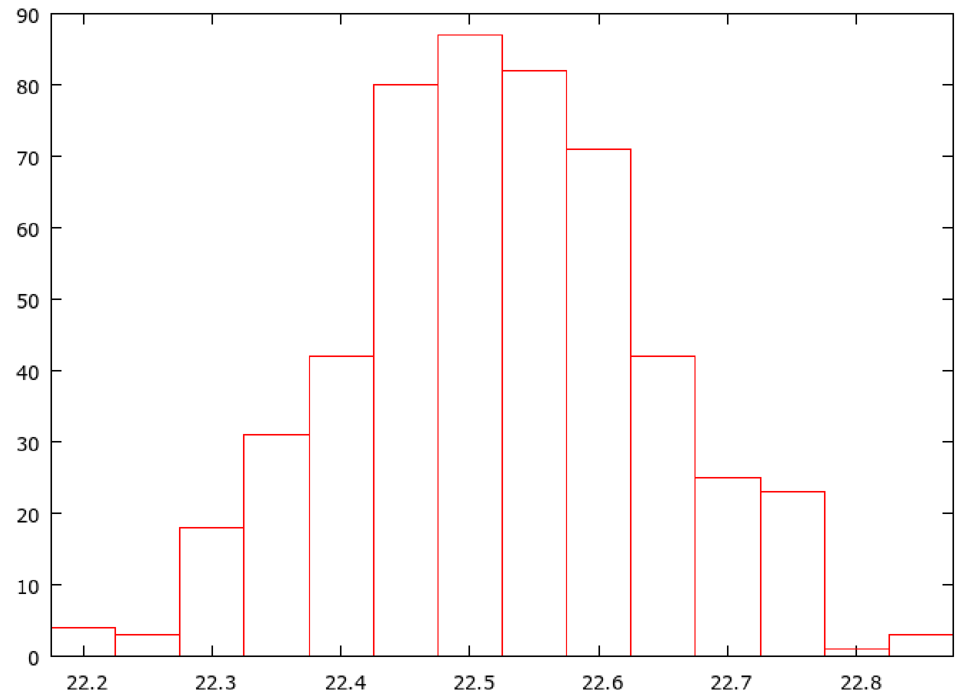

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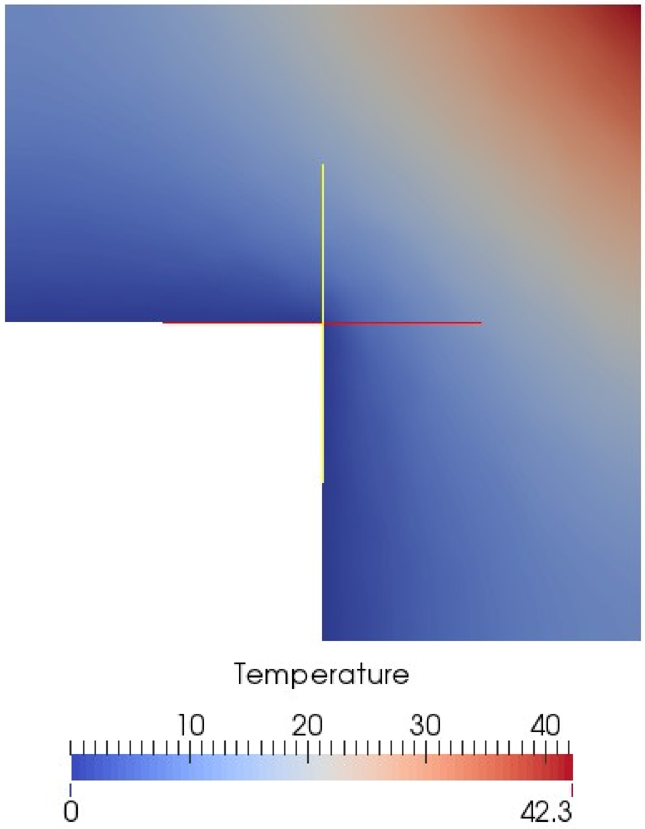

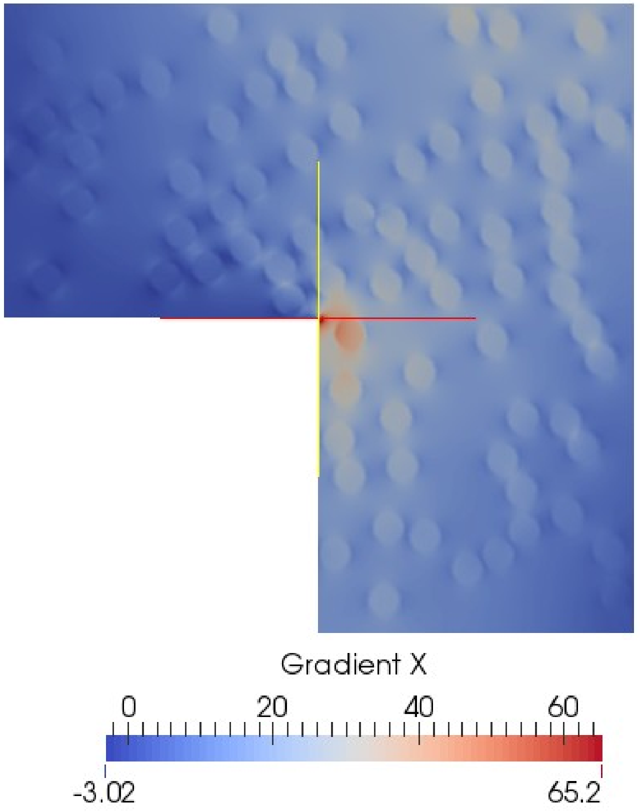

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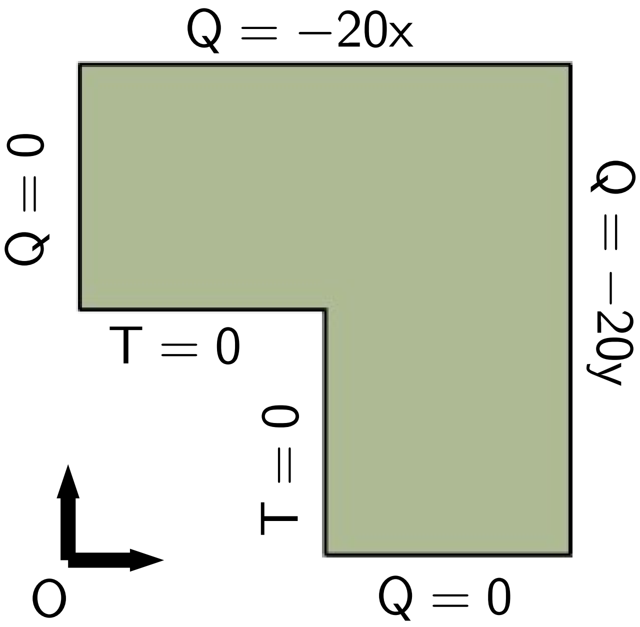
Studied in a domain homogenised through rule of mixture.



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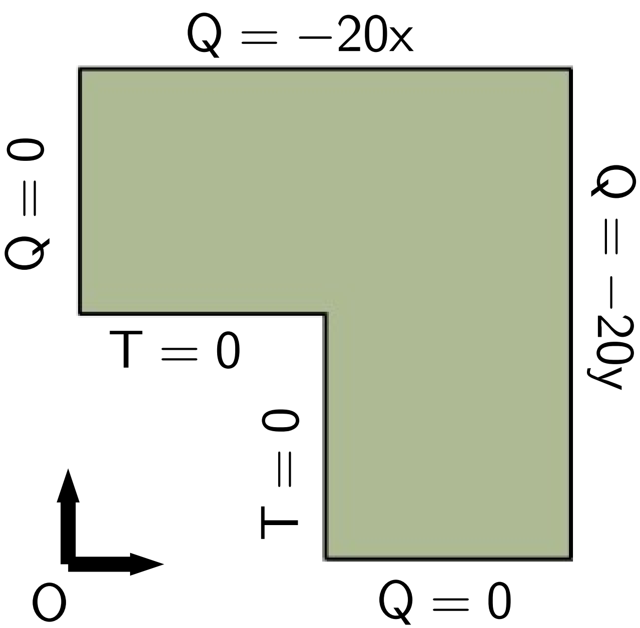

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Dual problem

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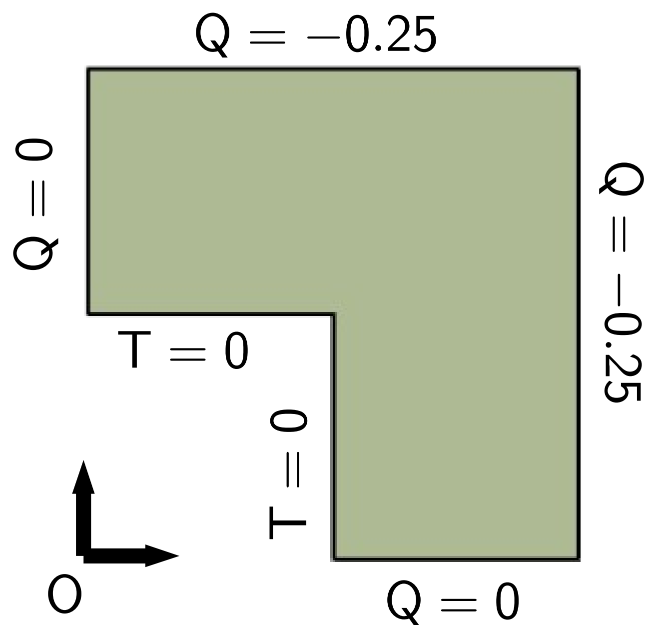

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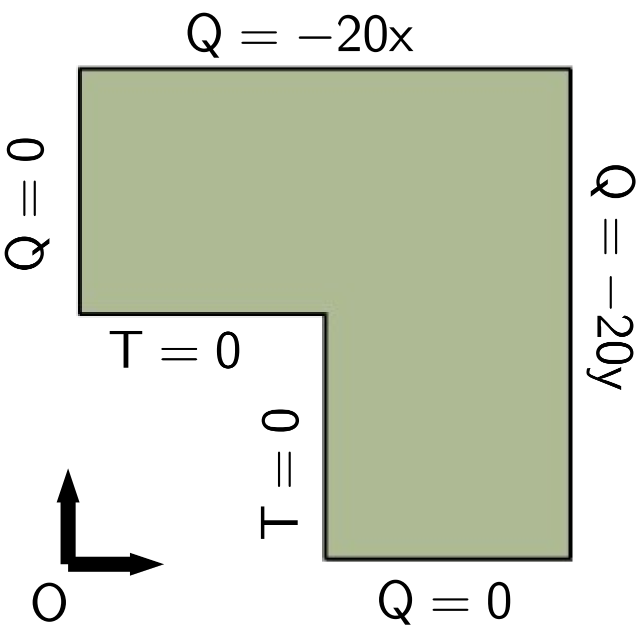

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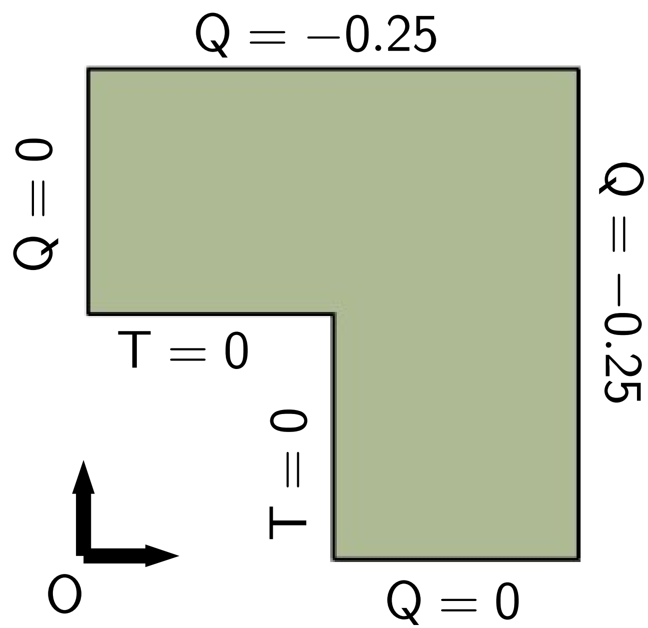

Two problems solved twice:

- Using “temperature” FE u^h, ϕ^h
- Using “flux” FE $\hat{Q}, \hat{Q}_\phi$

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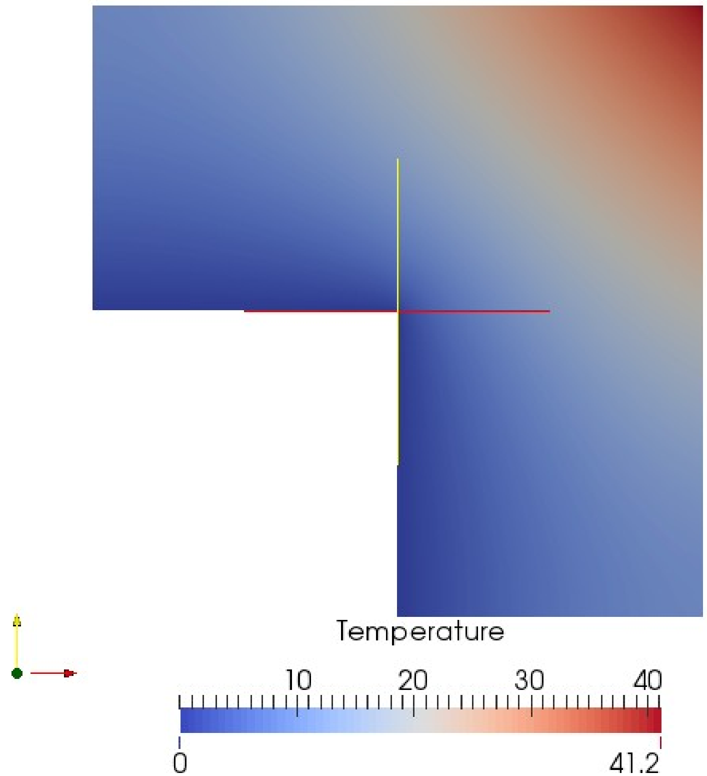
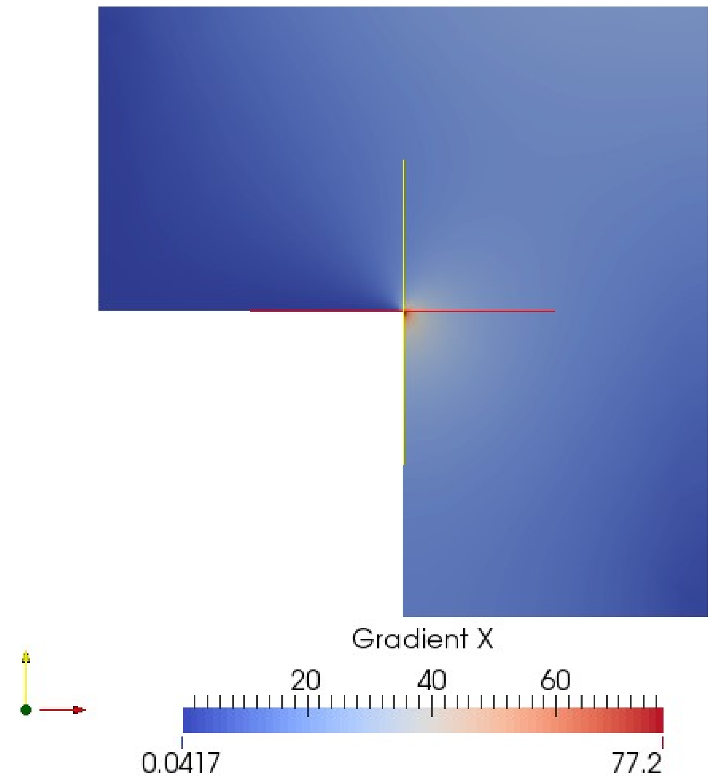




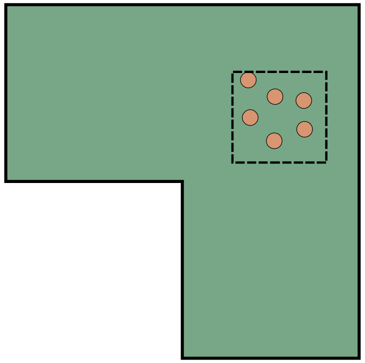
$q(u^h)$	ζ_l	$q(u) - q(u^h)$	$\leq \zeta_u$	$\zeta_l + q(u^h) \leq$	$q(u)$	$\leq \zeta_u + q(u^h)$
21.92	− 0.048	0.63	1.794	21.87	22.55	23.71

What if the bounds are not tight enough?

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

Two possible solutions

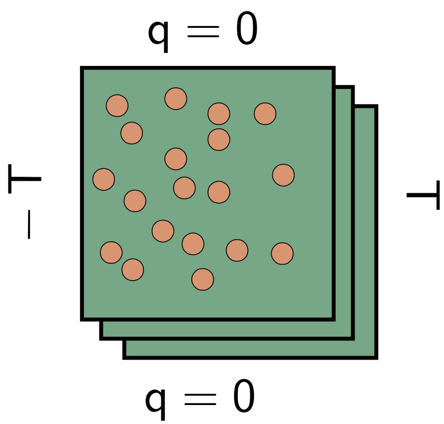
- **Adaptivity:** solve in a certain subdomain the heterogeneous problem

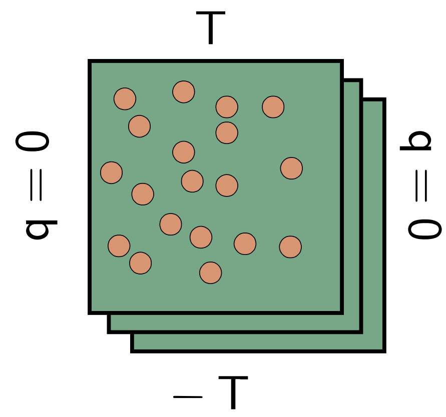


- **Enrichment:** solve an RVE and enrich the solution with its information

Enriched approximation

Idea: Solve RVEs, filter their solution





$u_x^{\mathrm{RVE}}(x, \theta)$ $\qquad$ $u_y^{\mathrm{RVE}}(x, \theta)$

to express our approximation as

$$u^h(x, \theta) = \sum N_i(x) u_i + u_x^{\mathrm{RVE}}(x, \theta) \sum N_i(x) a_i + u_y^{\mathrm{RVE}}(x, \theta) \sum N_i(x) b_i$$

Enriched approximation

Assembling the system of equations, 3 types of terms appear

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

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

$$a(N_i u_d^{\mathrm{RVE}}, N_j u_{d'}^{\mathrm{RVE}}) = \int_\Omega E[k u_d^{\mathrm{RVE}} u_{d'}^{\mathrm{RVE}}] \nabla N_i \nabla N_j + \int [k \nabla u_d^{\mathrm{RVE}} \nabla u_{d'}^{\mathrm{RVE}}] N_i N_j + \ldots$$

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

$$E[k],\ E[k u_d^{\mathrm{RVE}}],\ E[k u_d^{\mathrm{RVE}} u_{d'}^{\mathrm{RVE}}],\ E[k \nabla u_d^{\mathrm{RVE}} \nabla u_{d'}^{\mathrm{RVE}}], \ldots$$

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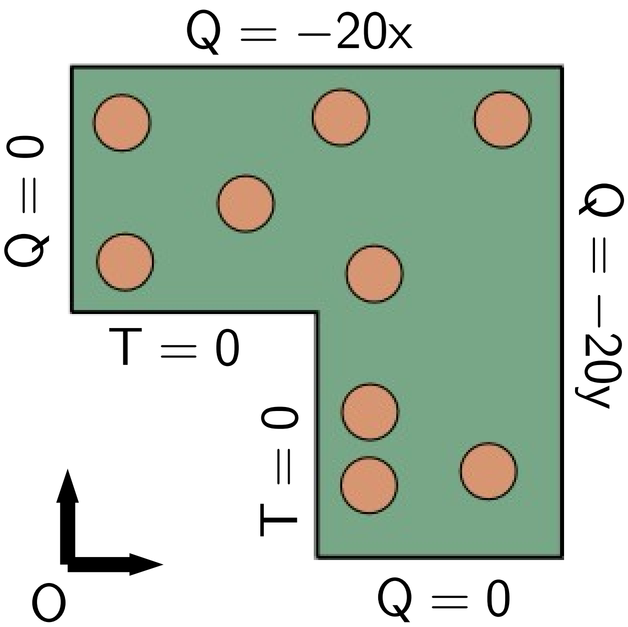
Remarks:

- 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



$$v_f = 0.196$$
$$k_I = 100$$
$$k_M = 1$$
$$R_I = 0.005$$

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

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