

# Error estimation in homogenisation

Strobl, 27<sup>th</sup> of January, 2015

Daniel Alves Paladim<sup>1</sup>

(alvesPaladimD@cardiff.ac.uk)

Pierre Kerfriden<sup>1</sup>

José Moitinho de Almeida<sup>2</sup>

Stéphane P. A. Bordas<sup>1,3</sup>

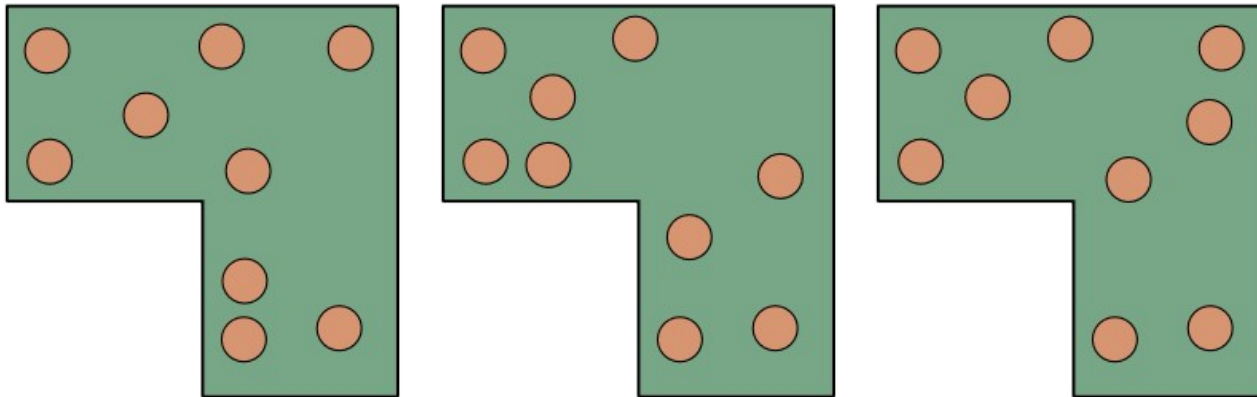
<sup>1</sup>School of Engineering, Cardiff University

<sup>2</sup>Instituto Superior Técnico, Universidade de Lisboa

<sup>3</sup>Faculté des Sciences, Université du Luxembourg

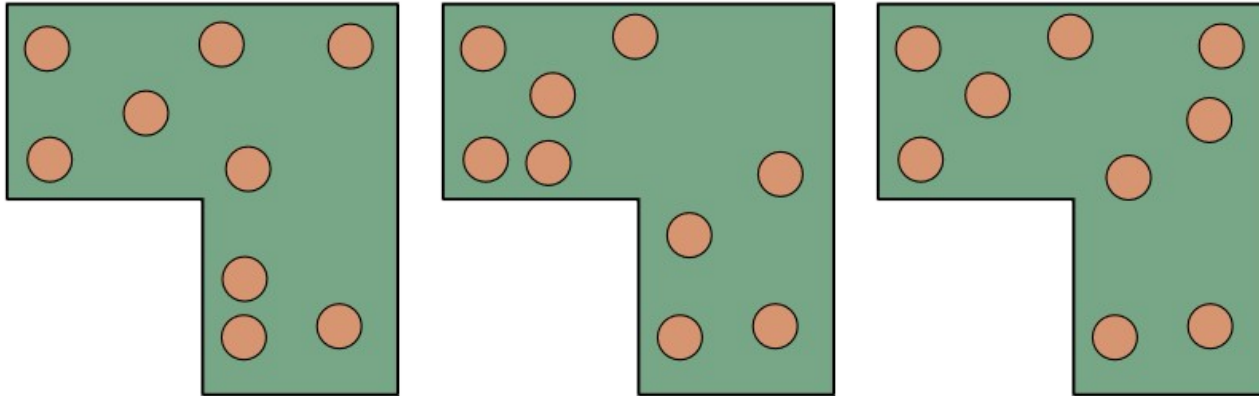
# Motivation

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

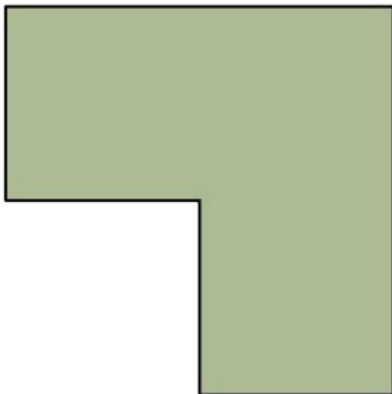


# Motivation

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

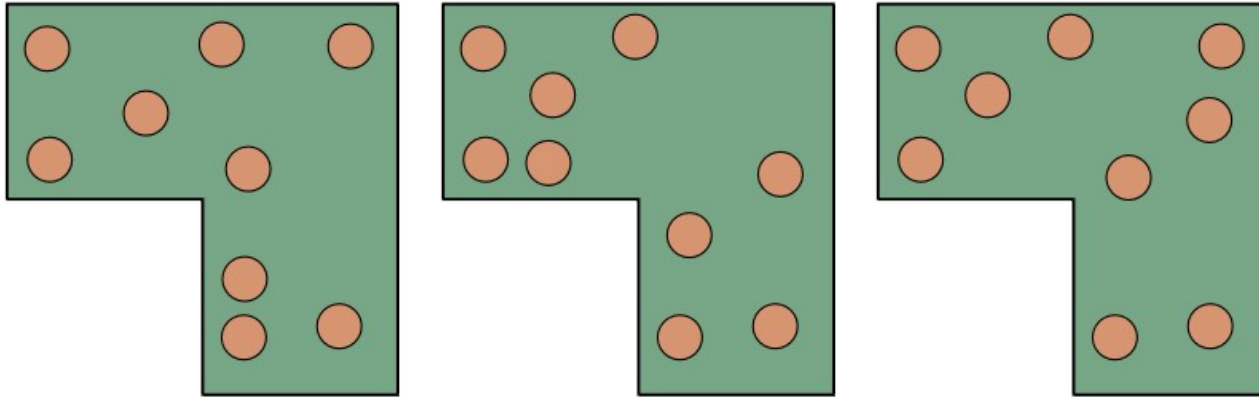


**Solution:** Homogenisation.

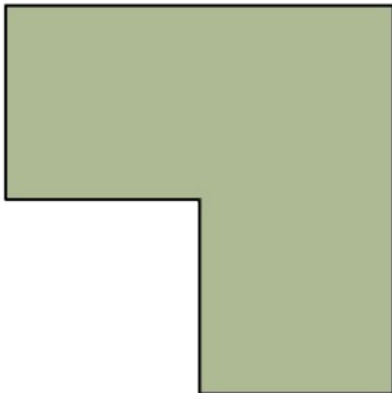


# Motivation

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



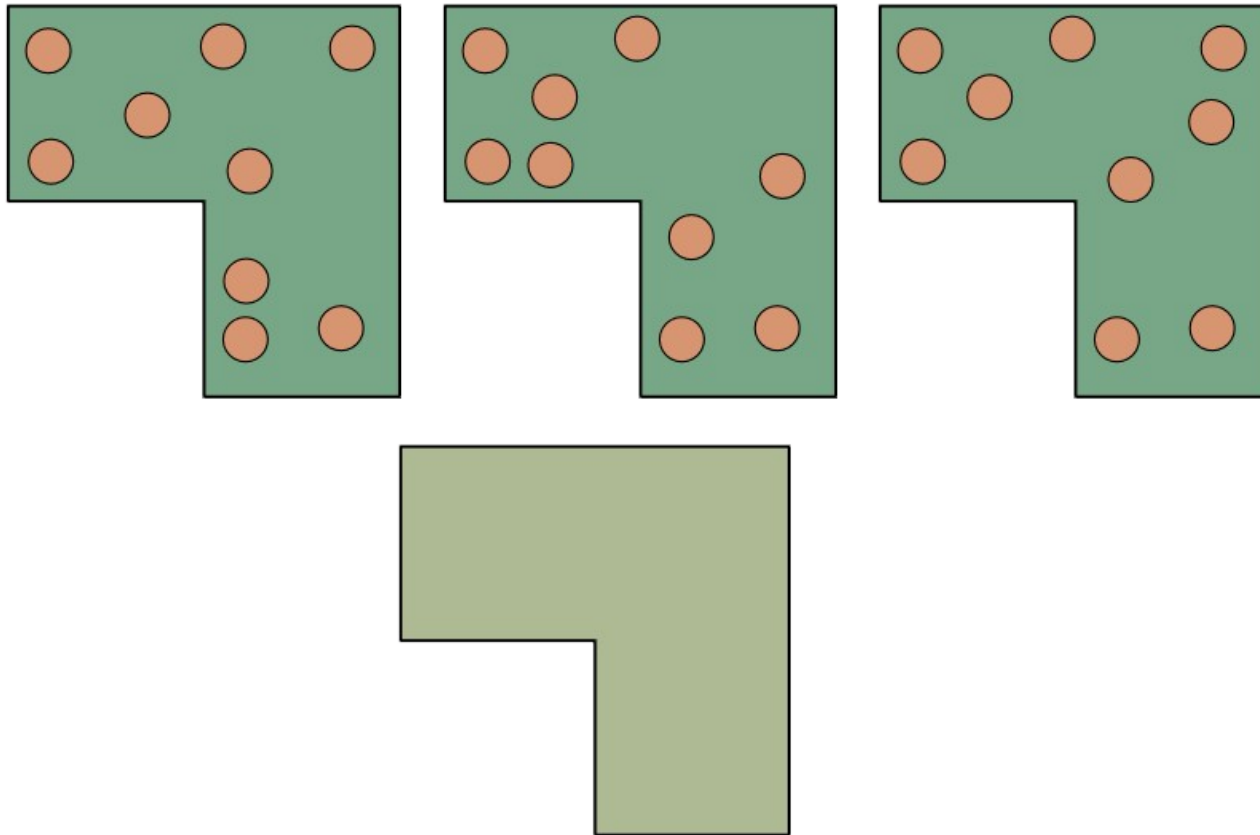
**Solution:** Homogenisation.



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

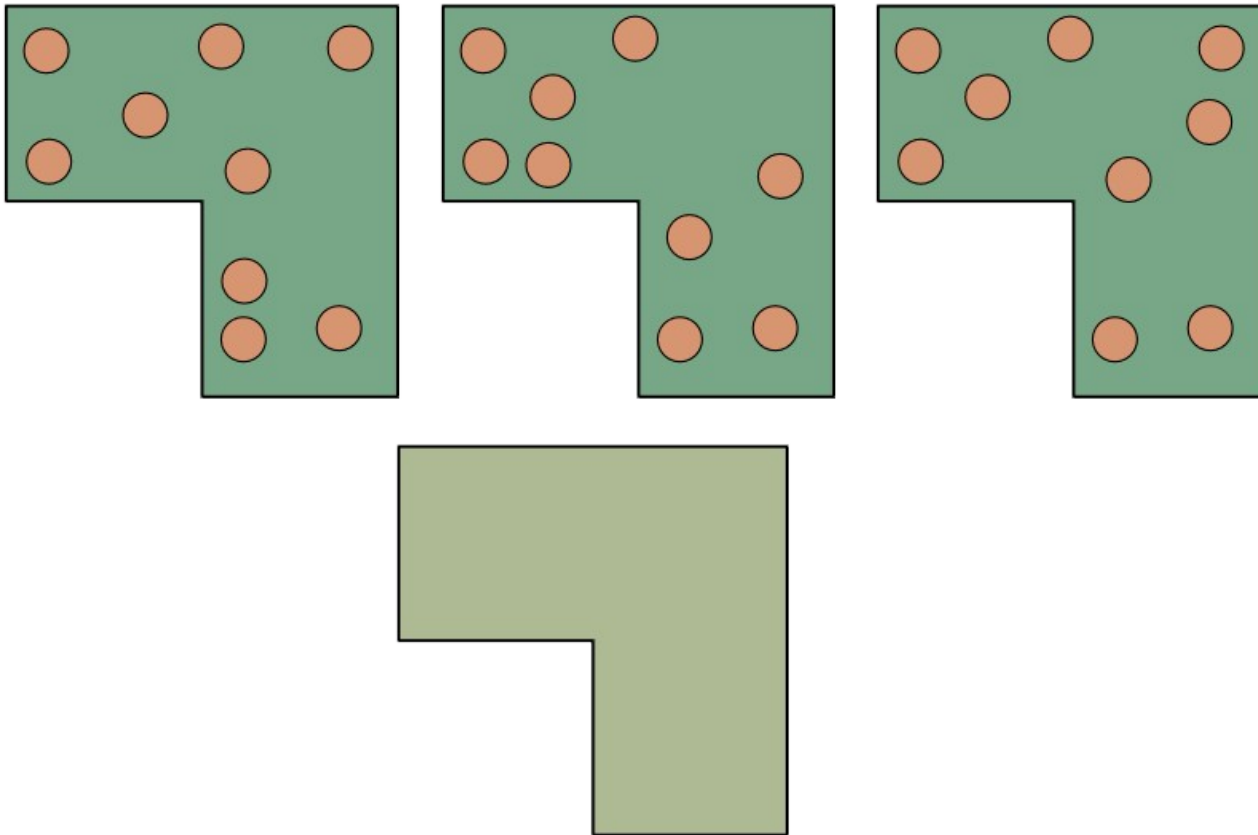
# Proposed solution

**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

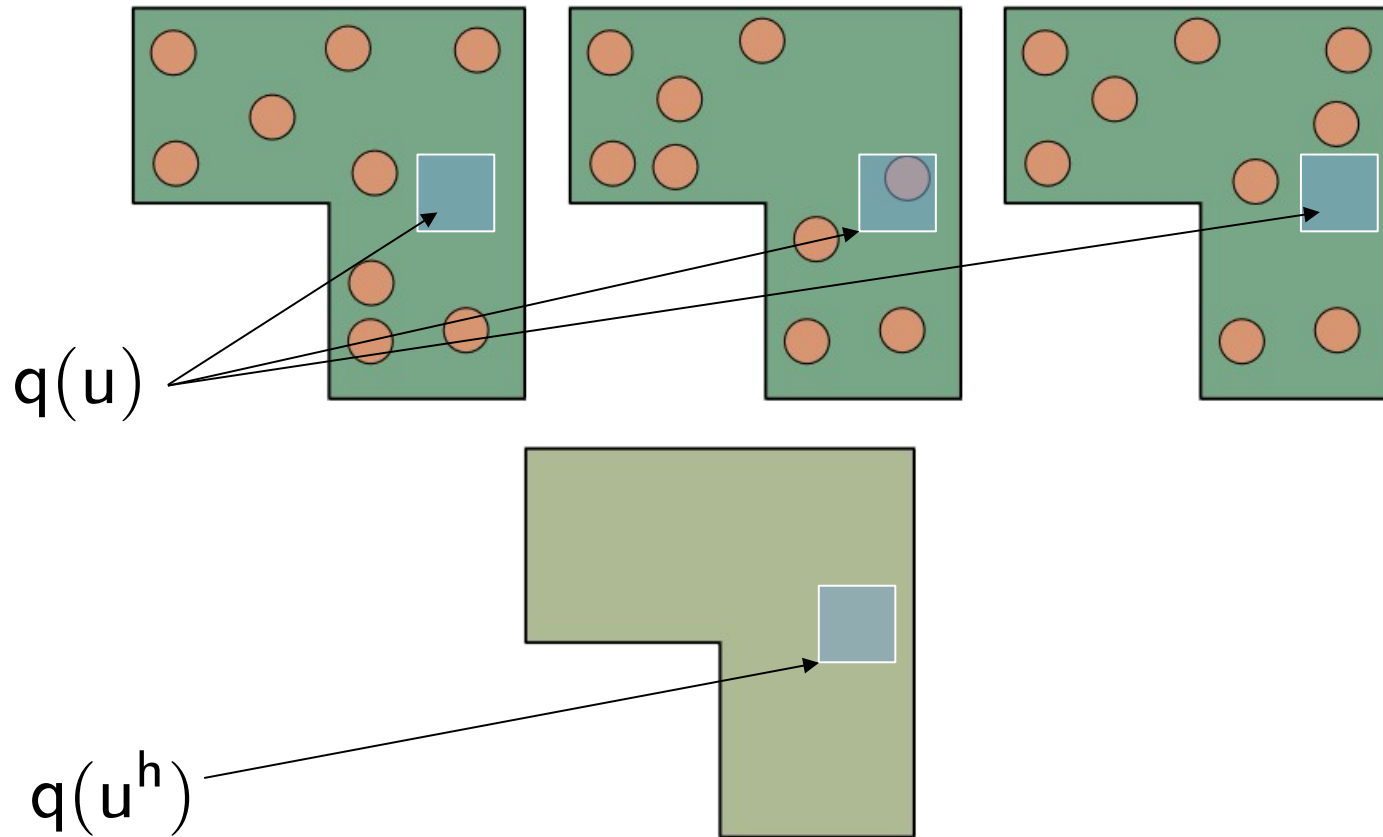
**SPDE:** Stochastic partial differential equation.  
Collection of parametric problems + probability density function



# Proposed solution

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

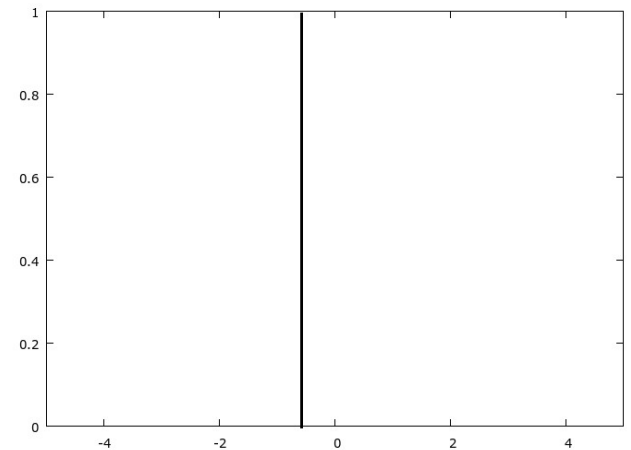
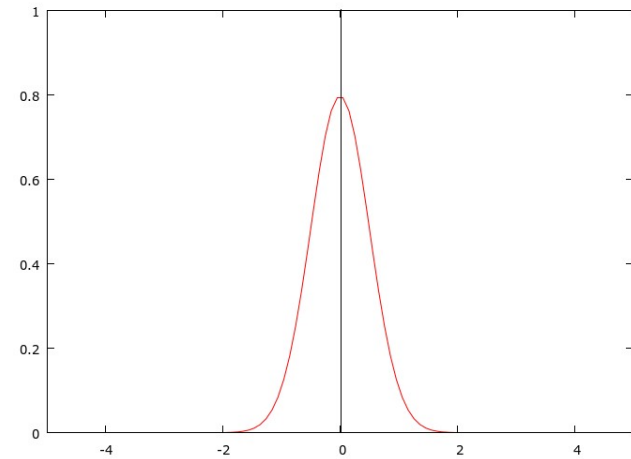
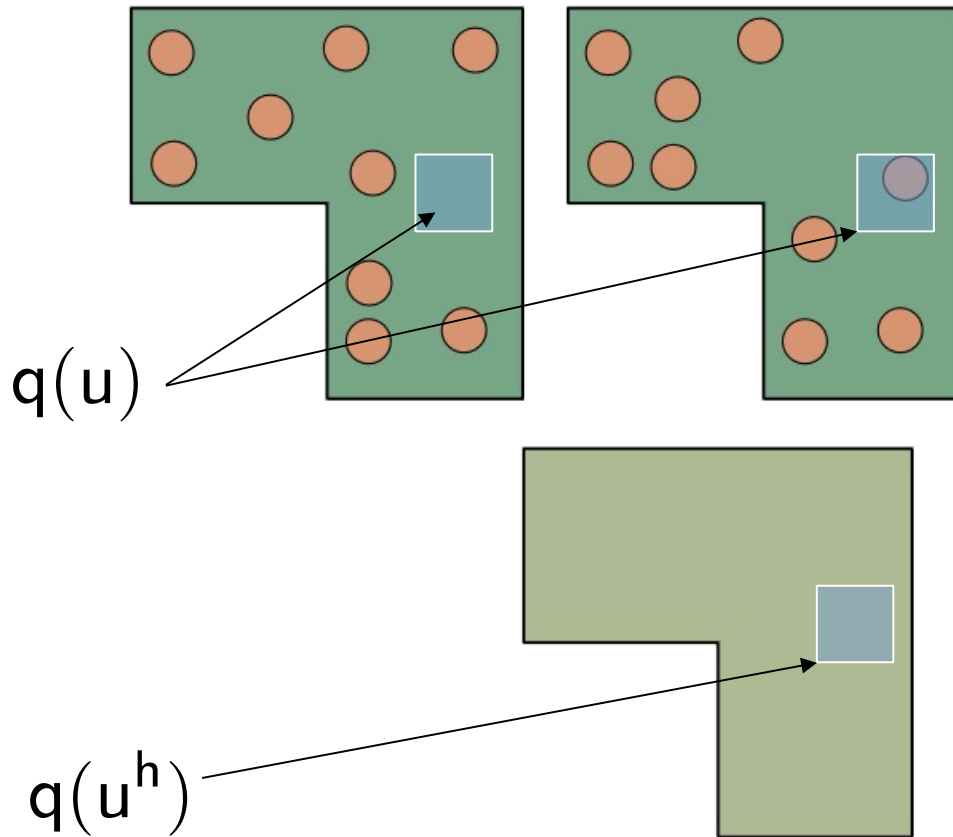
$$q(u) = \int_{\Omega} \int_{\Theta} \gamma(x) \cdot u(x, \theta) \quad (\text{linear})$$



# Proposed solution

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

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





## Heat equation

Heterogeneous problem

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

$$l(v) = \int_{\Omega} \int_{\Theta} f v - \int_{\partial\Omega} g v$$

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

## Heat equation

Heterogeneous problem

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

$$l(v) = \int_{\Omega} \int_{\Theta} f v - \int_{\partial\Omega} g v$$

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

Homogeneous problem

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

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

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

## Heat equation

Heterogeneous problem

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

$$l(v) = \int_{\Omega} \int_{\Theta} f v - \int_{\partial\Omega} g v$$

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

Homogeneous problem

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

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

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

**Aim:** Bound

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

The computation of the bound must be deterministic.

## **Hypothesis**

Deterministic boundary conditions

## Hypothesis

Deterministic boundary conditions

Constant volume fraction

$$\int_{\Omega} k(x, \theta) = v_f k_I + (1 - v_f) k_M \quad \forall \theta \in \Theta$$

## Hypothesis

Deterministic boundary conditions

Constant volume fraction

$$\int_{\Omega} k(x, \theta) = v_f k_I + (1 - v_f) k_M \quad \forall \theta \in \Theta$$

Constant PDF over the domain

$$\underbrace{\int_{\Theta} k(x, \theta)}_{E[k]} = v_f k_I + (1 - v_f) k_M \quad \forall x \in \Omega$$

The unknown is the flux field and

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

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

are fulfilled strongly.

The unknown is the flux field and

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

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

are fulfilled strongly.

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

$$u^h = h \quad x \in \partial\Omega_D$$



The unknown is the flux field and

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

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

are fulfilled strongly.

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

$$u^h = h \quad x \in \partial\Omega_D$$

In order to derive bounds, we will also need to use an homogenised “flux” FE solution  $\hat{Q}$

## Error in the energy norm

Rewriting the problem in terms of the flux and the temperature

$$\nabla \cdot \mathbf{Q} = f \quad \forall x \in \Omega \times \Theta$$

$$\mathbf{Q} \cdot \mathbf{n} = g \quad \forall x \in \partial\Omega_N \times \Theta$$

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

$$\mathbf{Q} + k\nabla u = 0 \quad \forall x \in \Omega \times \Theta$$

## Error in the energy norm

Rewriting the problem in terms of the flux and the temperature

$$\nabla \cdot \mathbf{Q} = f \quad \forall x \in \Omega \times \Theta$$

$$\mathbf{Q} \cdot \mathbf{n} = g \quad \forall x \in \partial\Omega_N \times \Theta$$

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

$$\mathbf{Q} + k\nabla u = 0 \quad \forall x \in \Omega \times \Theta$$

$\hat{\mathbf{Q}}$  will fulfill exactly the first 2 equations.

## Error in the energy norm

Rewriting the problem in terms of the flux and the temperature

$$\nabla \cdot \mathbf{Q} = f \quad \forall x \in \Omega \times \Theta$$

$$\mathbf{Q} \cdot \mathbf{n} = g \quad \forall x \in \partial\Omega_N \times \Theta$$

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

$$\mathbf{Q} + k\nabla u = 0 \quad \forall x \in \Omega \times \Theta$$

$\hat{\mathbf{Q}}$  will fulfill exactly the first 2 equations.

$u^h$  will fulfill exactly the 3<sup>rd</sup> equation.

## Error in the energy norm

Rewriting the problem in terms of the flux and the temperature

$$\nabla \cdot \mathbf{Q} = f \quad \forall x \in \Omega \times \Theta$$

$$\mathbf{Q} \cdot \mathbf{n} = g \quad \forall x \in \partial\Omega_N \times \Theta$$

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

$$\mathbf{Q} + k\nabla u = 0 \quad \forall x \in \Omega \times \Theta$$

$\hat{\mathbf{Q}}$  will fulfill exactly the first 2 equations.

$u^h$  will fulfill exactly the 3<sup>rd</sup> equation.

In general,  $\hat{\mathbf{Q}} + k\nabla u^h \neq 0$  Discrepancy = measure of the error

# Error in the energy norm

Formalizing this idea, it can be shown that

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

# Error in the energy norm

Formalizing this idea, it can be shown that

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

Expanding  $\eta^2$

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

# Error in the energy norm

Formalizing this idea, it can be shown that

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

Expanding  $\eta^2$

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

Deterministic quantity



# Error in the quantity of interest

The error in energy norm is not always relevant.

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

# Error in the quantity of interest

The error in energy norm is not always relevant.

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

Dual problem

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

# Error in the quantity of interest

The error in energy norm is not always relevant.

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

Dual problem

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

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

# Error in the quantity of interest

The error in energy norm is not always relevant.

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

Dual problem

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

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

Cauchy-Schwarz inequality

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

# Error in the quantity of interest

The error in energy norm is not always relevant.

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

Dual problem

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

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

Cauchy-Schwarz inequality

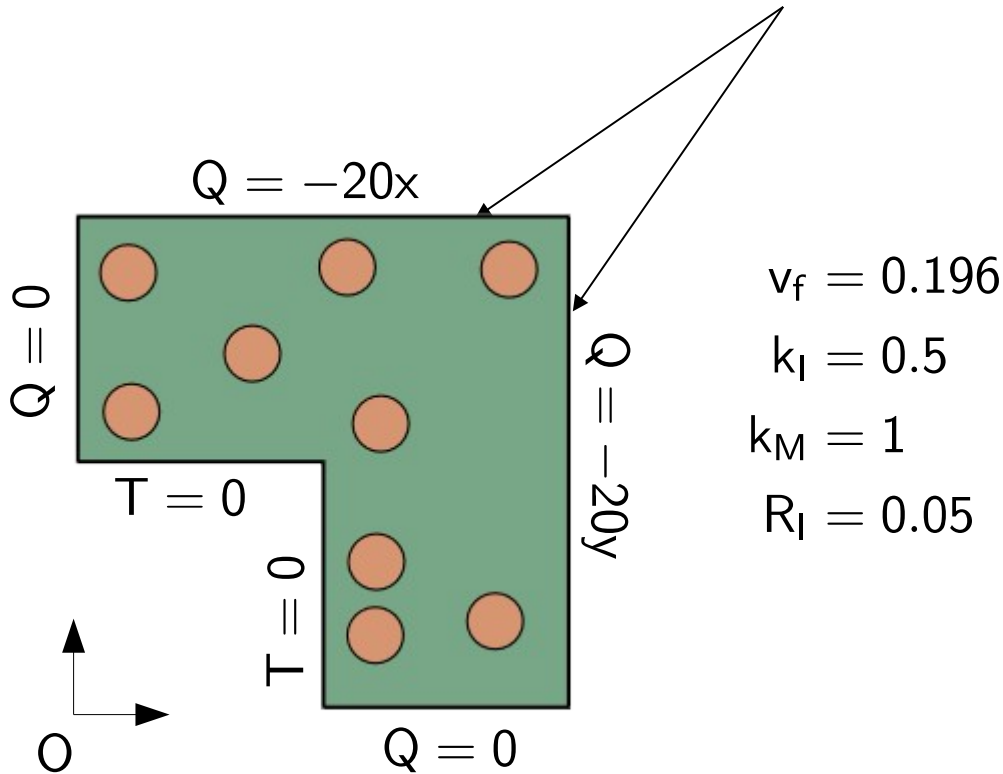
$$|a(e_\phi, e)| \leq \|e_\phi\| \|e\|$$

Use the bound in the energy norm,

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

# Validation

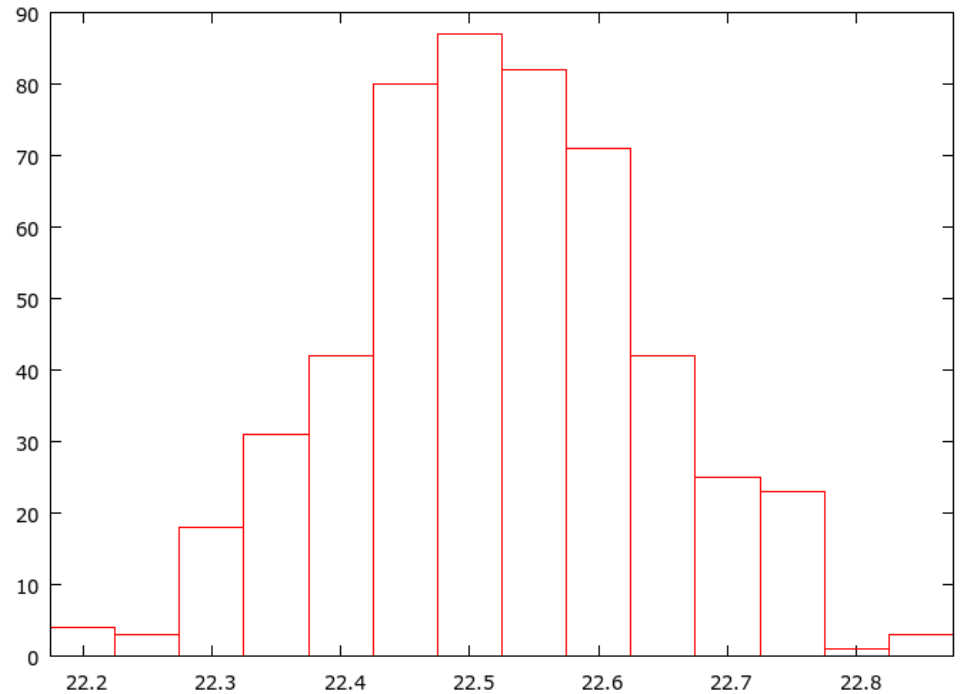
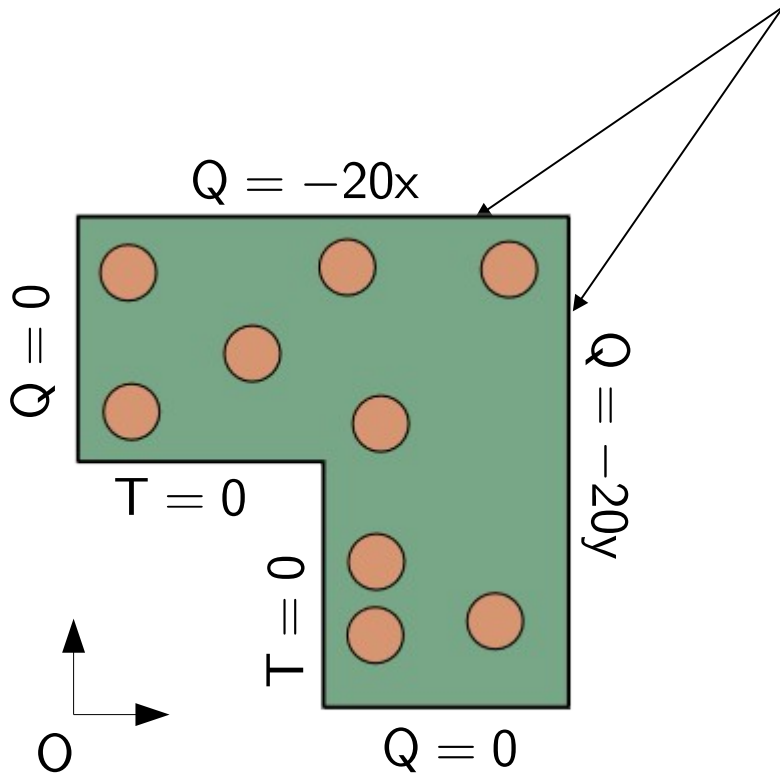
The quantity of the interest is the average temperature in the exterior faces.



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

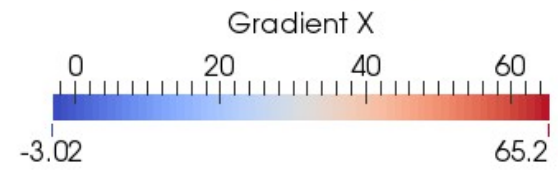
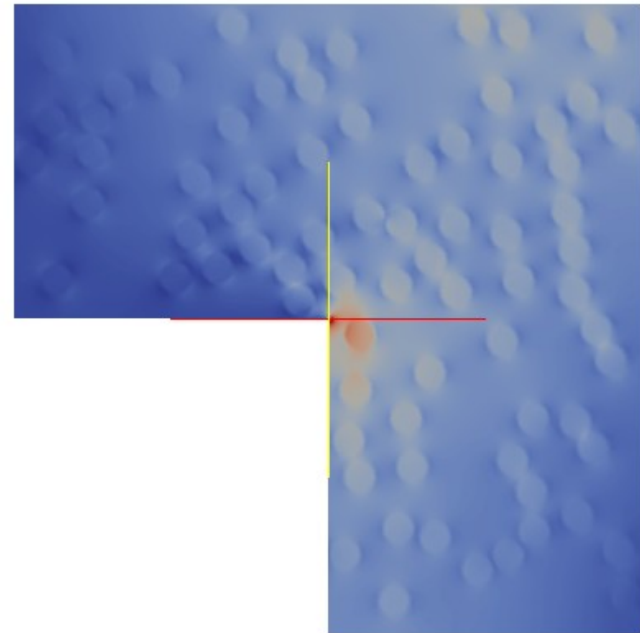
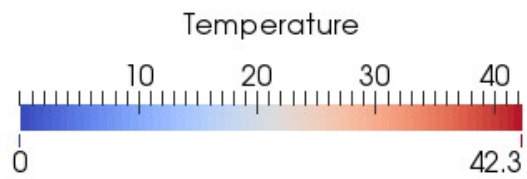
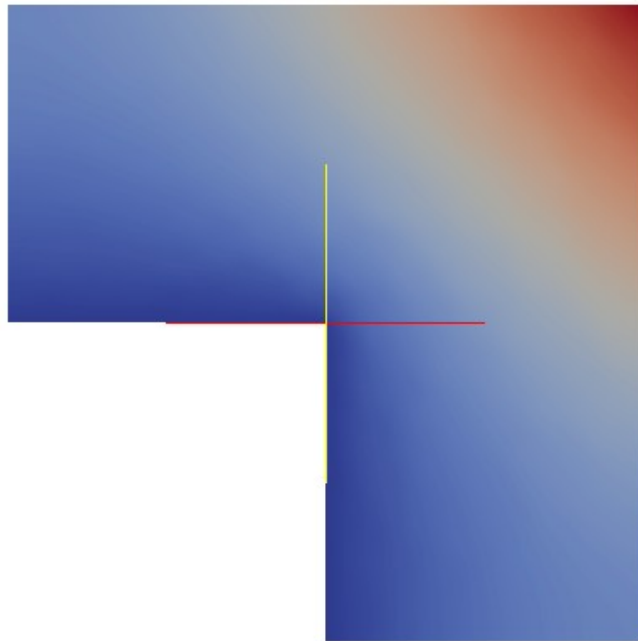
# Validation

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



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

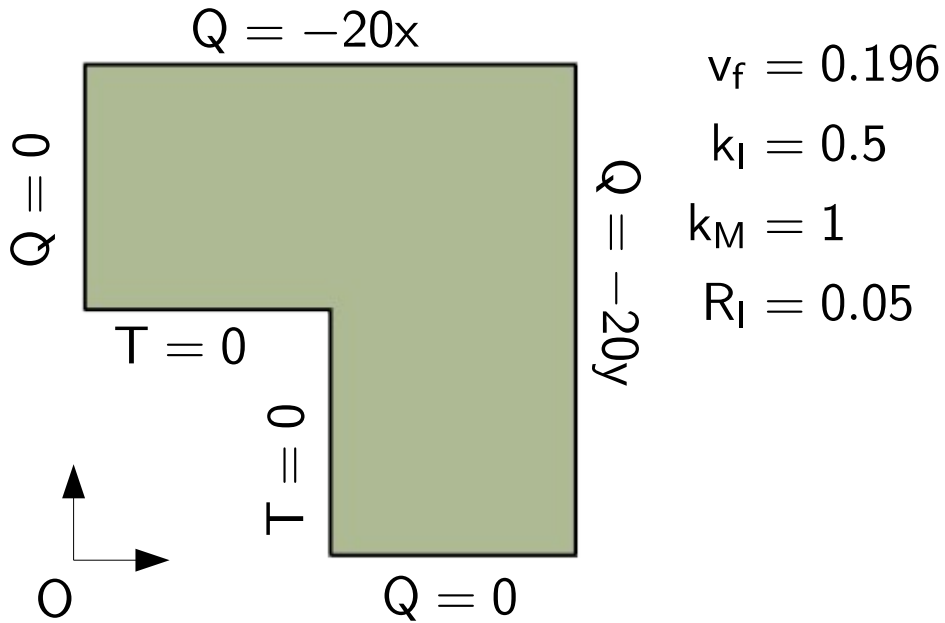
# Validation





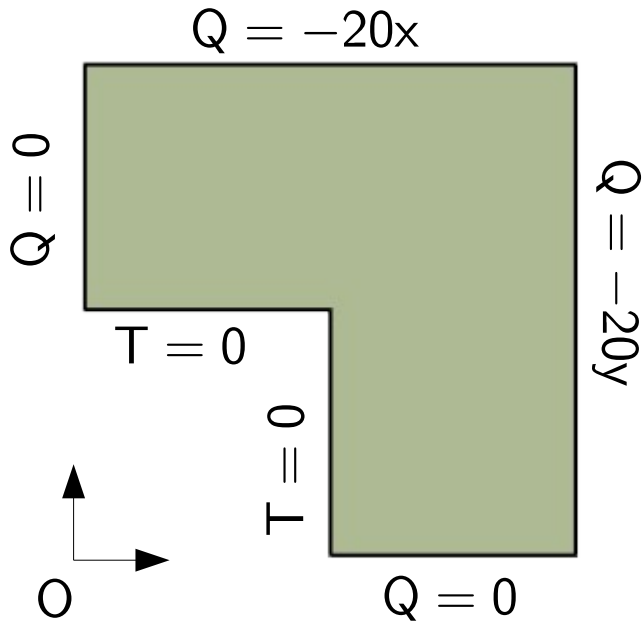
# Validation

Studied in a domain homogenised through rule of mixture.



# Validation

Studied in a domain homogenised through rule of mixture.



$$v_f = 0.196$$

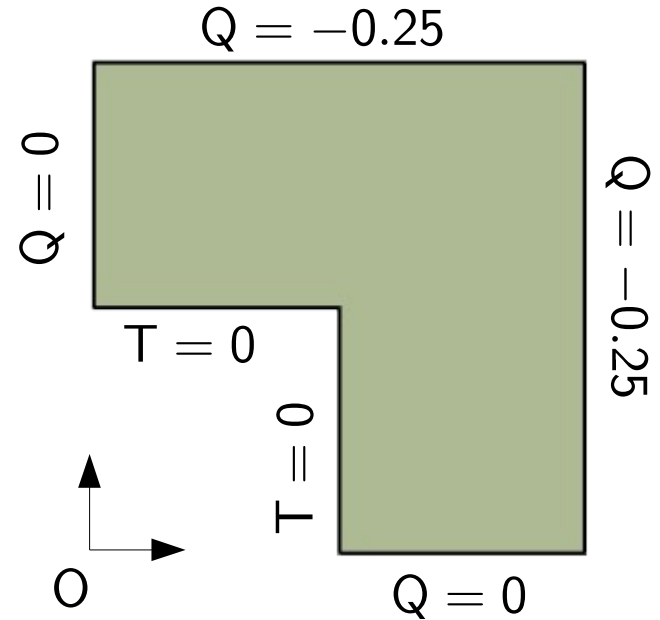
$$k_l = 0.5$$

$$k_M = 1$$

$$R_l = 0.05$$

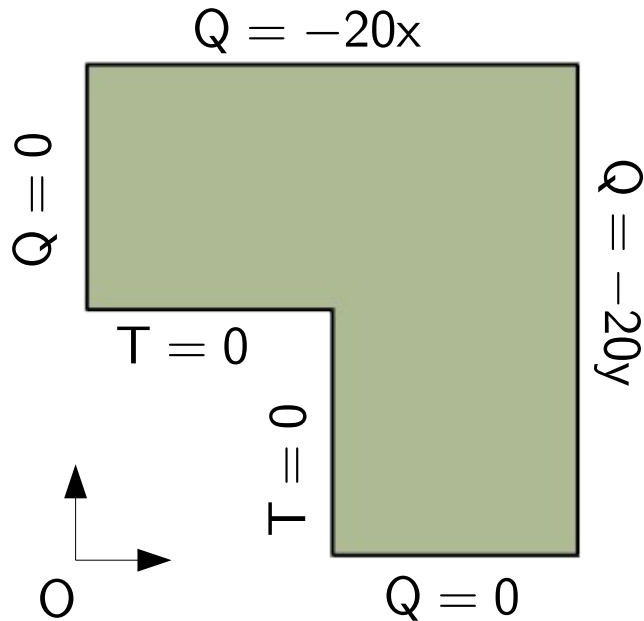
Dual problem

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



# Validation

Studied in a domain homogenised through rule of mixture.



$$v_f = 0.196$$

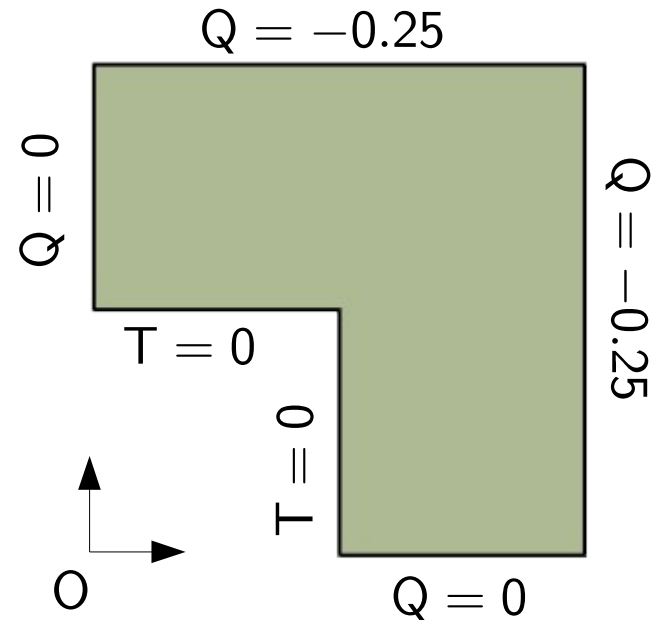
$$k_l = 0.5$$

$$k_M = 1$$

$$R_l = 0.05$$

Dual problem

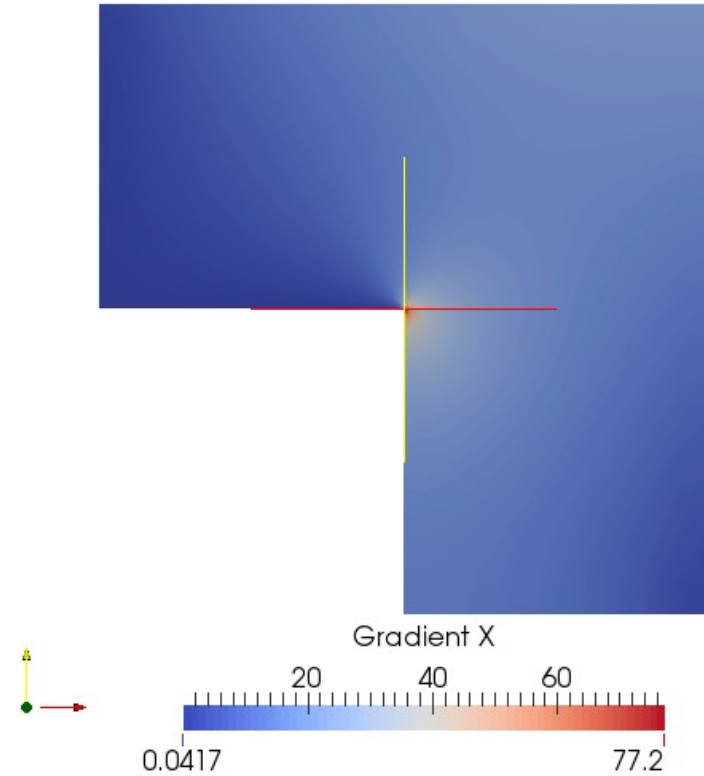
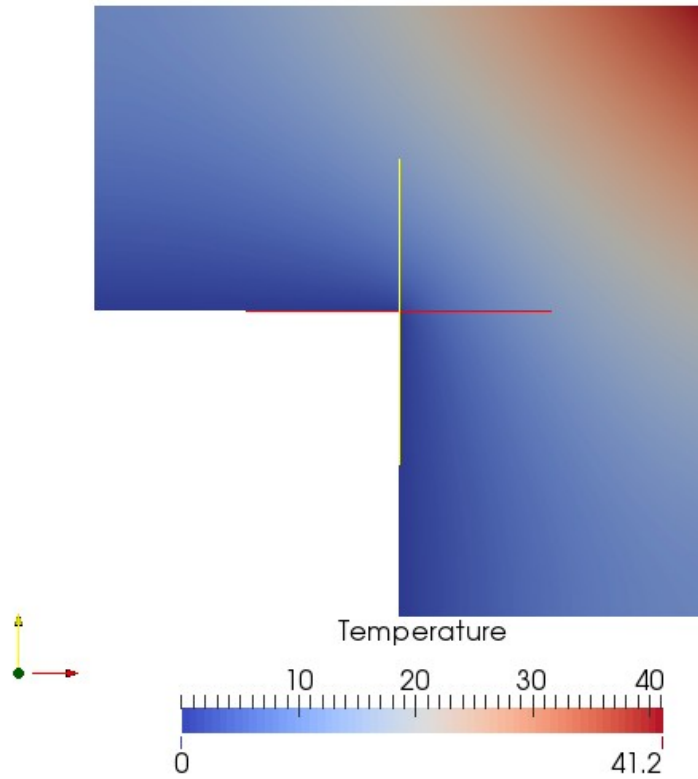
$$a_0(\phi^h, v) = q(v)$$



Two problems solved twice:

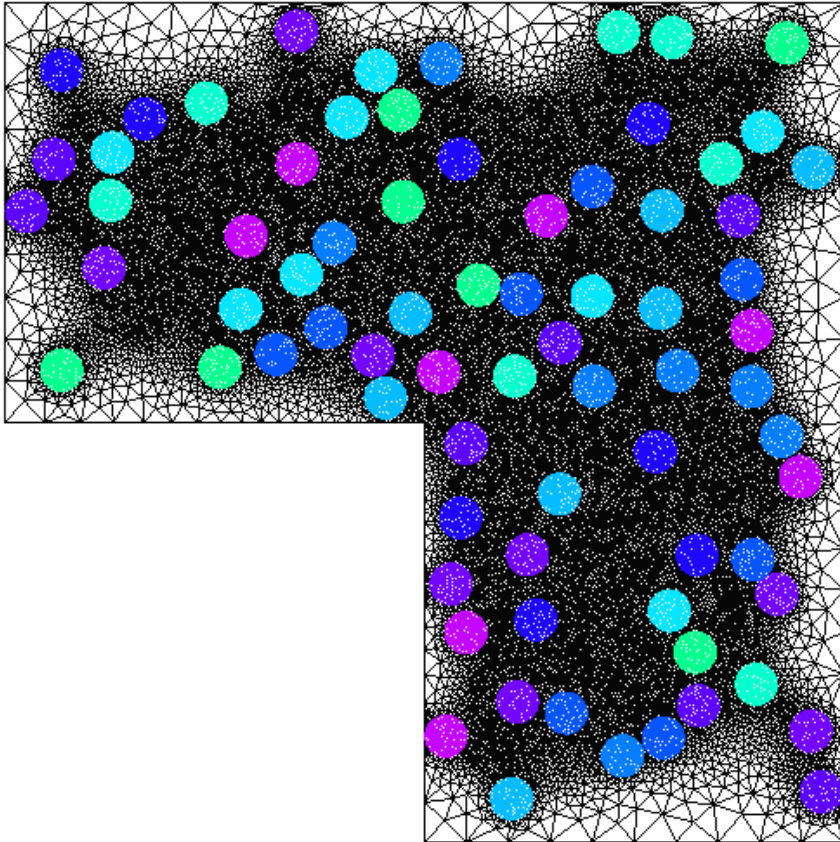
- Using "temperature" FE  $u^h, \phi^h$
- Using "flux" FE  $\hat{Q}, \hat{Q}_\phi$

# Validation

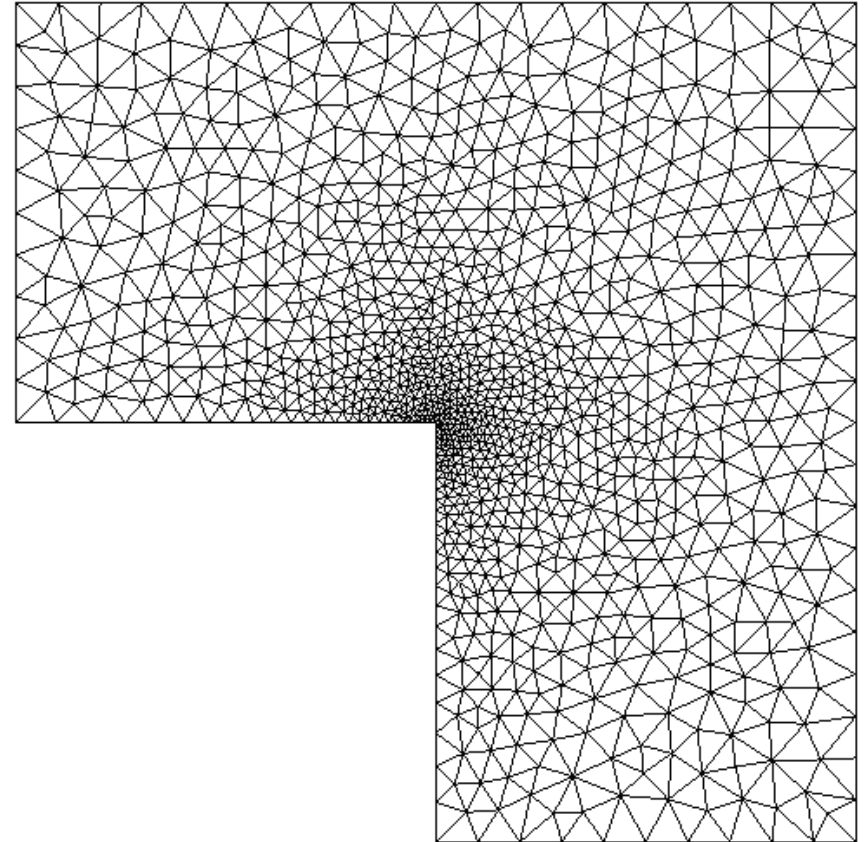


$q(u^h)$	$ q(u) - q(u^h) $	$\leq \zeta_u$	$\zeta_l + q(u^h) \leq$	$q(u)$	$\leq \zeta_u + q(u^h)$
21.92	0.63	1.84	20.08	22.55	23.76

# Validation



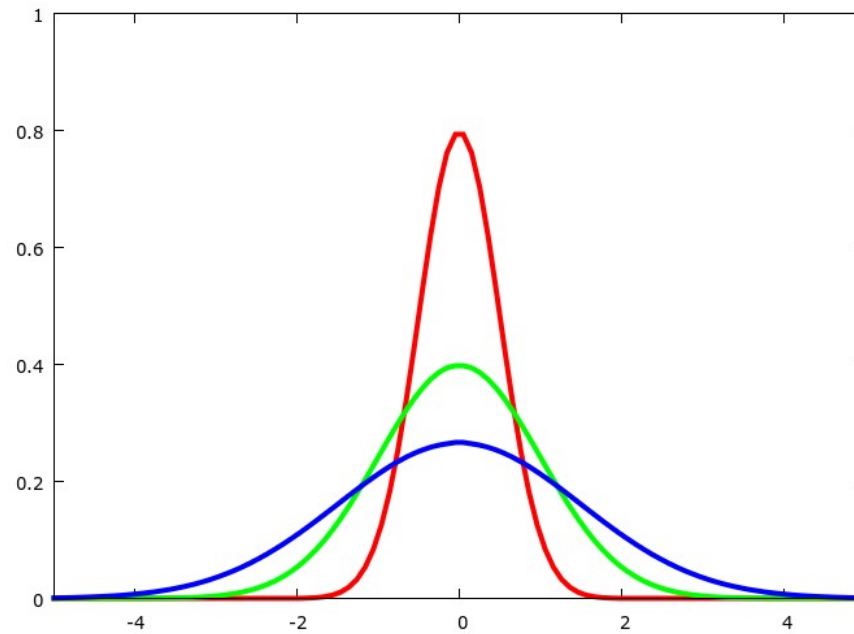
Around 60 000 elements  
512 problems, 512 different meshes  
Full PDF



Around 2000 elements  
4 problems, 1 mesh  
Bounds on the expectation

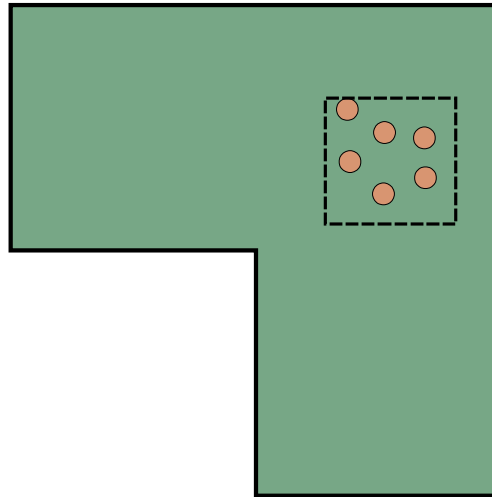
# Work in progress

- A bound on the variance.



# Work in progress

- Enhanced model. Insert patches with particles in parts of the domain.



# Summary

- A bound for the homogenisation error was presented.
- The computation of the bound is deterministic.
- The error estimate, should be used with care when there is a high contrast between the material properties.



# Summary

- A bound for the homogenisation error was presented.
- The computation of the bound is deterministic.
- The error estimate, should be used with care when there is a high contrast between the material properties.

Thank you for your attention.