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Uncertainty Updating in the Description of Coupled Transport Processes in Heterogeneous Materials

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ISUME 2011

1st International Symposium on Uncertainty Modelling in Engineering

Outline

- Motivation
- Bayesian updating of uncertainty
- Modelling of heterogeneities
- Dimensionality reduction – Karhunen-Loève expansion
- Acceleration by polynomial chaos expansion
- Heat and moisture transport by Künzel and Kiessl
- Conclusion and future work

Motivation

- Uncertainty quantification – why is that important?
  - Quantitative characterization and reduction of uncertainty in applications
  - Enabling of suitable reparation of buildings and extension of building's lifetime
  - Prevention of building's collapse with catastrophic consequences

- Bayesian inference provides:
  - probabilistic description of structural behaviour (model response)
  - incorporating different sources of information:
    expert's knowledge, results of measurements...
  - parameters estimation from noisy and limited data or imperfect forward model

[Marzouk & Najm, 2007&2009]

Bayesian updating of uncertainty

Let Y be a forward model of a real system: $\boldsymbol{Y}(\boldsymbol{q})+\boldsymbol{\eta}=\boldsymbol{z}$

- $\boldsymbol{z}$ are measurable quantities
- $\boldsymbol{q}$ are model input parameters
- $\boldsymbol{\eta}$ are uncertainties including ***observation errors*** together with ***model imperfections***

- Bayes's rule: $p(\boldsymbol{q}\,|\,\boldsymbol{z})=\kappa\cdot p(\boldsymbol{z}\,|\,\boldsymbol{q})p_q(\boldsymbol{q})$

a priori density function

- a posteriori density function:

$$\pi_m(\boldsymbol{q})=\int_D p(\boldsymbol{q}\,|\,\boldsymbol{z})\,\mathrm{d}\,\boldsymbol{z}=\kappa\cdot p_m(\boldsymbol{q})L(\boldsymbol{q})$$

likelihood function

- Assuming uncertainties $\boldsymbol{\eta}$ to be Gaussian:

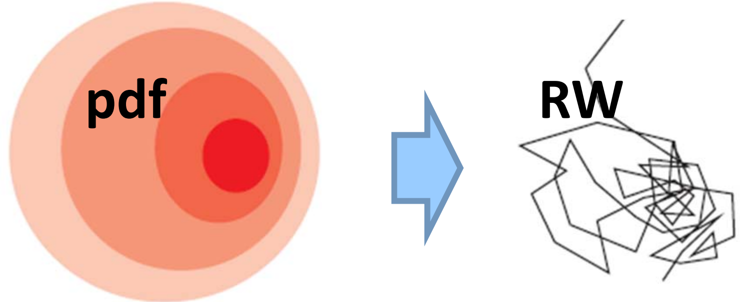
$$L(\boldsymbol{q})=\kappa\cdot\exp\left(-\frac{1}{2}\left(\boldsymbol{Y}(\boldsymbol{q})-\boldsymbol{z}_{\mathrm{obs}}\right)^T\mathbf{C}_{\mathrm{obs}}^{-1}\left(\boldsymbol{Y}(\boldsymbol{q})-\boldsymbol{z}_{\mathrm{obs}}\right)\right)$$

[Albert Tarantola, 2005, SIAM]

Sampling of a posteriori distribution:

Metropolis - Hastings algoritm

which is a Markov chain Monte Carlo method,
i.e., it is random (*Monte Carlo*) and has no memory in the sense that each step depends only on the previous step (*Markov chain*)



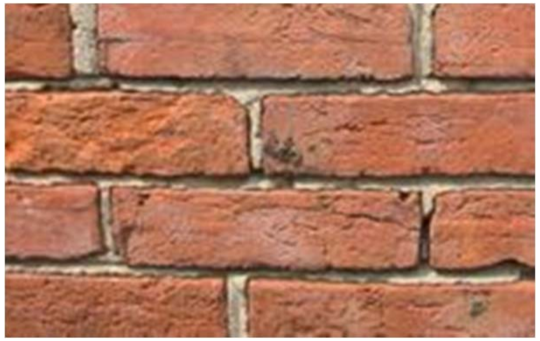
- start at $\boldsymbol{q}_i$
- generation of random walk $\boldsymbol{q}_j$ that samples the prior
- If $L(\boldsymbol{q}_j) \geq L(\boldsymbol{q}_i)$, then accept the proposed transition to $\boldsymbol{q}_j$
- If $L(\boldsymbol{q}_j) < L(\boldsymbol{q}_i)$, then accept the proposed transition to $\boldsymbol{q}_j$ with the probability $P_{i \to j} = L(\boldsymbol{q}_j) / L(\boldsymbol{q}_i)$, otherwise stay at $\boldsymbol{q}_i$

[Mosegaard & Tarantola, 2002, IHEES]

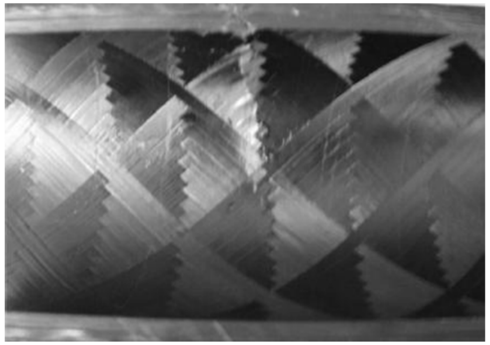
Modelling of heterogeneities

- homogenisation theories for materials with well-defined geometry:

Regular masonry



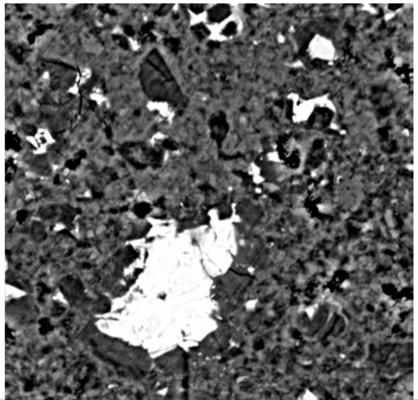
Wound composite tube



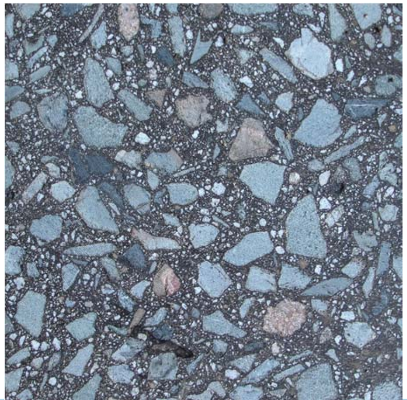
- describing uncertain material properties in time and/or space using stochastic processes and fields

Irregular masonry

Cement paste

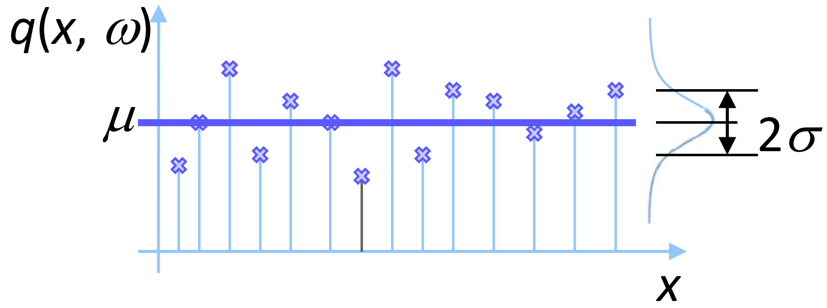


Asphalt

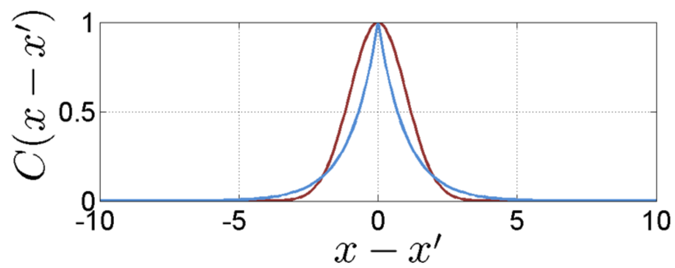


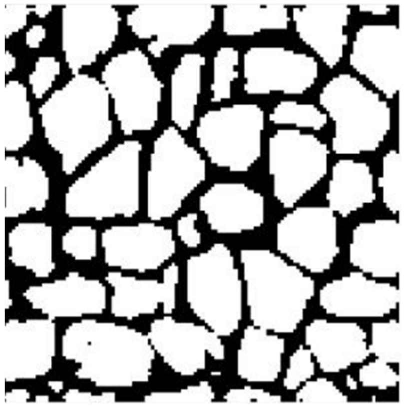
Description of random field

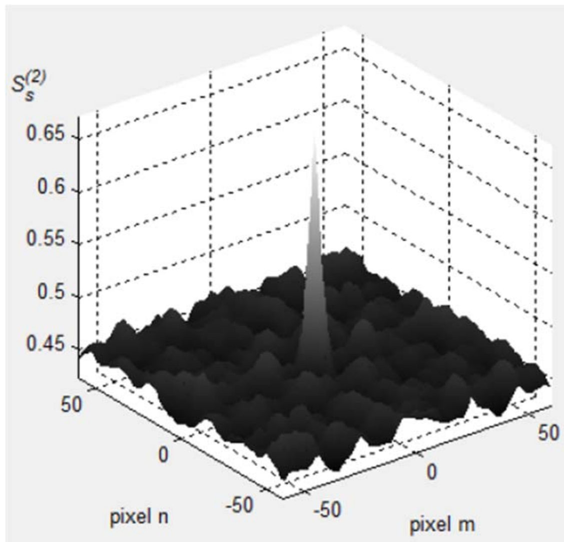
Random field $q(\boldsymbol{x},\omega)$ usually defined by:



- mean μ
- covariance function $C(\boldsymbol{x},\boldsymbol{x}')$
  - Gaussian covariance $C(x,x') = \sigma^2 \mathrm{e}^{-\frac{(x-x')^2}{2L_x^2}}$
  - Exponential covariance $C(x,x') = \sigma^2 \mathrm{e}^{-\left|\frac{x-x'}{L_x}\right|}$







Karhunen-Loève expansion

Since the covariance function is symmetric and positive definite , it can be represented by the ***spectral decomposition*** as

$$C(\boldsymbol{x},\boldsymbol{x}') = \sum_{i=1}^{\infty} \varsigma_i \psi_i(\boldsymbol{x}) \psi_i(\boldsymbol{x}')$$

ς_i ... eigenvalues

$\psi_i(\boldsymbol{x})$ ... eigenfunctions

– quite complex, solved only for one- or two-dimensional tasks

→ discretization of covariance according to *n* grid points:

$$\mathbf{C} = \sum_{i=1}^{M} \varsigma_i \psi_i \psi_i^T$$

ς_i ... eigenvalues

$\boldsymbol{\psi}_i$ ... eigenvectors

– where ς_i ,$\boldsymbol{\psi}_i$ are solution of eigenvalue problem $\mathbf{C}\boldsymbol{\psi}_i = \varsigma_i \boldsymbol{\psi}_i$

→ discretized field ***q*** can be written as ***Karhunen-Loève expansion***

$$\boldsymbol{q} = \boldsymbol{\mu} + \sum_{i=1}^{M} \sqrt{\varsigma_i}\, \xi_i \boldsymbol{\psi}_i$$

[e.g. Ghanem & Spanos, 1991, SFE or Matthies & Keese, 2005, CMAME]

Coupled heat and moisture transport

Model by Künzel and Kiessl, [Künzel and Kiessl, 1995]

Energy balance equation

$$\frac{\mathrm{d}H}{\mathrm{d}\Theta}\frac{\mathrm{d}\Theta}{\mathrm{d}t} = \nabla[\lambda\nabla\Theta] + h_v\nabla[\delta_p\nabla\{\varphi p_{\mathrm{sat}}(\Theta)\}]$$

Moisture balance equation

$$\frac{\mathrm{d}w}{\mathrm{d}\varphi}\frac{\mathrm{d}\varphi}{\mathrm{d}t} = \nabla[D_\varphi\nabla\varphi] + \nabla[\delta_p\nabla\{\varphi p_{\mathrm{sat}}(\Theta)\}]$$

H	$[\mathrm{Jm}^{-3}]$	enthalpy of the moist building material
w	$[\mathrm{kgm}^{-3}]$	water content of the building material
λ	$[\mathrm{Wm}^{-1}\mathrm{K}^{-1}]$	thermal conductivity
D_φ	$[\mathrm{kgm}^{-1}\mathrm{s}^{-1}]$	liquid conduction coefficient
δ_p	$[\mathrm{kgm}^{-1}\mathrm{s}^{-1}\mathrm{Pa}^{-1}]$	water vapour permeability
h_v	$[\mathrm{Jkg}^{-1}]$	evaporation enthalpy of the water
p_{sat}	$[\mathrm{Pa}]$	water vapour saturation pressure
Θ	$[^\circ\mathrm{C}]$	temperature
φ	$[-]$	relative humidity

$$\mathsf{K}_{\Theta\Theta}\mathbf{r}_\Theta + \mathsf{K}_{\Theta\varphi}\mathbf{r}_\varphi + \mathsf{C}_{\Theta\Theta}\frac{\mathrm{d}\mathbf{r}_\Theta}{\mathrm{d}t} = \mathbf{q}_{\mathrm{ext}}$$

$$\mathsf{K}_{\varphi\Theta}\mathbf{r}_\Theta + (\mathsf{K}^w_{\varphi\varphi} + \mathsf{K}^v_{\varphi\varphi})\mathbf{r}_\varphi + \mathsf{C}_{\varphi\varphi}\frac{\mathrm{d}\mathbf{r}_\varphi}{\mathrm{d}t} = \mathbf{g}_{\mathrm{ext}}$$

Coupled heat and moisture transport

Thermal conductivity - $$\lambda = \lambda_0 \left(1 + \frac{b_{\text{tcs}} w_f (b-1)\varphi}{\rho_s (b-\varphi)}\right)$$

Evaporation enthalpy of water - $$h_v = 2.5008 \cdot 10^6 \left(\frac{273.15}{\theta}\right)^{(0.167+3.67 \cdot 10^{-4}\theta)}$$

Water vapour saturation pressure - $$p_{\text{sat}} = 611 \exp\left(\frac{17.08\theta}{234.18+\theta}\right)$$

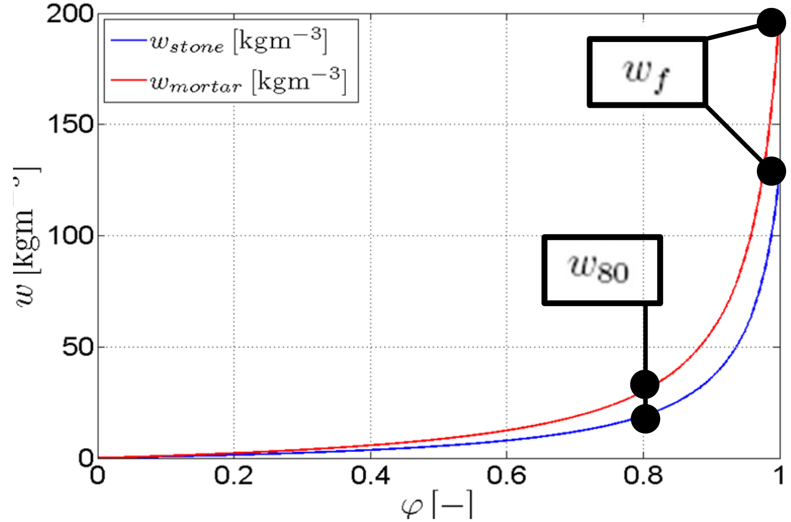
Water vapour permeability - $$\delta_p = \frac{1.9446 \cdot 10^{-12}}{\mu} \cdot (\theta + 273.15)^{0.81}$$

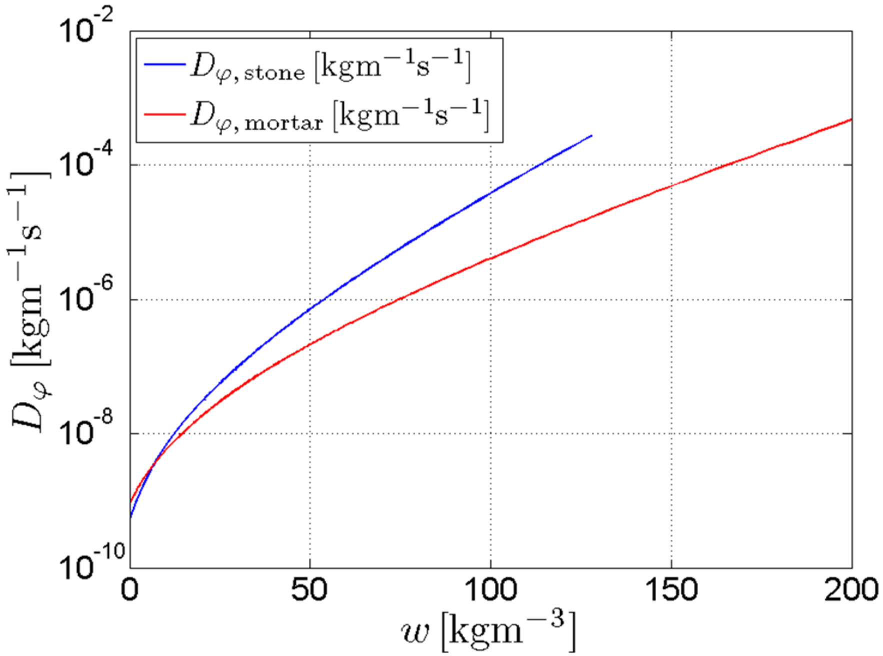
Liquid conduction coefficient - $$D_\varphi = 3.8 \frac{a^2}{w_f} \cdot 10^{\frac{3w_f(b-1)\varphi}{(b-\varphi)(w_f-1)}} \cdot \frac{b(b-1)}{(b-\varphi)^2}$$

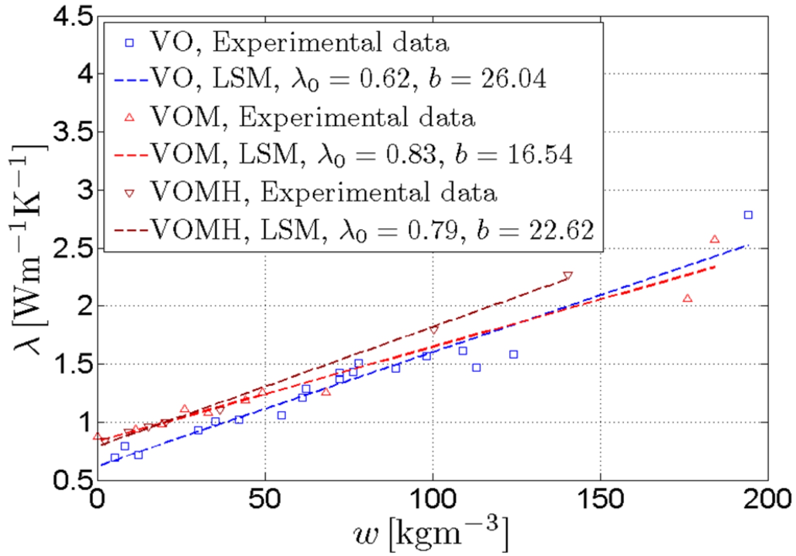
Total enthalpy - $$H = \rho_s c_s \theta$$

Model parameters

w_f	$[\mathrm{kgm^{-3}}]$	free water saturation
w_{80}	$[\mathrm{kgm^{-3}}]$	water content at 80 % relative humidity
λ_0	$[\mathrm{Wm^{-1}K^{-1}}]$	thermal conductivity of dry building material
b	$[-]$	thermal conductivity supplement
ρ_s	$[\mathrm{kgm^{-3}}]$	bulk density of dry building material
μ	$[-]$	water vapour diffusion resistance factor
A	$[\mathrm{kgm^{-2}s^{-0.5}}]$	water absorption coefficient



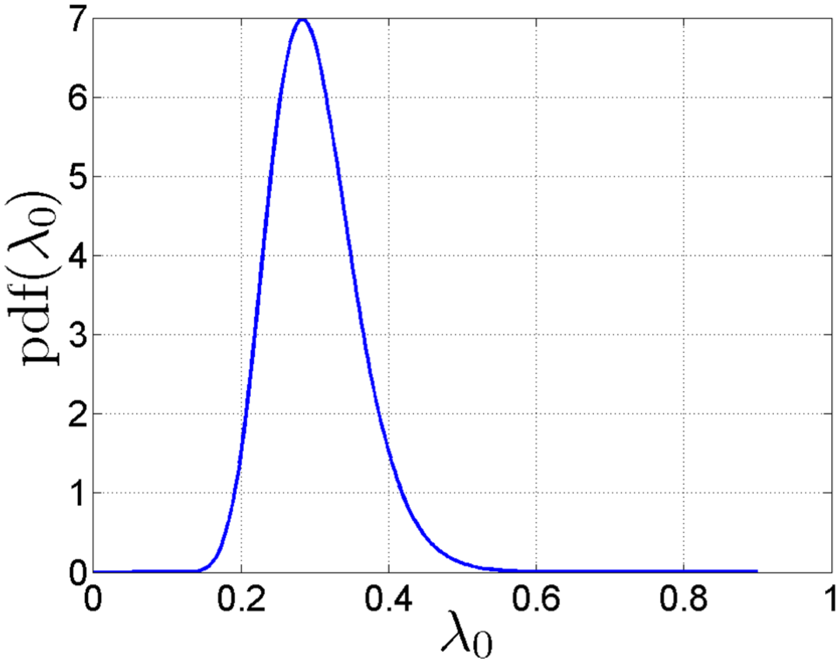




Variation of thermal conductivity as a function of water content

Model parameters

- Lognormal distribution
  - ⇨ Lognormal random field $\boldsymbol{q}(\boldsymbol{x},\omega)$



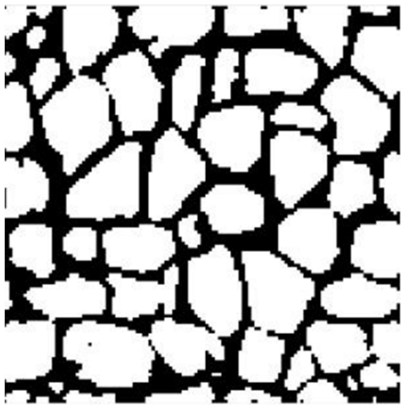
nonlinear transformation of standard

Gaussian random field $\boldsymbol{g}(\boldsymbol{x},\omega)$

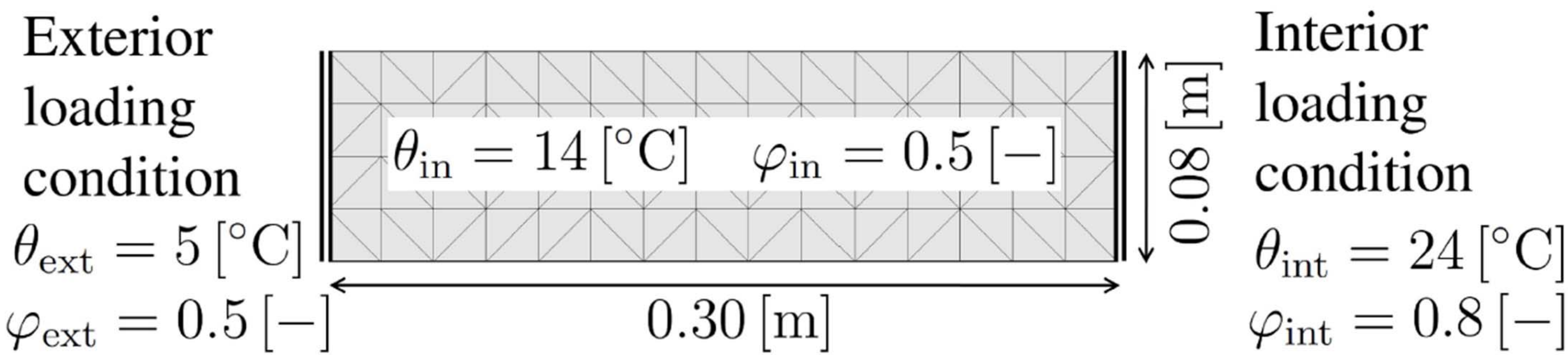
$$\boldsymbol{q}(\boldsymbol{x},\omega) = \exp(\mu_g+\sigma_g\,\boldsymbol{g}(\boldsymbol{x},\omega))$$

$$\boldsymbol{g} = \sum_{i=1}^{M} \sqrt{\varsigma_i}\,\xi_i\,\gamma_i \qquad \sigma_g^2 = \ln\left(1+\left(\frac{\sigma_{\mathrm{q}}}{\mu_{\mathrm{q}}}\right)^2\right) \qquad \mu_g = \ln\mu_{\mathrm{q}} - 0.5\sigma_g^2$$

- Assumption: fully correlated parameters
  - ⇨ differ only in second order statistics μ_g, σ_g, the shape $\boldsymbol{g}$ is the same



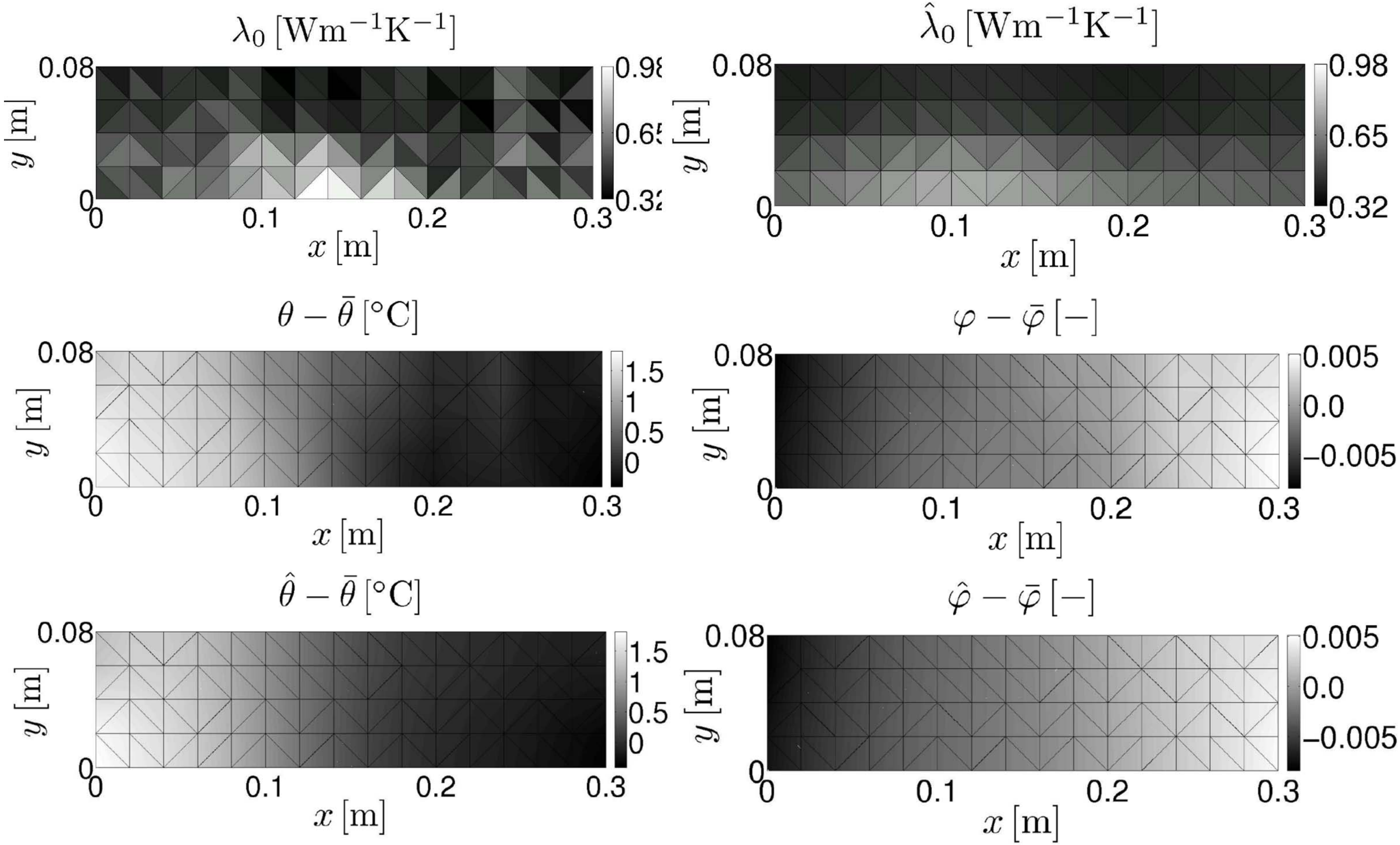
Numerical example



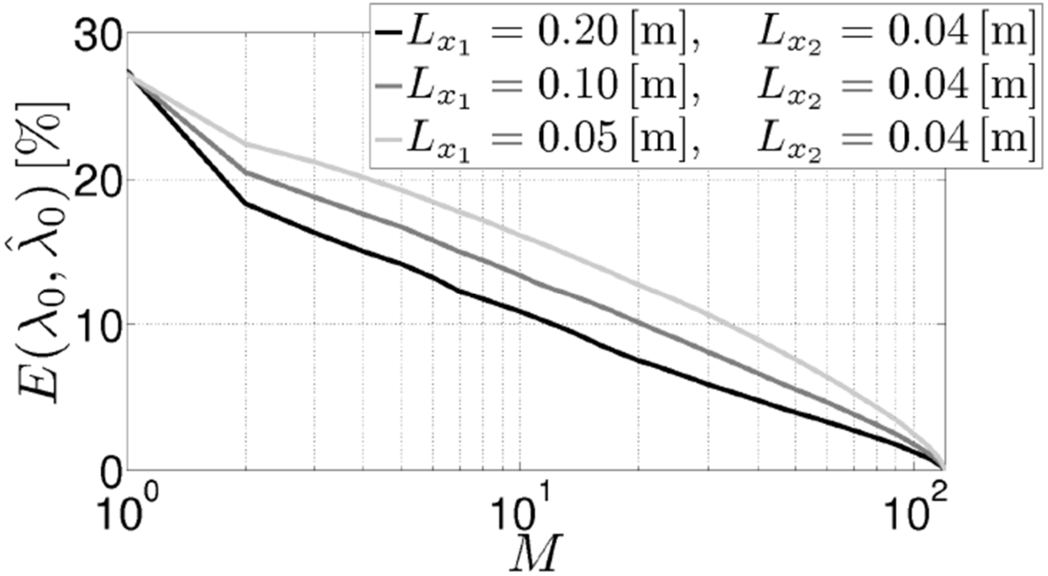
- Exponential covariance kernel $C(\boldsymbol{x},\boldsymbol{x}') = \sigma^2 \mathrm{e}^{-\left|\frac{x-x'}{L_x}\right| - \left|\frac{y-y'}{L_y}\right|}$
- Lognormal random field with second order statistics:

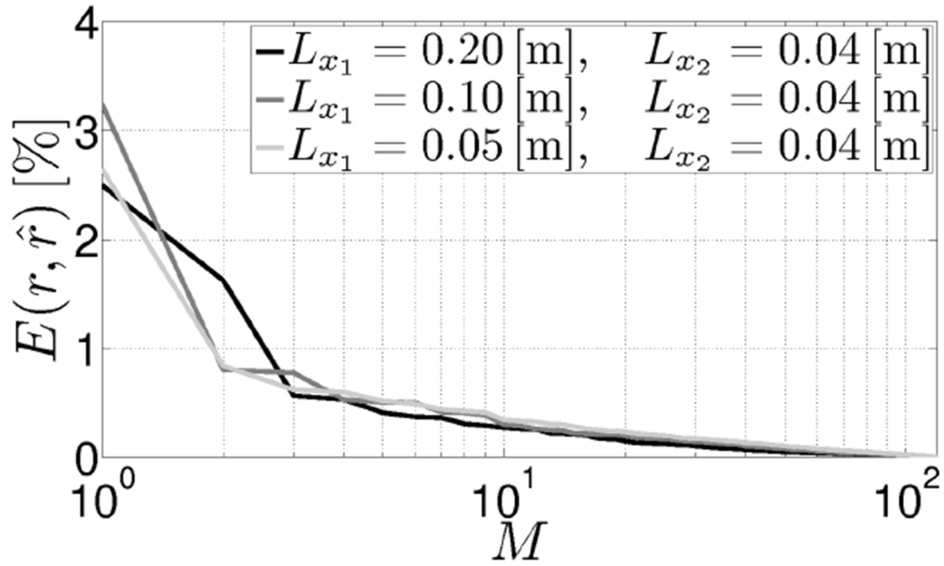
parameter	w_f [kgm^{-3}]	w_{80} [kgm^{-3}]	λ_0 [Wm^{-1}K^{-1}]	b [-]	ρ_s [kgm^{-3}]	μ [-]	A [kgm^{-2}s$^{-0.5}$]
Mean	75	25	0.3	10	1700	20	0.2
Std	15	5	0.06	2	340	4	0.04

$M = 7,\ L_x = 0.1$



λ0 [Wm−1K−1]
λ̂0 [Wm−1K−1]
θ − θ̄ [°C]
φ − φ̄ [−]
θ̂ − θ̄ [°C]
φ̂ − φ̄ [−]
y [m]
x [m]
0.08
0
0.1
0.2
0.3
0.98
0.65
0.32
1.5
1
0.5
0.005
0.0
−0.005





$$E(\boldsymbol{q}, \hat{\boldsymbol{q}}) = \frac{1}{100} \sum_{j=1}^{100} \frac{1}{120} \sum_{i=1}^{120} \frac{|q_i(\boldsymbol{\xi}_j) - \hat{q}_i^{(M)}(\boldsymbol{\xi}_j)|}{q_i(\boldsymbol{\xi}_j)}$$

Polynomial chaos expansion

Each material parameter is approximated by KL expansion:

$$\hat{\boldsymbol{q}}_0 = \boldsymbol{\mu} + \sum_{i=1}^{M} \sqrt{\varsigma_i}\, \xi_i\, \boldsymbol{\psi}_i$$

Model response can be approximated by PC expansion:

in i-th node: $\tilde{r}_i(\xi) = \sum_{\alpha} \beta_{\alpha,i} H_\alpha(\xi(\omega)) = \boldsymbol{H}^*(\xi(\omega)) \cdot \boldsymbol{\beta}_i$

in all nodes: $\tilde{\boldsymbol{r}}(\xi) = \sum_{\alpha} \boldsymbol{\beta}_\alpha H_\alpha(\xi(\omega)) = \left(\mathbf{I} \otimes \boldsymbol{H}^*(\xi(\omega))\right) \cdot \boldsymbol{\beta}$

where $\boldsymbol{\beta}^T = \left(\ldots, \boldsymbol{\beta}_i^T, \ldots\right)$ are PC coefficients and $H_\alpha(\xi(\omega))$ are multivariate Hermite polynomials:

$$H_\alpha(\xi(\omega)) = \prod_{j=1}^{\infty} h_{\alpha_j}(\xi_j(\omega))$$

[e.g. Ghanem & Spanos, 1991, SFE
or Matthies & Keese, 2005, CMAME]

Enthalpy at i-th triangular element becomes:

$$\widetilde{H}_i\left(\widetilde{\boldsymbol{\theta}}(\xi)\right)=\hat{\rho}_s(\xi)c_s(\xi)\frac{1}{3}\sum_{j=1}^{3}\widetilde{\theta}_{i,j}(\xi)=$$

$$=\left(\mu_{\rho_s}+\sum_{j=1}^{M}\sqrt{\varsigma_{\rho_s,j}}\,\xi_j\boldsymbol{\psi}_j\right)\left(\mu_{c_s}+\sum_{j=1}^{M}\sqrt{\varsigma_{c_s,j}}\,\xi_j\boldsymbol{\psi}_j\right)\left(\frac{1}{3}\sum_{j=1}^{3}\boldsymbol{H}^*\xi\cdot\boldsymbol{\beta}_j\right)$$

Balance equation becomes:

$$\mathbf{K}\left(\boldsymbol{\beta},\xi(\omega)\right)\otimes\boldsymbol{H}^*\left(\xi(\omega)\right)\cdot\boldsymbol{\beta}-\boldsymbol{q}_{ext}=\boldsymbol{0}$$

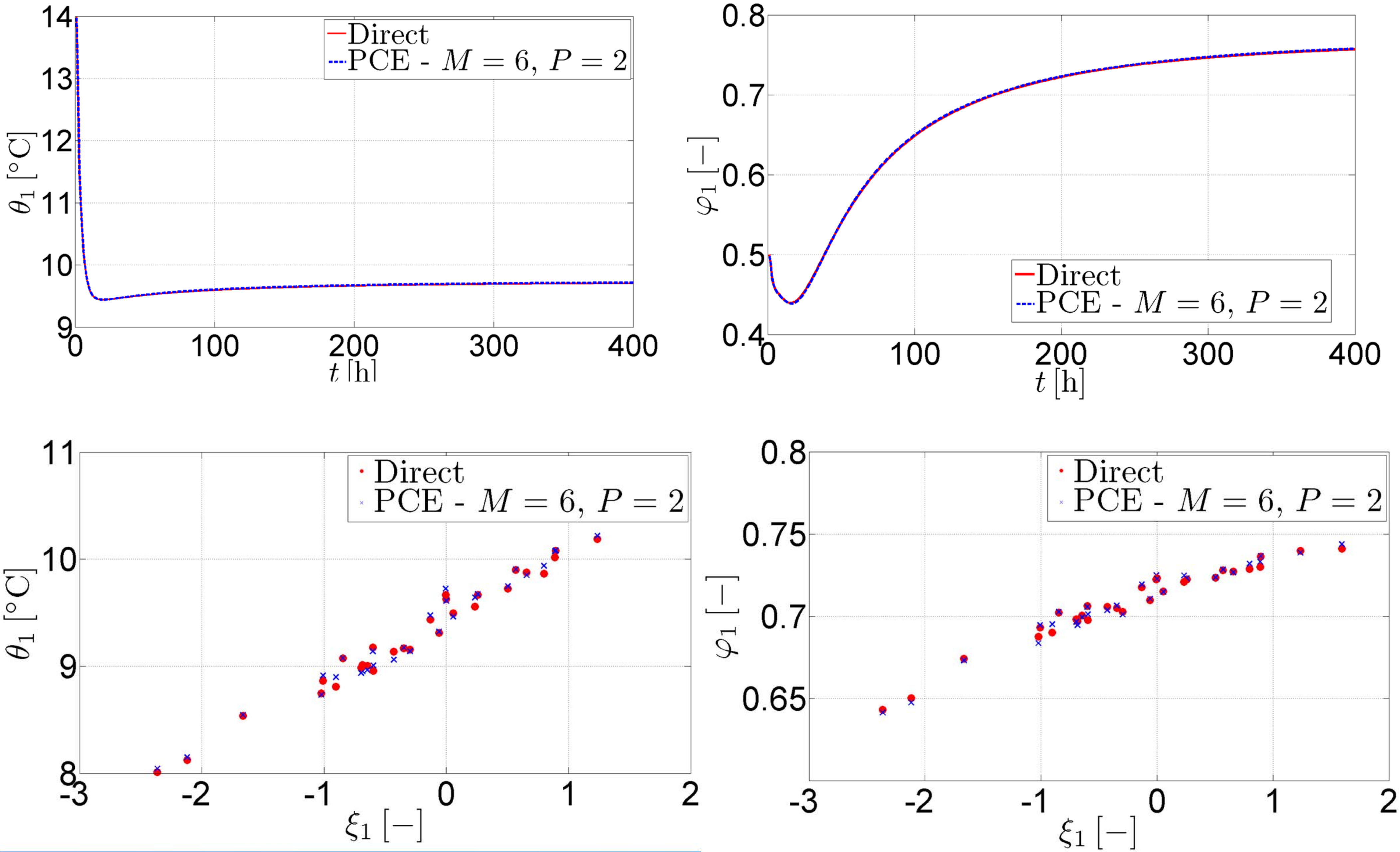
and can be solved using Galerkin projection:

$$\int_{\Omega}\boldsymbol{H}\left(\xi(\omega)\right)\otimes\mathbf{K}\left(\boldsymbol{\beta},\xi(\omega)\right)\otimes\boldsymbol{H}^*\left(\xi(\omega)\right)\mathrm{dP}(\omega)\cdot\boldsymbol{\beta}-$$

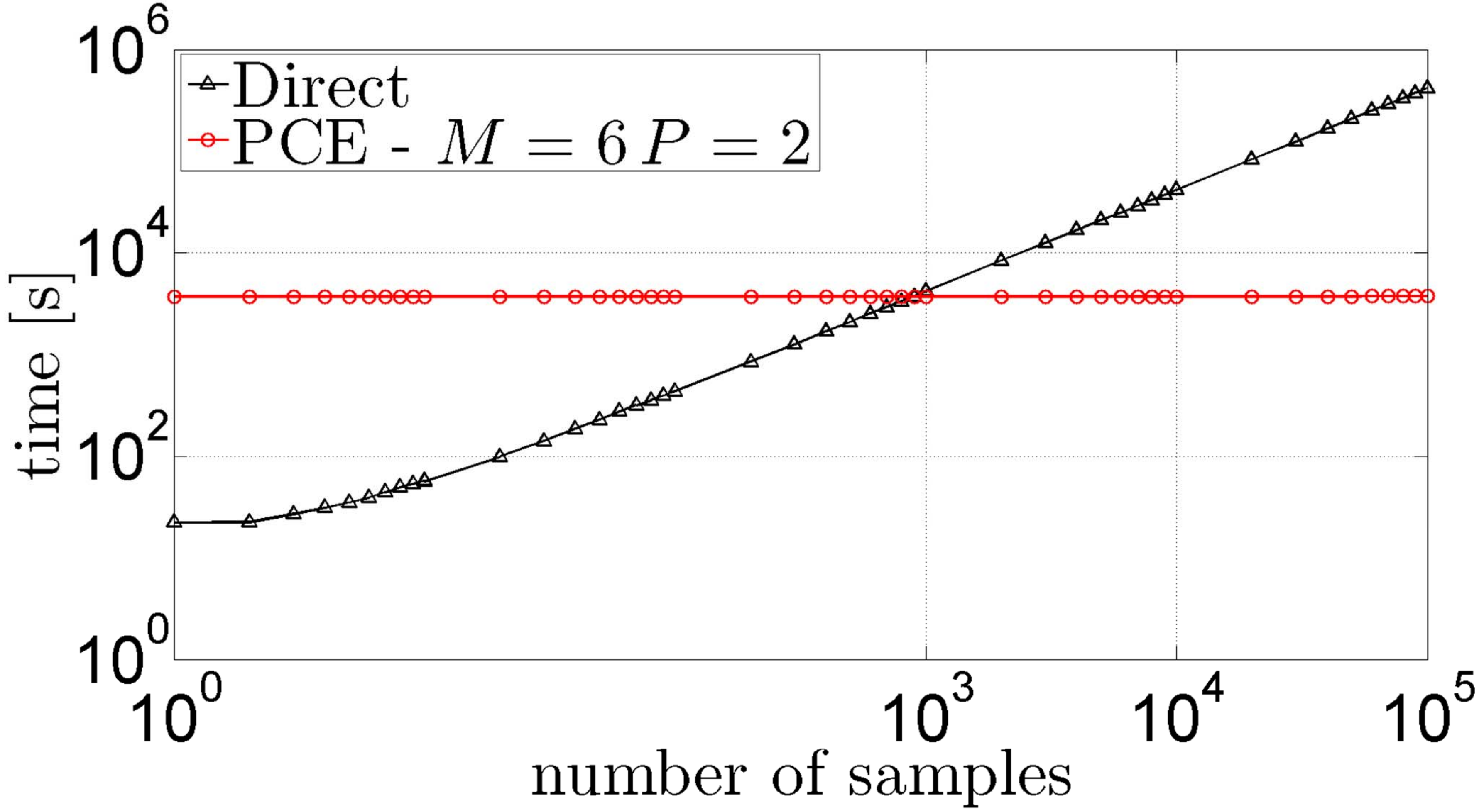
$$-\int_{\Omega}\boldsymbol{H}\left(\xi(\omega)\right)\mathrm{dP}(\omega)\otimes\boldsymbol{q}_{ext}=\boldsymbol{0}$$

Nonlinear system is solved by Newton-Raphson method.

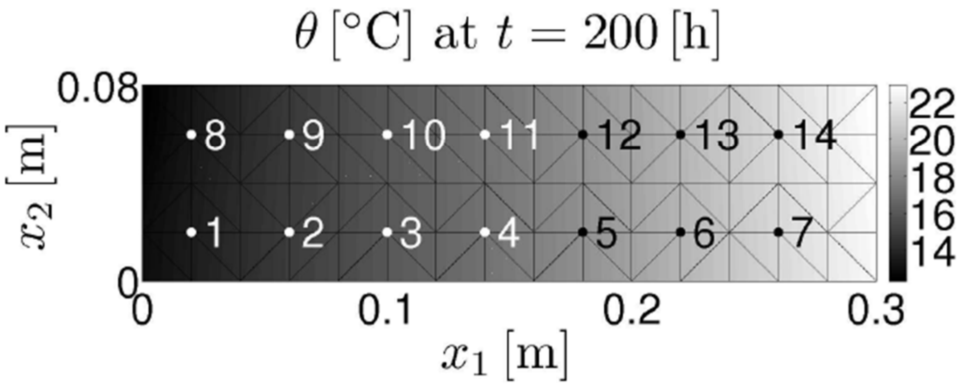
PCE - accuracy

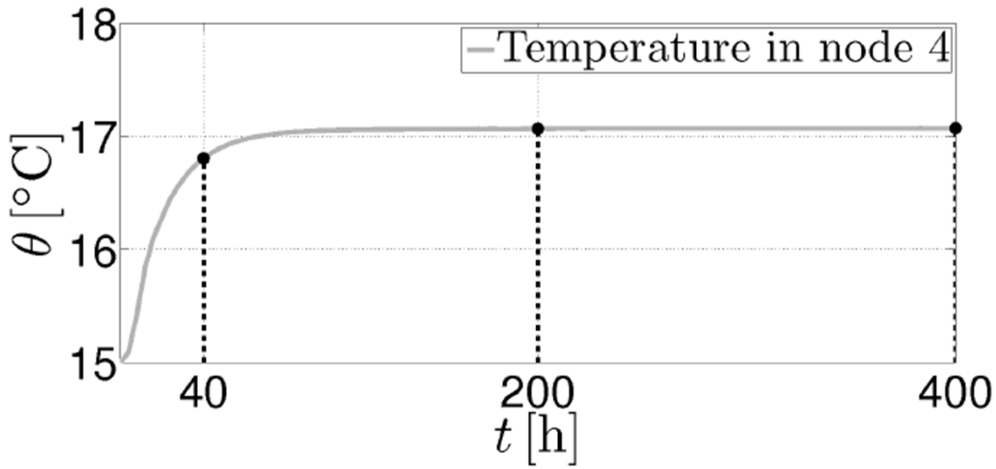


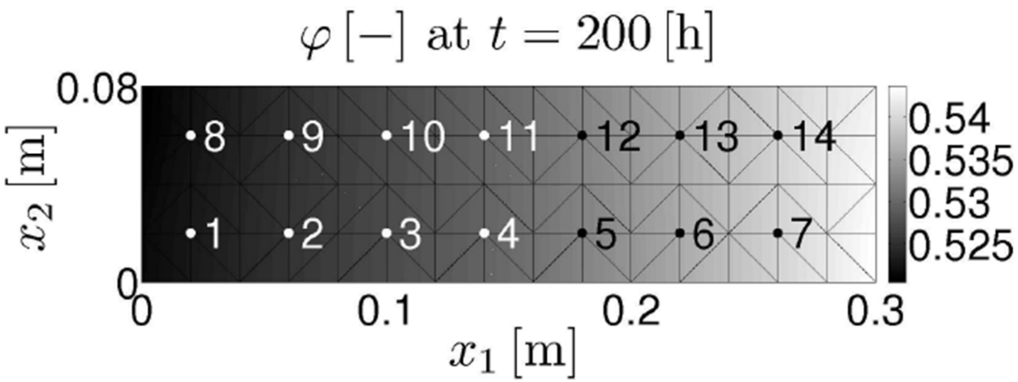
PCE - acceleration

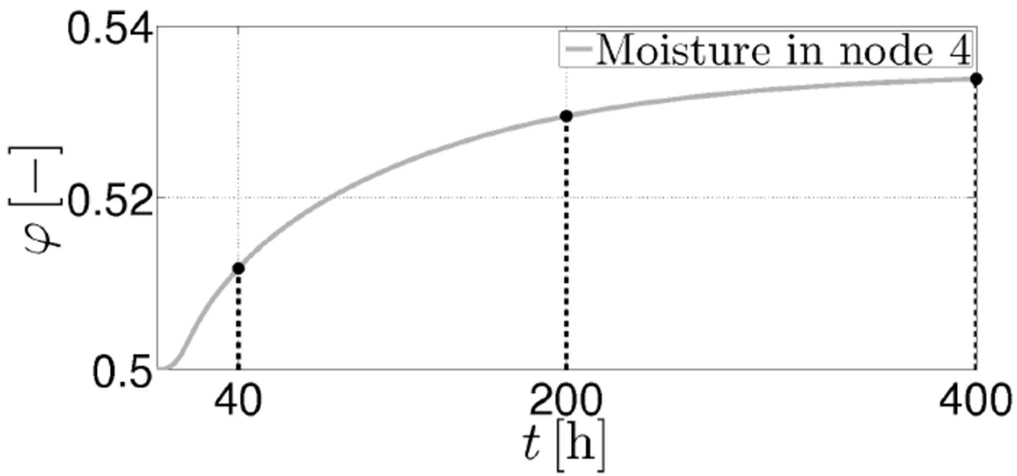


Experimental setup

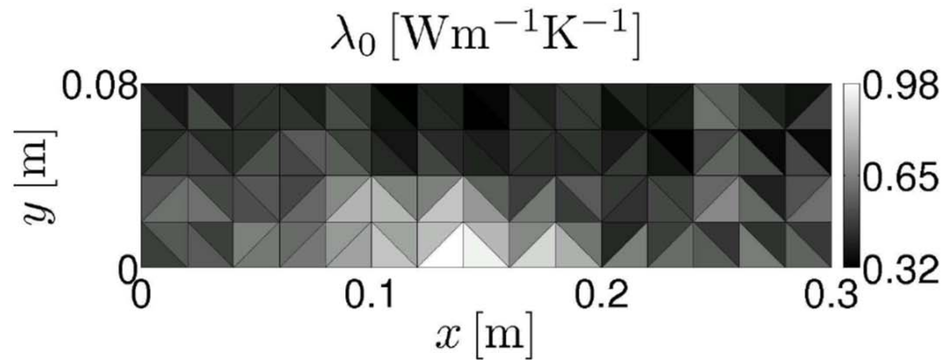








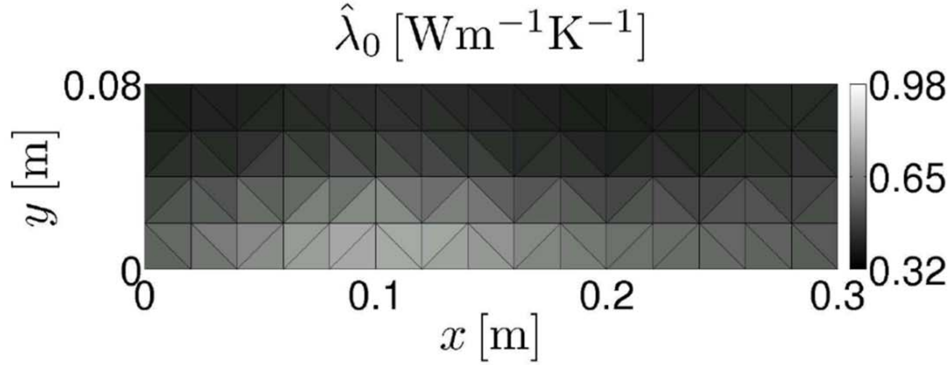
Bayesian update

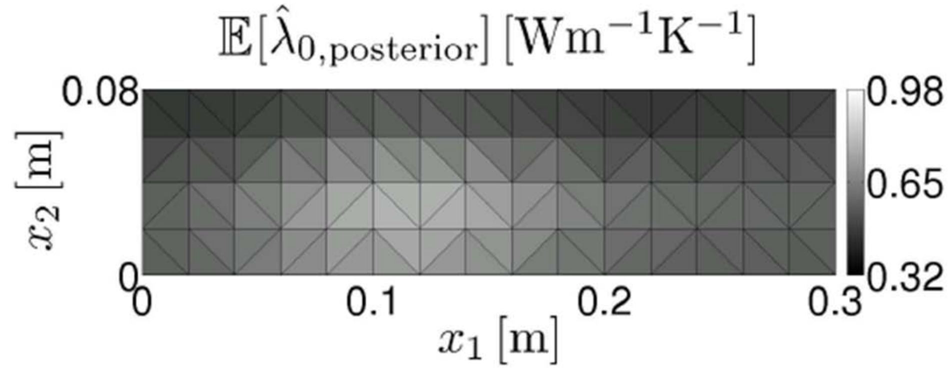


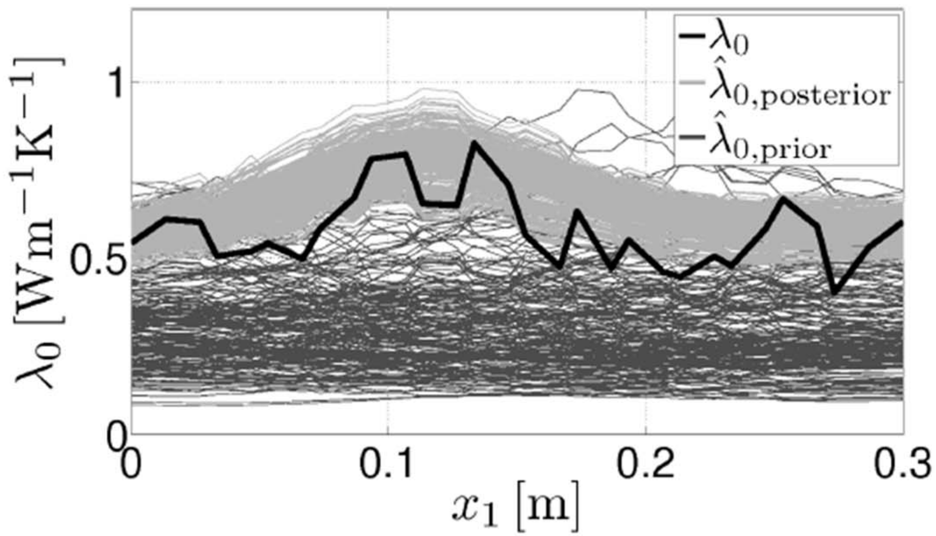
$$L_x = 0.1\,\mathrm{m}, L_y = 0.04\,\mathrm{m}$$

$$M = 7$$

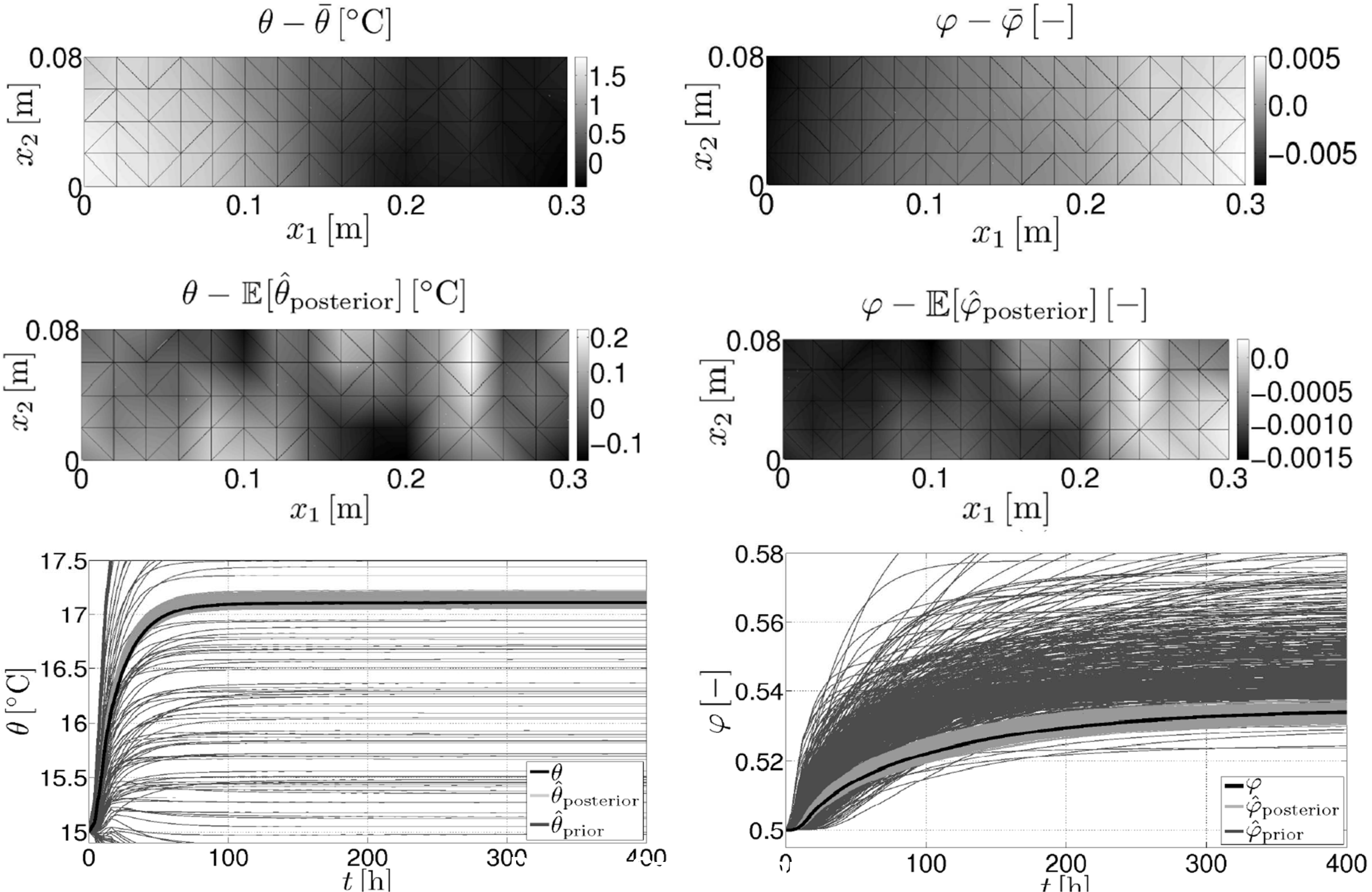
80000 samples







Bayesian update



Conclusions and future perspectives

- Bayesian approach provides a foundation for inference from noisy and limited data
- Karhunen-Loève expansion enables an efficient description of input parameters defined as random field
- Polynomial chaos expansion can be used to approximated the model response and accelerate the Bayesian inference even for highly nonlinear models

Future work:

- More reliable description of correlated input random fields