Surrogate-based Bayesian Inversion for the Model Calibration of Fire Insulation Panels

Author(s):
Wagner, Paul-Remo; Fahrni, Reto; Klippel, Michael; Sudret, Bruno

Publication date:
2018-04

Permanent link:
https://doi.org/10.3929/ethz-b-000279670

Surrogate-based Bayesian Inversion for the Model Calibration of Fire Insulation Panels

P.-R. Wagner[a], R. Fahrni[b], M. Klippel [b], B. Sudret[a]

[a]Chair of Risk, Safety and Uncertainty Quantification - ETH Zürich
[b]Chair of Timber Structures - ETH Zürich

SIAM UQ 2018, Garden Grove, California, USA, 16.04.2018

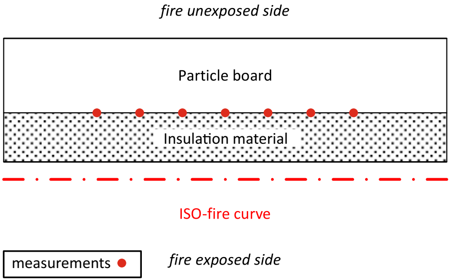
Motivation

Efficient inversion

Timber engineering relies on accurate model calibration for:

- simulation of fire hazards (component additive method)
- code based design

Experiments are carried out under standardized conditions for different insulation materials.



Breu (2016), Isofloc Insulation

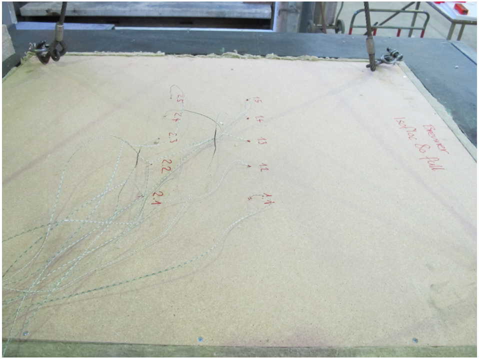
Motivation

Efficient inversion

Timber engineering relies on accurate model calibration for:

- simulation of fire hazards (component additive method)
- code based design

Experiments are carried out under standardized conditions for different insulation materials.



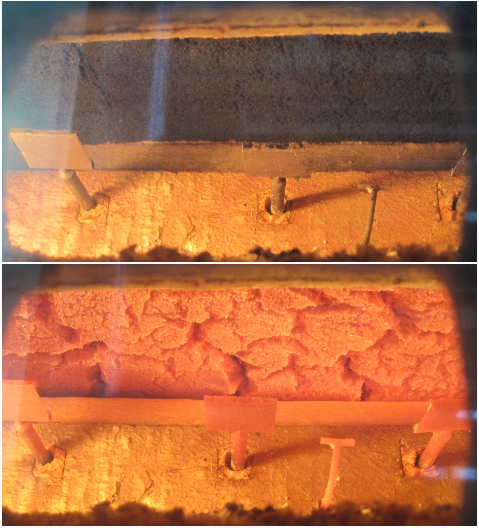
Motivation

Efficient inversion

Timber engineering relies on accurate model calibration for:

- simulation of fire hazards (component additive method)
- code based design

Experiments are carried out under standardized conditions for different insulation materials.



Motivation

Efficient inversion

Timber engineering relies on accurate model calibration for:

- simulation of fire hazards (component additive method)
- code based design

Experiments are carried out under standardized conditions for different insulation materials.

Outline

Experimental data and forward model

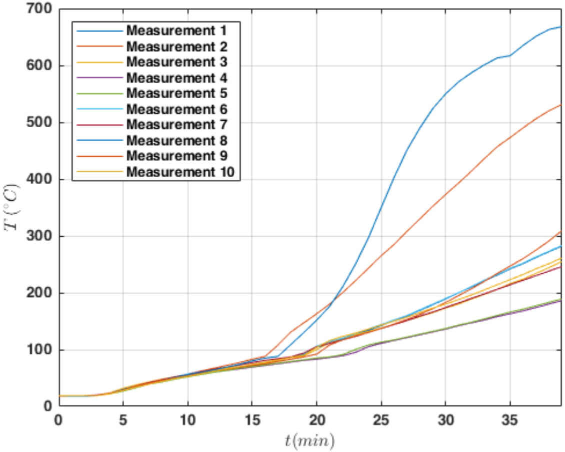
Experimental data y

Huge variations in measurements due to:

- cracking
- inhomogeneous insulation material

Forward model $\mathcal{M}(X)$

1D heat transfer problem with temperature dependent effective material parameters solved with FEM.



Experimental data and forward model

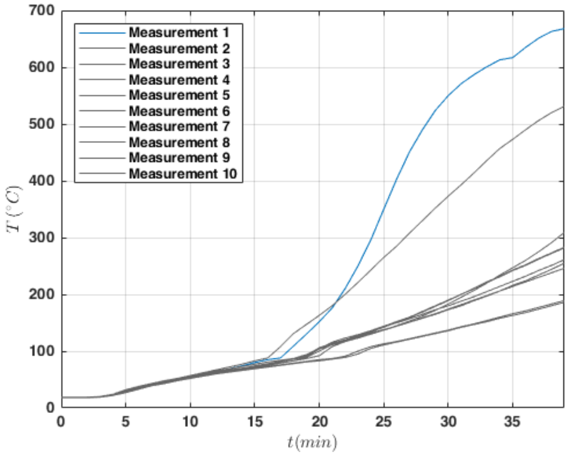
Experimental data y

Huge variations in measurements due to:

- cracking
- inhomogeneous insulation material

Forward model $\mathcal{M}(X)$

1D heat transfer problem with temperature dependent effective material parameters solved with FEM.



Experimental data and forward model

Experimental data $\boldsymbol{y}$

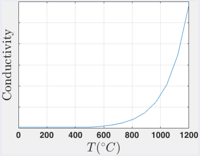
Huge variations in measurements due to:

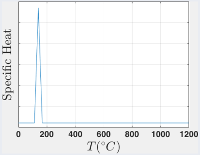
- cracking
- inhomogeneous insulation material

Forward model $\mathcal{M}(\boldsymbol{X})$

1D heat transfer problem with temperature dependent effective material parameters solved with FEM.

Temp. dependent parameters



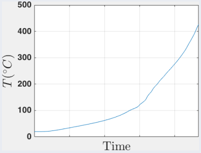


$\Rightarrow$

$\mathcal{M}(\boldsymbol{x})$

$\Rightarrow$

output temperature



Inverse problem

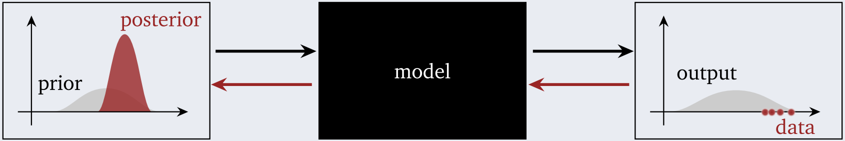
Bayes' theorem

With observed data regarded as $\boldsymbol{Y}|\boldsymbol{x} \sim \pi(\boldsymbol{y}|\boldsymbol{x})$

$$\pi(\boldsymbol{x}|\boldsymbol{y}) \propto \pi(\boldsymbol{y}|\boldsymbol{x})\pi(\boldsymbol{x})$$

with the Posterior $\pi(\boldsymbol{x}|\boldsymbol{y})$, the Prior $\pi(\boldsymbol{x})$ and the Likelihood $\pi(\boldsymbol{y}|\boldsymbol{x})$

Black-Box model



Prior in insulation problem

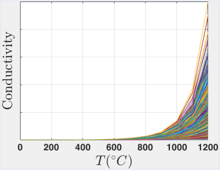
Parametrization

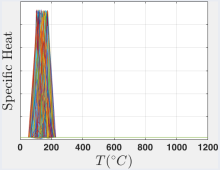
Define prior $\pi(\boldsymbol{x})$ on temp. dependent parameter curve parameters:

$$\boldsymbol{x} \sim \mathcal{U}(\boldsymbol{x}_l, \boldsymbol{x}_u)$$

$\Rightarrow$

Temp. dependent parameters



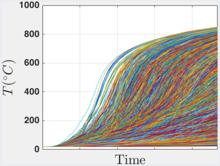


$\Rightarrow$

$\mathcal{M}(\boldsymbol{x})$

$\Rightarrow$

output temperature



Likelihood in insulation problem

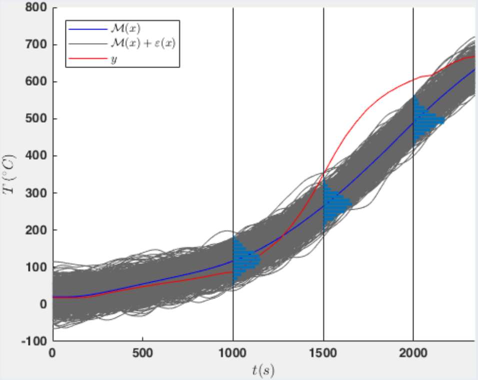
Likelihood function $\pi(\boldsymbol{y}|\boldsymbol{x})$

Pdf of the data $\boldsymbol{y}$ conditioned on the parameters $\boldsymbol{x}$ as a function of these parameters:

$$\boldsymbol{Y}|\boldsymbol{x} \sim \mathcal{N}(\mathcal{M}(\boldsymbol{x}) - \boldsymbol{y}, \boldsymbol{\Sigma}(\boldsymbol{x}))$$

Normal distribution describes the discrepancy between the model predictions $\mathcal{M}(\boldsymbol{x})$ and the observed data $\boldsymbol{y}$.

Experimental curve vs. predictions



Outline

Inversion with surrogate forward modelling

Method

Two-stage procedure:

- build a sufficiently accurate surrogate model of $\mathcal{M}(\boldsymbol{X})$
  1. run N forward runs of $\boldsymbol{y} = \mathcal{M}(\boldsymbol{x})$
  2. construct $\mathcal{M}^{PC}(\boldsymbol{X}) \approx \mathcal{M}(\boldsymbol{X})$
- perform inference
  1. set up a standard method (MAP, MLE, MCMC, etc.)
  2. use $\mathcal{M}^{PC}(\boldsymbol{X})$ instead of $\mathcal{M}(\boldsymbol{X})$

PCE + PCA

Principal Component Analysis

The $N = 235$ output dimensions of $\boldsymbol{Y} = \mathcal{M}(\boldsymbol{X})$ are compressed to $N' = 7$ dimensions of a set of principal components $\boldsymbol{Z}$ through PCA:

$$\log(\boldsymbol{Y}) \approx \bar{\boldsymbol{\mu}}_{\boldsymbol{Y}} + \sum_{p=1}^{N'} \tilde{z}_p(\boldsymbol{X})\bar{\phi}_p$$

with the empirical mean $\bar{\boldsymbol{\mu}}_{\boldsymbol{Y}}$ and a set of N' eigenvectors of the empirical covariance matrix $\bar{\phi}_p$ of $\log(\boldsymbol{Y})$.

Polynomial Chaos Expansion

The N' retained principal components are expanded using an orthogonal polynomial basis $\boldsymbol{\Psi}_{\boldsymbol{\alpha}}(\boldsymbol{X})$:

$$\tilde{z}_p(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}^M} a_{p,\boldsymbol{\alpha}} \boldsymbol{\Psi}_{\boldsymbol{\alpha}}(\boldsymbol{X}) \approx \sum_{\boldsymbol{\alpha}\in\mathcal{A}_\gamma} a_{p,\boldsymbol{\alpha}} \boldsymbol{\Psi}_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

Surrogate model $\mathcal{M}^{PC}(\boldsymbol{x})$

$\mathcal{M}^{PC}(\boldsymbol{x})$

- After computing the coefficients the response random vector can be represented as:

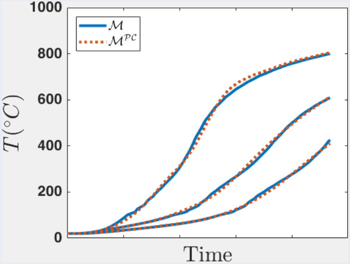
$$\boldsymbol{Y} \approx \exp\left[\bar{\boldsymbol{\mu}}_{\boldsymbol{Y}} + \sum_{p=1}^{N'}\left(\sum_{\boldsymbol{\alpha}\in\mathcal{A}_\gamma} a_{p,\boldsymbol{\alpha}}\boldsymbol{\Psi}_{\boldsymbol{\alpha}}(\boldsymbol{X})\right)\bar{\phi}_p\right]$$

which can be used as a metamodel for $\mathcal{M}(\boldsymbol{x})$.

- The transformation to the log-space assures:

$$\mathcal{M}^{PC}(\boldsymbol{x}) \in \mathbb{R}_+^N$$

Comparison of $\mathcal{M}$ and $\mathcal{M}^{PC}$



The surrogate model is accurate enough!

MCMC

Solution of the inverse problem

We are interested in sampling from the posterior distribution $\pi(\boldsymbol{x}|\boldsymbol{y})$:

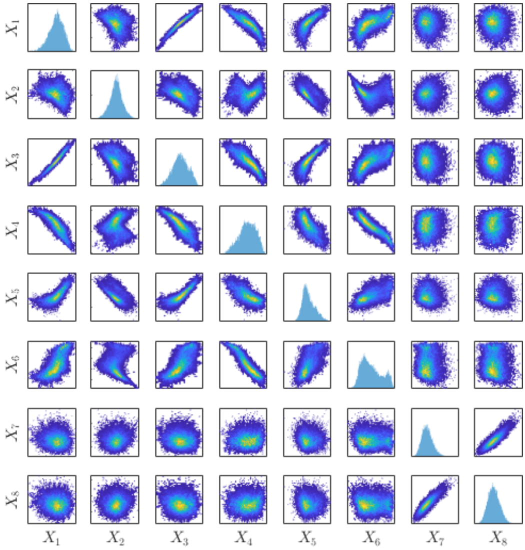
$$\boldsymbol{X}|\boldsymbol{y} \sim \pi(\boldsymbol{x}|\boldsymbol{y})$$

AIES

We use the affine-invariant ensemble sampler (AIES) presented in Goodman, Weare (2010)

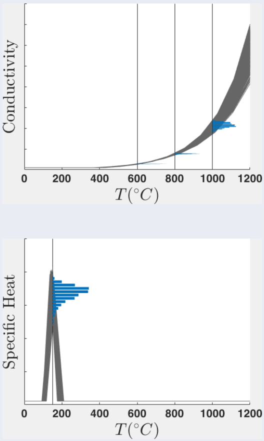
+ invariant under affine transformations of the target distribution
+ multiple parallel chains simultaneously explore the target distribution
+ little tuning necessary
− slow (no parallelization)

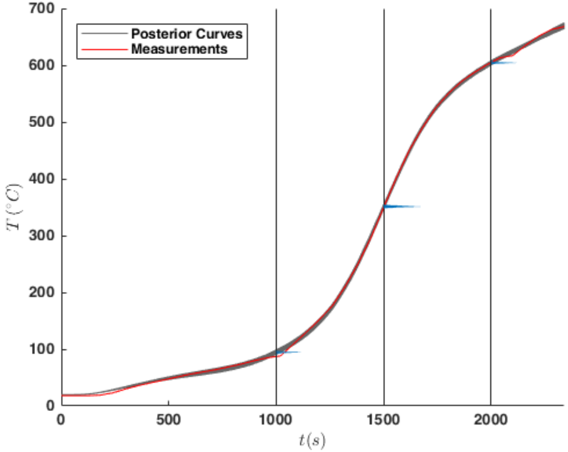
Posterior distribution $\pi(\boldsymbol{x}|\boldsymbol{y})$



Posterior curves

Posterior Parameters





Outline

Inversion with surrogate likelihood

Method

One-stage procedure:

- build sufficiently accurate surrogate model of $\pi(\boldsymbol{y}|\boldsymbol{x})$
  1. run N forward runs of $\mathcal{L}(\boldsymbol{x}) = \pi(\boldsymbol{y}|\boldsymbol{x})$
  2. construct $\mathcal{L}^{PC}(\boldsymbol{X}) \approx \mathcal{L}(\boldsymbol{X})$
  3. inference is merely post-processing of $\mathcal{L}^{PC}(\boldsymbol{X})$

Spectral likelihood expansion

directly build a surrogate model for the likelihood:

$$\mathcal{L}(\boldsymbol{X}) \approx \mathcal{L}^{PC}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}_\gamma} a_{\boldsymbol{\alpha}} \boldsymbol{\Psi}_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

Nagel, J. and Sudret, B., Spectral likelihood expansions for Bayesian inference, J. Comp. Phys. (2016)

Spectral likelihood expansion

Inference

- By post-processing the coefficients $a_{\boldsymbol{\alpha}}$, an approximation to the posterior distribution can be derived easily:

$$\pi(\boldsymbol{x}|\boldsymbol{y}) \approx \frac{1}{a_{\mathbf{0}}}\mathcal{L}^{PC}(\boldsymbol{x})\pi(\boldsymbol{x})$$

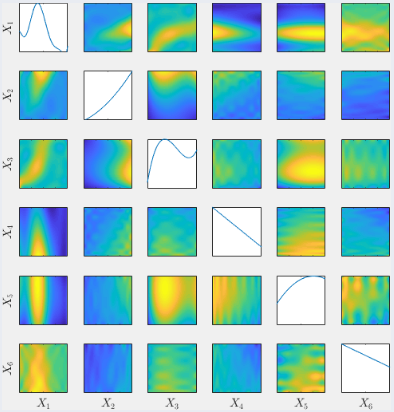
- The posterior moments of the marginals can be derived analytically:

$$\mathrm{E}[X_j|\boldsymbol{y}] \approx \frac{1}{a_{\mathbf{0}}}\left\langle x_j, \mathcal{L}_j^{PC}\right\rangle_{L^2_{\pi_j}}$$

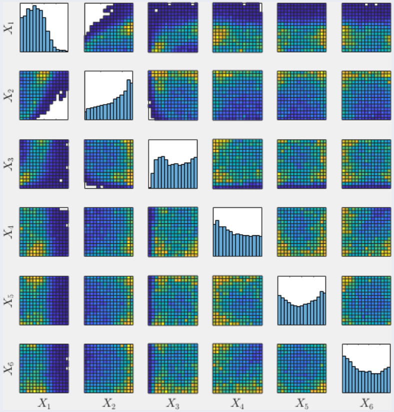
$$\mathrm{Var}[X_j|\boldsymbol{y}] \approx \frac{1}{a_{\mathbf{0}}}\left\langle (x_j - \mathrm{E}[X_j|\boldsymbol{y}])^2, \mathcal{L}_j^{PC}\right\rangle_{L^2_{\pi_j}}$$

Posterior distribution $\pi(\boldsymbol{x}|\boldsymbol{y})$ SLE vs. MCMC

$\pi(\boldsymbol{x}|\boldsymbol{y})$ SLE



$\pi(\boldsymbol{x}|\boldsymbol{y})$ MCMC



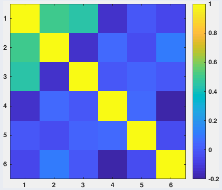
Large model error assumed!

Posterior moments of $\pi(\boldsymbol{x}|\boldsymbol{y})$ SLE vs. MCMC

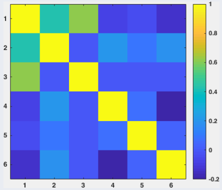
Comparison

	X_1	X_2	X_3	X_4	X_5	X_6
$\mathrm{E}[X_j\|\boldsymbol{y}]_{\mathsf{MCMC}}$	427.4	$3.308 \cdot 10^{-4}$	0.016	$5.12 \cdot 10^{4}$	142	51.11
$\mathrm{E}[X_j\|\boldsymbol{y}]_{\mathsf{SLE}}$	446.5	$3.708 \cdot 10^{-4}$	0.015	$4.431 \cdot 10^{4}$	144	50.3
ε (%)	4.47	12.09	6.25	13.46	1.41	1.58
$\mathrm{Var}[X_j\|\boldsymbol{y}]_{\mathsf{MCMC}}$	$5.667 \cdot 10^{3}$	$1.669 \cdot 10^{-9}$	$6.616 \cdot 10^{-5}$	$1.118 \cdot 10^{9}$	628.1	758.3
$\mathrm{Var}[X_j\|\boldsymbol{y}]_{\mathsf{SLE}}$	$4.707 \cdot 10^{3}$	$9.242 \cdot 10^{-9}$	$6.265 \cdot 10^{-5}$	$8.855 \cdot 10^{8}$	475.3	652.9
ε (%)	20.4	81.94	5.6	26.26	32.15	16.14

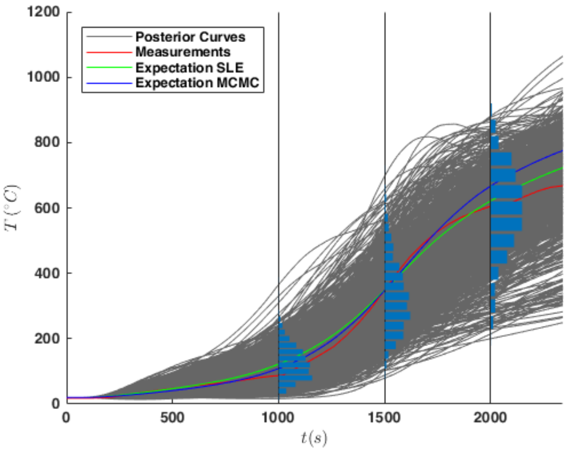
$\rho_{X_iX_j,\mathsf{MCMC}}$



$\rho_{X_iX_j,\mathsf{SLE}}$



Posterior curves



SLE pros/cons

- \+ sampling free
- \+ deterministic approach for inversion
- \+ only one source of error (Quality of PCE)
- – does not work with spiked likelihood functions (yet!)
- – high dimensions (PCE based)

Outline

Conclusion & outlook

- Bayesian inversion is suitable for calibrating transient heat conduction models of fire experiments
- Classical MCMC can be used together with advanced surrogate models (principal component analysis + polynomial chaos expansion)
- Spectral likelihood expansion is a promising, sampling free approach that requires some further tuning
- Multiple experiments shall be combined using hierarchical Bayesian models

www.uqlab.com

Thank You!

Questions?