

**Czech Technical University in Prague**  
Faculty of Civil Engineering

**České vysoké učení technické v Praze**  
Fakulta stavební

**doc. Ing. Anna Kučerová, Ph.D.**

**Probabilistic modelling of material properties**

**Pravděpodobnostní modelování materiálových vlastností**

## SUMMARY

Reliable modeling of heterogeneous materials, such as concrete or composites, requires an accurate probabilistic description of their internal structure, inherent randomness, and associated uncertainties. A crucial step is the extraction of detailed information from digital microstructure images. In this area, the work focuses on representing the heterogeneous microstructure using a set of statistically representative cells that enable the modeling of non-periodic media. To improve their morphology, attention is given to augmenting the commonly used two-point probability by the lineal-path function and its computational acceleration on graphics processing units. Further morphological improvement is offered by the use of Convolutional Neural Networks. Their training, however, requires a sufficiently large dataset, which is typically difficult to obtain for concrete. Therefore, attention is directed towards the automatic phase identification in low-contrast XCT images of concrete using modern deep learning methods and semantic segmentation. To probabilistically capture the internal randomness of the material, a transition from a statistical description to a random field-based description is introduced, enabling the generation of synthetic specimens.

In situations where the probabilistic model needs further refinement or when microstructure images are completely lacking, material properties can be identified by using macroscopic measurements of the material response. The calibration of material models from limited and uncertain data is formulated as an inverse problem solved via Bayesian inference. Its computational demand, stemming from the sampling of posterior uncertainties using Markov chains, was effectively suppressed by employing fast surrogate models based on polynomial chaos. The work presents the inference of both spatially varying properties characterized by random fields and effective parameters for complex nonlinear models, such as the discrete particle model or the macroscopic damage-plasticity model. To adequately capture the inherent randomness of material parameters within a set of specimens and to separate it from the epistemic uncertainty arising from a lack of knowledge, a hierarchical formulation of Bayes' theorem is introduced, alongside an alternative method based on the nonlinear transformation of random variables, which does not require strong prior assumptions about the probability distribution.

Despite persisting theoretical challenges, the developed procedures have found application in engineering practice, e.g., in the calibration of a viscoplastic damage model for metal alloys used in combustion chambers of launchers, or in the identification of thermal boundary conditions and the calibration of a concrete creep model directly from long-term in-situ measurements on the Temelín Nuclear Power Plant containment.

## SOUHRN

Spolehlivé modelování heterogenních materiálů, jako je beton či kompozity, vyžaduje přesný pravděpodobnostní popis jejich vnitřní struktury, vlastní náhodnosti i souvisejících nejistot. Zásadní krok představuje získání detailních informací z digitálních snímků mikrostruktury. Práce se v této oblasti věnuje reprezentaci heterogenní mikrostruktury pomocí souboru statisticky reprezentativních buněk, které umožňují modelovat neperiodické médium. Pro zlepšení jejich morfologie je pozornost věnována doplnění běžně užívané dvoubodové pravděpodobnosti o deskriptor založený na lineární cestě a jeho výpočetnímu urychlení na grafických procesorech. Další zlepšení morfologie nabízí využití konvolučních neuronových sítí, které však pro své natrénování vyžadují dostatečný soubor dat, jenž je u betonu těžko dostupný. Pozornost je proto věnována automatické identifikaci fází v nízkokontrastních XCT snímcích betonu pomocí moderních metod hlubokého učení a sémantické segmentace. Pro pravděpodobnostní uchopení vnitřní náhodnosti materiálu je představen přechod od statistického popisu k popisu založenému na náhodných polích, který umožňuje generování syntetických vzorků i následně zpřesňování pravděpodobnostního modelu při získání nových dat.

V situacích, kdy je nutné pravděpodobnostní model dále zpřesnit, nebo snímky mikrostruktury zcela chybí, vstupují do hry makroskopická měření odezvy materiálu. Kalibrace materiálových modelů z omezených a nejistých dat je formulována jako inverzní problém řešený pomocí Bayesovské inference. Její výpočetní náročnost plynoucí ze vzorkování aposteriorních nejistot Markovovými řetězci byla efektivně potlačena využitím rychlých náhradních modelů založených na polynomiálním chaosu. Práce představuje inferenci jak prostorově proměnných vlastností charakterizovaných náhodnými poli, tak i efektivních parametrů pro komplexní nelineární modely, jako je částicový model či makroskopický model poškození a plasticity. Pro adekvátní zachycení vlastní náhodnosti materiálových parametrů napříč souborem vzorků a její oddělení od epistemické nejistoty plynoucí z nedostatku znalostí je dále představena hierarchická formulace Bayesova teorému a jako alternativa metoda založená na nelineární transformaci náhodných veličin, která nevyžaduje silné počáteční předpoklady o pravděpodobnostním rozdělení.

Navzdory přetrvávajícím teoretickým výzvám nalezly vyvinuté postupy uplatnění v inženýrské praxi, např. při kalibraci viskoplastického modelu poškození kovových slitin využitých ve spalovacích motorech nosných raket nebo při tvorbě prediktivního digitálního dvojčete kontejnmentu Jaderné elektrárny Temelín pro identifikaci nejistých teplotních okrajových podmínek a kalibraci modelu dotvarování betonu přímo z dlouhodobých in-situ měření.

### ***Keywords***

random heterogeneous materials; statistical descriptors; Wang tiles; uncertainty quantification; inverse analysis; parameter identification; Bayesian inference; surrogate models; polynomial chaos; artificial neural networks

### ***Klíčová slova***

heterogenní materiály; statisticky deskriptory; Wangovo dláždění; modelování nejistot; inverzní analýza; identifikace parametrů; Bayesovská inference; náhradní modely; polynomiální chaos; umělé neuronové sítě

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# 1 INTRODUCTION

The accurate characterization and reliable modeling of material properties represent a fundamental step in the multiscale modeling of complex heterogeneous materials, such as concrete, porous media, or composites [Torquato, 2005]. Due to their complex internal structure and inherent variability, traditional deterministic approaches are often insufficient, which is why this text presents a comprehensive framework for the probabilistic modeling of materials, relying on advanced methods for microstructure characterization [Bostanabad et al., 2018] and parameter identification via inverse analysis [Tarantola, 2005].

Methods for material characterization can generally be divided based on their input data into two main categories: those relying on high-resolution scans of the material’s internal structure, and those based on macroscopic response measurements. The methods in the first category use digital image analysis of X-ray computed tomography (XCT) scans to extract key statistical descriptors necessary for the robust reconstruction of computational domains [Bostanabad et al., 2018]. The following section discusses in more detail several computational difficulties encountered in the characterization of materials using image data, such as statistical artifacts arising when the material representation is based on single statistically equivalent periodic cells [Novák et al., 2012] and qualities of alternative statistical descriptors such as the lineal path function [Havelka et al., 2016]. Furthermore, it addresses the challenge of the automatic segmentation of low-contrast concrete images [Das et al., 2026], which is crucial for obtaining a sufficient amount of data for subsequent analysis and the creation of a credible material representation. While representations based on one or multiple statistically representative cells rely purely on a statistical description of the input images—resulting in a domain that is either entirely deterministic (in the case of a single periodic cell) or generated by a stochastic assembly of a predefined set of cells—a powerful alternative is the probabilistic description discussed at the end of the chapter. In this approach, specific spatial characteristics, such as correlation lengths or eigenfunctions characterizing the arrangement of material phases, are derived from the statistical descriptors, but the material morphology itself is formulated probabilistically using random fields [Kučerová, 2020, Šilhánek, 2021]. Crucially, this probabilistic formulation opens the possibility for further systematic refinement of the material description based on macroscopic measurements, seamlessly bridging to the second category of methods.

This second category of methods addresses a fundamental bottleneck of probabilistic modeling: the precise prior probability distributions of the input parameters are often highly uncertain, but they can be updated by using

additional data from macroscopic testing of the material or data collected from probes placed on the existing structure. Once such measurements are performed, inverse analysis based on Bayesian inference [Tarantola, 2005, Gelman et al., 2013] can be employed to systematically update the initial probabilistic models. The subsequent chapter details this Bayesian framework and addresses the computational exhaustion associated with traditional sampling methods, such as Markov chain Monte Carlo (MCMC). It demonstrates how to significantly accelerate the identification process using dimensionality reduction via the Karhunen-Loève Expansion [Marzouk and Najm, 2009, Havelka et al., 2019] and fast surrogate models based on Polynomial Chaos Expansion (PCE) [Marzouk et al., 2007, Kučerová and Sýkora, 2013]. Ultimately, these advanced stochastic tools provide a robust mechanism not only for updating the probabilistic description via random fields, but also for identifying effective material properties as demonstrated on calibration of advanced concrete failure models [Janouchová et al., 2021, Kučerová et al., 2023].

The aforementioned probabilistic description—whether using random fields to characterize spatial variations within an existing structure or random variables to represent effective material properties—reflects epistemic uncertainty arising from a lack of knowledge and data. It assumes that the sought material characteristics possess a true, deterministic value that simply cannot be determined with absolute certainty. The final part of the chapter, however, addresses a more complex formulation of the probabilistic material description, where material properties are considered inherently random, meaning they genuinely vary across individual specimens. The goal then becomes to identify their underlying probability distribution, which is itself uncertain, thus explicitly distinguishing between the inherent randomness of the properties (aleatory uncertainty) and the lack of knowledge (epistemic uncertainty) [Kočková and Kučerová, 2026].

## **2 MICROSTRUCTURE CHARACTERIZATION FOR RANDOM HETEROGENEOUS MATERIALS**

Microstructure characterization is a fundamental step in the multiscale modeling of heterogeneous materials such as concrete, porous media, or composites [Torquato, 2005]. Current state-of-the-art procedures rely primarily on digital image analysis (e.g., from XCT scans), which allows for the extraction of key statistical descriptors—most notably  $n$ -point probability functions, phase size distributions, or lineal-path functions [Bostanabad et al., 2018]. These methods aim to define a Statistically Representative Volume Element (SVE) that faithfully represents the effective properties of the real material in a numerical model, see [Bargmann et al., 2018] for a thorough review of SVE

generation. Traditionally, this is achieved through a Statistically Equivalent Periodic Unit Cell (SEPUC) [Zeman and Šejnoha, 2007], which is optimized to minimize the discrepancy between the statistical characteristics of the real specimen and its idealized periodic representation.

However, relying on a single periodic cell (SEPUC) introduces several computational and physical artifacts. The most significant is the artificially imposed periodicity, which does not reflect the inherent randomness of real-world materials. This can lead to systematic errors in predicting localized failure or transport processes where the directional orientation of the microstructure is crucial. Furthermore, the size of a SEPUC is always a compromise: a cell that is too small fails to capture long-range correlations, while one that is large enough to be truly representative significantly increases computational costs.

### 2.1 Aperiodic Microstructure Representation via Stochastic Wang Tilings

To overcome the limitations associated with a single periodic unit cell, a modern alternative based on the concept of stochastic Wang tilings has been proposed [Novák et al., 2012]. Instead of relying on a single, heavily compromised representative cell, this approach utilizes a small, finite set of distinct square domains—Wang tiles—to compress and reconstruct disordered microstructures, see Fig. 2.2. Originally introduced in discrete mathematics, Wang

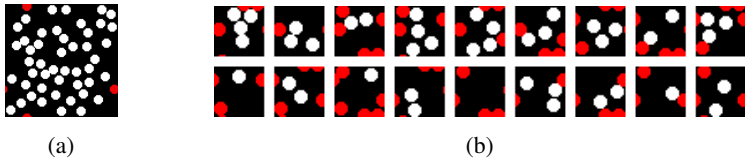


Figure 2.1: Building blocks of microstructure compression based on (a) a PUC and (b) a set of 18 Wang tiles with 49 disks assigned to tile edges (red) and interiors (white). Novák et al. [2012]

tiles are defined by specific edge codes that permit their mutual assembly strictly in a geometrically compatible manner, meaning that the morphological patterns on contiguous boundaries must always match.

Unlike the deterministic periodic extension of a SEPUC, Wang tiles are assembled to cover macroscopic domains using a fast stochastic tiling algorithm (such as the Cohen-Shade-Hiller-Deussen algorithm). This stochastic assembly ensures that the resulting generated microstructure is strictly aperiodic, effectively mitigating the strong, repetitive long-range correlations that are inevitably tied to the dimensions of a single unit cell. Consequently, this

concept allows for the synthesis of arbitrarily large, naturally looking microstructural domains that accurately reproduce long-range orientation orders at a negligible computational cost.

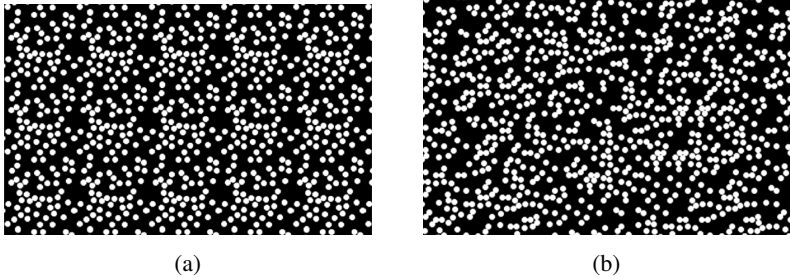


Figure 2.2: Microstructures assembled from (a) a PUC and (b) a set of 18 Wang tiles. Novák et al. [2012]

Similarly to the SEPUC generation, the internal morphological features of the Wang tiles are carefully designed through an optimization procedure to match the target spatial statistics of the real material, most commonly evaluated via the two-point probability function. Furthermore, to be applicable in advanced multiscale computations (such as generalized partition of unity or hybrid Trefftz finite element schemes), the tiles can be optimized not only for geometric statistics but also to ensure that microstructural enrichment functions (e.g., stress or traction fluctuations) remain compatible across the contiguous tile edges. This tiling-based representation thus maintains consistency in both the statistical properties of the random morphology and the continuity of the synthesized mechanical fields across the entire non-periodic macroscopic domain [Novák et al., 2013].

## **2.2 Enhancing Microstructural Representation via Accelerated Lineal-Path Function**

While the aforementioned stochastic Wang tilings and periodic unit cells are most commonly optimized using the two-point probability function [Karsanina et al., 2015], this statistical descriptor has inherent limitations. Specifically, it often struggles to accurately capture phase-connectedness and specific short-range morphological features, such as the precise shape of solid particles or thin continuous walls.

A superior alternative for characterizing these short-range effects and preserving phase continuity is the lineal-path function [Li et al., 2012]. However, its application in microstructural compression and reconstruction has

historically been restricted by its enormous computational requirements. Consequently, past approaches often had to rely on rough Monte Carlo-based approximations that introduce slow convergence and significant geometric errors into the reconstructed microstructures. To overcome this critical bottleneck, an accelerated numerical evaluation of the entire lineal-path function was developed by porting the core algorithm to a graphics processing unit (GPU) using the CUDA programming environment as presented in [Havelka et al., 2016]. This massive acceleration makes it computationally feasible to employ the exact lineal-path function within exhaustive iterative optimization processes. By utilizing this accelerated descriptor, the optimization procedure successfully preserves complex geometric shapes and continuous phase features that the standard two-point probability function systematically fails to capture, see Fig. 2.3.

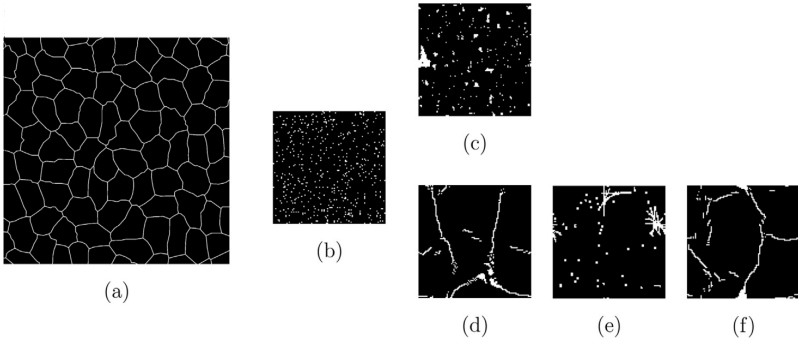


Figure 2.3: Epithelial cells: (a) original medium; (b) random initial structure; (c) compressed  $S_2$ -based image; (d) compressed  $L_2^b$  and  $L_2^w$ -based image; (e) compressed  $L_2^w$ -based image; (f) compressed  $L_2^b$ -based image. Havelka et al. [2016]

### 2.3 Data Scarcity and Semantic Segmentation in Concrete

Before statistical descriptors can be extracted and utilized for microstructure reconstruction or compression, the raw digital images (such as XCT scans) must be precisely partitioned into distinct material phases. In multiphase materials like concrete, this pre-characterization step poses a unique and fundamental challenge. The core of the problem lies in the fact that concrete aggregates and mortar exhibit very similar X-ray attenuation coefficients, resulting in extremely low-contrast grayscale images where phase boundaries are difficult to discern, see Fig. 2.4a.

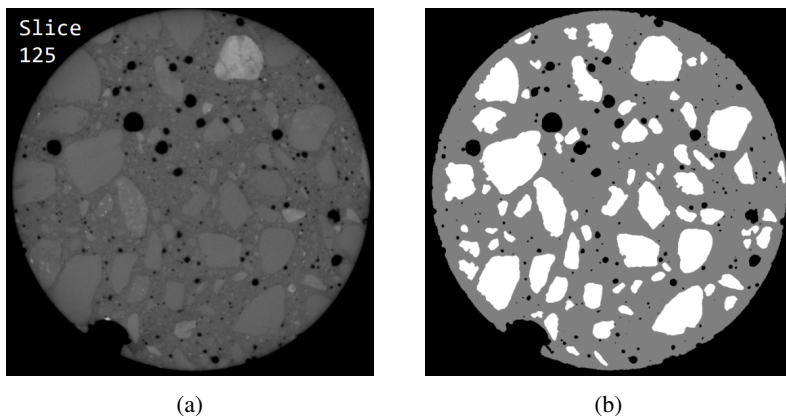


Figure 2.4: XCT slice of concrete (a) and its segmented representation (b). Das et al. [2026]

While deep Convolutional Neural Networks (CNNs) represent the current state-of-the-art for image segmentation, their standard application is heavily dependent on supervised learning [Werner et al., 2025]. This means they require massive amounts of precisely annotated (labeled) training data. In materials science, and particularly for new XCT datasets of concrete, such labeled ground truths are exceedingly rare, largely unavailable, and practically too resource-intensive to produce manually.

To bypass this critical lack of labeled data, recent advancements are shifting towards unsupervised semantic segmentation approaches. Therefore, self-annotation methodologies have been successfully introduced to process low-contrast concrete XCTs in [Das et al., 2026]. The core of this approach relies on combining a U-Net architecture (Fig. 2.5) with a self-annotation pipeline based on superpixels. Initially, the raw image is partitioned into perceptually similar, spatially contiguous local regions—superpixels—using algorithms like SLIC [Achanta et al., 2010]. Unlike supervised learning, which minimizes a standard cross-entropy loss against fixed target labels, this unsupervised framework employs a dynamically evolving target label. During each training iteration, the CNN predicts pixel-wise class probabilities. These predictions are then constrained by the predefined superpixels to enforce spatial contiguity: the most frequently predicted class within a given superpixel is uniformly assigned to all its pixels, thereby creating a "dynamic image label" for that specific iteration.

The network's parameters are subsequently updated by minimizing a modified cross-entropy loss function formulated using these dynamic labels.

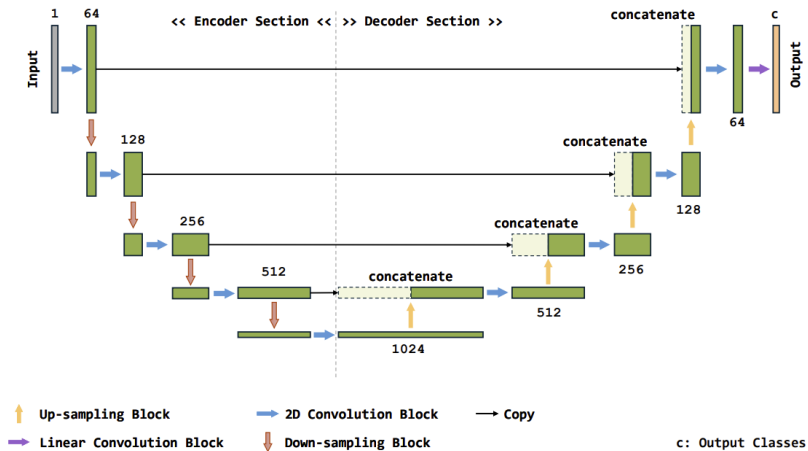


Figure 2.5: The U-Net model architecture. Das et al. [2026]

By iteratively updating both the model weights and the target labels, see Fig. 2.6, the network learns global-local spatial relationships and autonomously

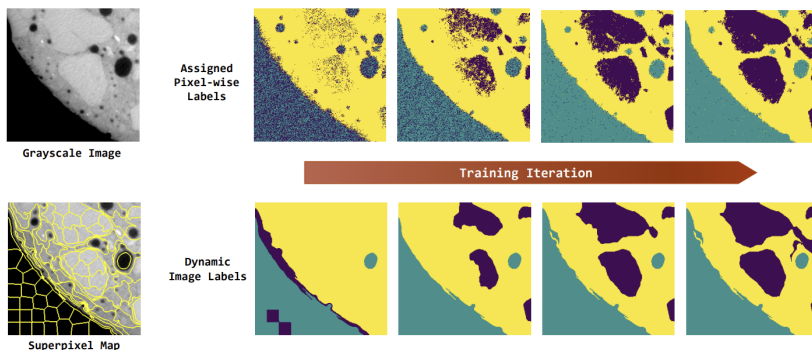


Figure 2.6: The U-Net model architecture. Das et al. [2026]

identifies semantically similar structures. This fully unsupervised capability allows for reliable separation of aggregates, mortar, and porosity (cf. Fig. 2.4b) without any reliance on pre-annotated training datasets, providing a crucial enabler for subsequent high-throughput multiscale modeling.

## 2.4 Generation of Concrete Microstructures: Random Fields and Deep Learning

While the aforementioned techniques address the characterization and segmentation of existing microstructures, generating entirely new computational domains for concrete brings its own set of challenges. One traditional statistical approach to modeling the spatial variability of heterogeneous materials utilizes random fields. A prominent technique in this domain is the Karhunen-Loève Expansion (KLE), which generates samples of a random field based on a covariance function and a set of underlying random variables [Lombardo et al., 2009]. The eigenfunctions (see Fig. 2.7) and corresponding samples

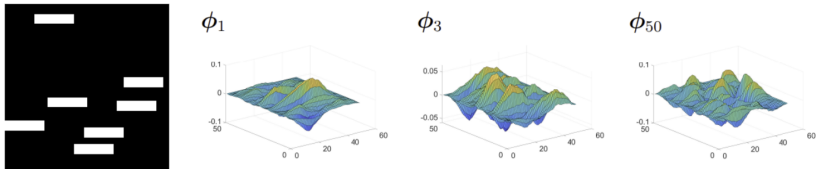


Figure 2.7: Illustrative two-phase medium and its first, third, and 50<sup>th</sup> eigenfunctions. Šilhánek [2021]

of eigenvariables can be derived from image analysis as presented e.g. in Bachelor thesis [Šilhánek, 2021] written in Czech or in Habilitation thesis [Kučerová, 2020]. Alternatively, recent advancements proposed in [Das et al., 2025] utilize deep learning models directly as interpretable microstructure generators. In this novel approach, a multi-headed autoencoder architecture processes a small, tractable set of inputs—specifically state descriptors (such as the aggregate’s area to control its size) and shape constants (based on scale-invariant image moments)—to output realistic 2D aggregate shapes.

Despite the distinct advantages and capabilities of both tools, they ultimately encounter the same fundamental bottleneck: the probabilistic description of their respective input parameters remains unresolved. In the KLE approach, the true joint probability distribution of the driving random variables is generally unknown and mathematically difficult to describe. Consequently, methods often have to rely on drawing from simplified independent standard normal distributions, which then require arbitrary thresholding to represent the binary phases of the material, complicating the accurate sampling process. Similarly, while the neural network generator relies on physically meaningful and tractable geometric descriptors, defining the precise joint probability distribution of these specific inputs for a given real-world concrete mixture is not trivial. In both methods, because the joint probability distribution of the necessary input parameters is highly complex and difficult to mathematically

formalize, see Fig. 2.8, accurately sampling from it to unconditionally gen-

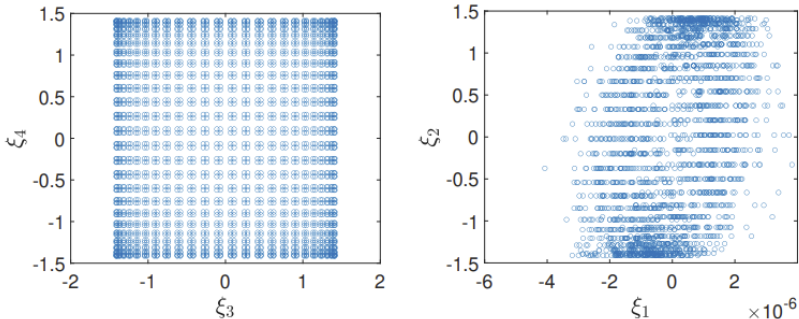


Figure 2.8: Two examples of sampled joint distributions of KLE eigenvariables derived by samples from the image analysis of two-phase medium. Šilhánek [2021]

erate new, strictly representative microstructures remains a significant open challenge.

### 3 INVERSE ANALYSIS: BAYESIAN INFERENCE

In Chapter 2, we explored how the microstructure of heterogeneous materials can be characterized to formulate a probabilistic description, such as utilizing image analysis to derive random fields. However, as discussed previously, the precise joint probability distributions of the corresponding random variables are often unknown or highly uncertain prior to actual macroscopic testing. Once a macroscopic sample is available or the structure is built, practical measurements can be performed. Inverse analysis allows us to use these observations to systematically update the initial probabilistic models, leading to a more accurate and reliable estimate of the material’s spatial properties.

To achieve this, the parameter identification is cast within a probabilistic setting using Bayesian inference [Tarantola, 2005] governed by

$$p(\mathbf{x}|\mathbf{z}) \propto p(\mathbf{z}|\mathbf{x})p(\mathbf{x}), \quad (3.1)$$

where  $p(\mathbf{x})$  stands for the prior distribution of the identified parameters  $\mathbf{x}$ , expressing the prior expert knowledge;  $p(\mathbf{z}|\mathbf{x})$  represents the likelihood function quantifying how well the modelled response fits the observed data; and  $p(\mathbf{x}|\mathbf{z})$  gives the posterior distribution of the identified parameters, i.e., the posterior state of knowledge about the identified parameters updated by the data. Traditional deterministic approaches to inverse boundary value problems

often suffer from ill-posedness, where small variations in measured data can result in large, unstable changes in the identified parameters. In contrast, the Bayesian framework naturally regularizes the inverse problem by modeling the unknown parameters as random variables [Gelman et al., 2013, Rosic et al., 2013]. A major advantage of this approach is that it provides a rigorous mechanism for combining prior expert knowledge—such as physical constraints or initial random field covariance structures—with noisy and limited experimental observations. Consequently, rather than yielding a single optimal point estimate, Bayesian updating results in a well-posed problem that yields a posterior probability distribution. This posterior distribution comprehensively summarizes all available information and quantifies any remaining uncertainty in the estimated material properties.

Throughout this chapter, Bayesian inference serves as the central unifying framework for the parameter identification. However, the exact formulation and interpretation of this Bayesian updating depend fundamentally on the specific nature of the system being modeled as described in detail in the following sections.

### **3.1 *Updating Random Fields***

When the objective is to characterize one specific laboratory specimen or a localized structural domain and spatial variability of the material properties within its domain—such as thermal conductivity, heat capacity, or moisture transport coefficients—can be described using random fields [Adler and Taylor, 2009, Vanmarcke, 2010]. Prior to testing, the exact spatial distribution is unknown, representing an epistemic prior uncertainty. While the Bayesian framework elegantly regularizes this identification by yielding a posterior probability distribution [Tarantola, 2005], its practical execution encounters a severe computational bottleneck. The posterior distributions are typically complex and high-dimensional, and they are primarily evaluated using sampling techniques, such as Markov chain Monte Carlo (MCMC) methods (e.g., the Metropolis-Hastings algorithm) [Gelman et al., 2013]. This sampling procedure requires up to millions of sequential evaluations of the forward numerical model.

To make this sampling practically feasible, substantial mathematical treatments are introduced. First, physical constraints must be respected. Because material parameters must remain strictly positive, non-Gaussian distributions, most notably log-normal random fields, are utilized for their prior description [Matthies, 2007, Rosić and Matthies, 2008]. However, the spatial discretization of these continuous random fields within a finite element model introduces a massive number of random variables.

To mitigate this infinite dimensionality, a dimensionality reduction is

achieved via the Karhunen-Loève expansion (KLE) [Ghanem and Spanos, 2003, Khoromskij and Litvinenko, 2008]. The KLE decomposes the underlying covariance matrix of the random field into a set of orthogonal eigenfunctions and corresponding eigenvalues. This allows the spatial variability to be accurately approximated by a truncated, finite set of uncorrelated standard Gaussian random variables. The correlation lengths and covariance structures necessary for the KLE can be derived from preliminary microstructural characterization, linking back to the image analysis techniques discussed in Chapter 2.

Consequently, the strictly positive unknown random fields can be parameterized via the truncated KLE and a non-linear log-normal transformation as

$$\hat{x}(\omega) = \exp \left( \mu_g + \sigma_g \sum_{k=0}^m \sqrt{\varsigma_k} \xi_k(\omega) \psi_k \right), \quad (3.2)$$

where  $\hat{x}(\omega)$  represents the approximated spatial material parameter field,  $\mu_g$  and  $\sigma_g$  are the mean and standard deviation of the underlying standard Gaussian field's natural logarithm, respectively,  $m$  is the truncation order defining the number of retained eigenmodes,  $\varsigma_k$  and  $\psi_k$  denote the corresponding positive eigenvalues and orthogonal eigenfunctions of the covariance matrix, and  $\xi_k(\omega)$  is a set of independent standard Gaussian random variables [Matthies, 2007, Havelka et al., 2019].

Once the unknown random fields are parameterized, Bayesian inference is utilized to systematically update these prior standard Gaussian random variables  $\xi_k(\omega)$  based on macroscopic experimental observations, such as boundary temperature or moisture responses, according to

$$p(\boldsymbol{\xi}|\mathbf{z}) \propto p(\mathbf{z}|\mathbf{x}(\boldsymbol{\xi}))p(\boldsymbol{\xi}). \quad (3.3)$$

Second, even with the reduced dimensionality provided by the KLE, the computationally exhaustive finite element evaluations within the MCMC sampling must be accelerated. This is effectively handled by substituting the computationally expensive forward numerical model with a fast surrogate model, typically constructed using Polynomial Chaos Expansion (PCE) [Marzouk et al., 2007, Marzouk and Najm, 2009]. By applying an intrusive stochastic Galerkin method [Babuška et al., 2004, Matthies and Keese, 2005], the model's response is projected onto a basis of multivariate orthogonal polynomials [Xiu and Karniadakis, 2002] of the independent random variables.

The specific capabilities, applications, and limitations of the aforementioned methodologies are demonstrated in detail across three key studies. First, the Bayesian framework, combined with KLE, was applied to investigate the spatial fluctuations of material properties in complex heterogeneous structures,

such as quarry masonry [Kučerová and Sýkora, 2013]. It was demonstrated that the probabilistic approach successfully refines the highly uncertain prior estimates of eight distinct transport parameters of the coupled heat and moisture Künzels model used to predict the temperature and moisture field within a rectangular domain, see Fig. 3.1

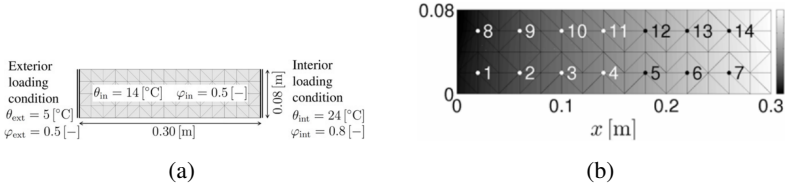


Figure 3.1: Experimental setup (a) and spatial arrangement of probes (b). Kučerová et al. [2012]

However, the direct evaluation of the numerical model within the MCMC sampling revealed a severe computational burden. To overcome this limitation, the implementation of the PCE-based surrogate model, constructed via the intrusive stochastic Galerkin method, was introduced and validated to reduce the sample evaluation time by orders of magnitude, see Fig. 3.2, [Kučerová et al., 2012]. This study showed that rigorous Bayesian updating becomes

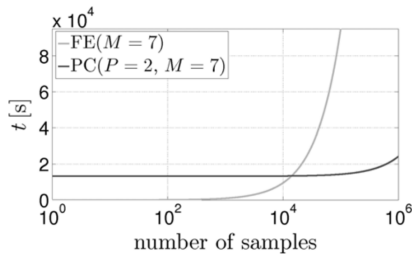


Figure 3.2: Comparison of time necessary for evaluation of samples directly by finite element method (FE) and its polynomial chaos-based surrogate (PC). Kučerová et al. [2012]

feasible even for highly complex transport processes without compromising the accuracy of the resulting posterior distributions.

Finally, the limits and capabilities of the dimensionality reduction itself were rigorously examined in the context of thermal tomography [Havelka et al., 2019]. This study focused on identifying the spatial distribution of thermal conductivity and volumetric heat capacity from boundary temperature measurements, see Fig. 3.3, highlighting the profound impact of the chosen

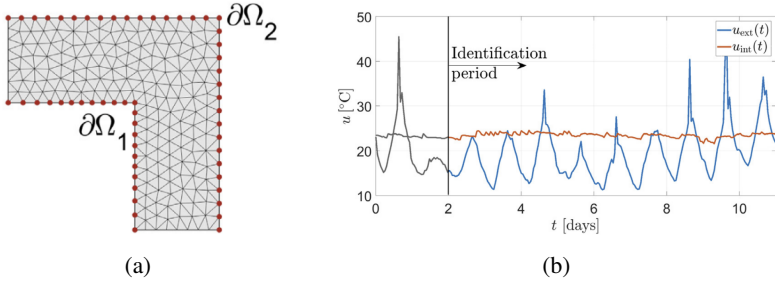


Figure 3.3: Geometrical L-shaped domain with highlighted boundary conditions (a) and ambient boundary conditions b). Havelka et al. [2019]

prior correlation lengths and the number of retained KLE eigenmodes on the accuracy of the reconstructed material fields, see Fig. 3.4.

### 3.2 Sampling-Free Bayesian Updating

While the introduction of surrogate models substantially accelerates the evaluation of the forward problem, the traditional Bayesian inference still relies on Markov chain Monte Carlo (MCMC) methods. This sampling procedure remains inherently burdensome due to slow convergence, the generation of correlated samples, and the necessity of burn-in periods. Alternatively, the Bayesian update can be expressed in terms of conditional expectation. This approach leaves the underlying probability measure unchanged and instead updates the measurable function—the random variable itself. To make this mathematically elegant concept computationally efficient, a functional approximation based on the Polynomial Chaos Expansion (PCE) is utilized in [Rosić et al., 2013] and further elaborated in [Rosić et al., 2016]. Instead of generating random samples, both the prior material parameters and the numerical model response are projected onto a basis of orthogonal polynomials. Consequently, the Bayesian update is reformulated into a linear, deterministic algebraic procedure, often referred to as the Polynomial Chaos-based Linear Bayesian Update.

By directly updating the PCE coefficients of the identified random variables, this spectral approach completely eliminates the need for any Monte Carlo sampling. However, the accuracy of this method is fundamentally limited by the linear approximation inherent in the update formula. The performance strongly depends on the nonlinearity of the measurement operator and the chosen prior distribution [Rosić et al., 2016]. If the actual parameter value lies in a region of low prior probability and the measurement relationship

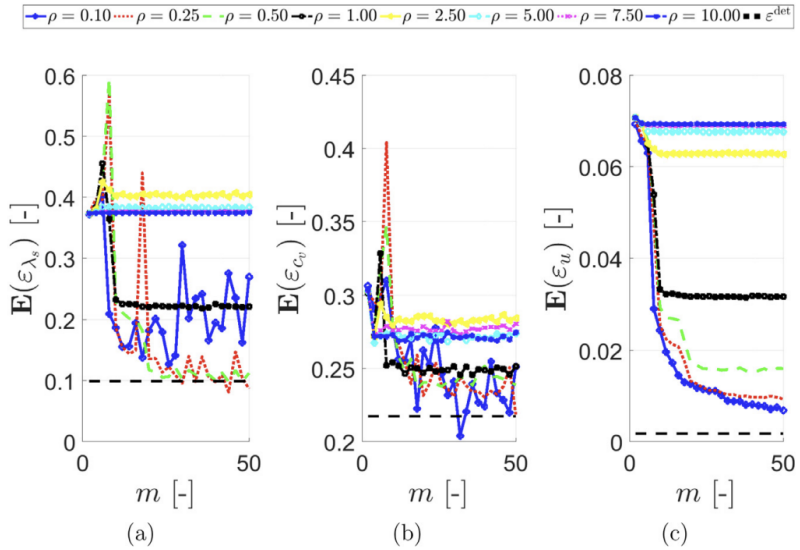


Figure 3.4: Averaged errors in (a) thermal conductivity, (b) volumetric heat capacity and (c) temperature as a function of the number of eigenmodes  $m$  and correlation length  $\rho$ . Havelka et al. [2019]

is highly nonlinear, the linear approximant tends to overshoot, meaning the procedure can be safely applied primarily to measurement operators with slight nonlinearities [Rosić et al., 2016]. Furthermore, strong physical nonlinearities, such as elasto-plasticity, render the identification process exceedingly difficult. Because the elasto-plastic response manifests only locally in regions where the yield stress has been reached, any features of the true material field that have little effect on the observed macroscopic response remain inherently uncertain and cannot be successfully identified.

### 3.3 Identification of Concrete Material Properties from Loading Tests

When the engineering focus shifts from characterizing the exact spatial distribution of properties within a specific object to describing an entire material class, the complex spatial variability is often abstracted. In [Janouchová et al., 2021, Kučerová et al., 2023], the identified parameters represent effective material properties, which are considered to be spatially constant within the employed macroscopic or mesoscopic computational models. The identification process aims here to extract these effective properties from a few repetitions of laboratory loading tests, such as unconfined compression and three-point bending tests in [Janouchová et al., 2021], or a set of confined compression tests in [Kučerová et al., 2023]. However, the inherent heterogeneity of the concrete material inevitably causes a significant variance, manifesting as a wide spread in the measured stress-strain diagrams or load-deflection curves across different test specimens, see Fig. 3.5.

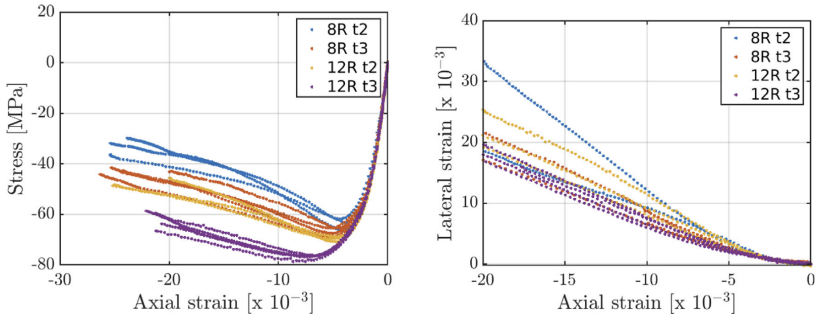


Figure 3.5: Experimental data obtained from confined compression test on concrete cylinders with four different types of reinforcement. Kučerová et al. [2023]

Attempting to fit the response of each specimen individually would be problematic, as a single test typically lacks sufficient information to distinguish

the influence of all considered material properties, often leading to random or physically nonsensical parameter values. While fitting all available experimental data simultaneously increases the overall amount of information, it still might not be sufficient for a unique identification of all parameters. In such cases, a traditional deterministic approach would fail to reveal that some parameters remain practically unidentifiable [Kučerová et al., 2023]. The employed Bayesian inference naturally regularizes this ill-posed problem and yields a posterior probability density reflecting the remaining uncertainty in the estimated parameter values [Tarantola, 2005, Gelman et al., 2013]. Consequently, the probabilistic description clearly quantifies which parameters are identified with high confidence and which remain highly uncertain, with the degree of uncertainty being easily comprehensible through a direct comparison with the prescribed prior distribution.

The width and shape of this posterior distribution reflect several distinct sources of uncertainty that are explicitly combined within the likelihood function. First, the experimental measurement error encompasses both the inaccuracy of the measurement instrumentation and the aforementioned variance caused by the material heterogeneity [Kučerová et al., 2023]. Second, to make the MCMC sampling computationally feasible, the time-consuming forward numerical models are replaced by computationally efficient surrogate models based on Polynomial Chaos Expansion (PCE) [Ghanem and Spanos, 2003, Marzouk et al., 2007]. The discrepancy between the exact numerical model and its polynomial approximation introduces a quantifiable theoretical model error [Janouchová et al., 2021, Kučerová et al., 2023]. Finally, when the forward numerical model is inherently stochastic—such as the Lattice Discrete Particle Model (LDPM) [Cusatis et al., 2011b,a], where the random generation of the internal particle configuration causes response oscillations (see Fig. 3.6 even for a fixed set of macroscopic material parameters—an additional theoretical uncertainty estimating the response variance for a given parameter set is included in the likelihood formulation too [Janouchová et al., 2021].

This unified identification strategy consisting of surrogate model construction (see Fig. 3.7) and sampling-based identification of material parameters' posterior distribution together with posterior predictions of model responses (see Fig. 3.8) has proven to be highly robust and versatile. In the case of the stochastic LDPM, it successfully identified seven mesoscale material parameters using a combination of unconfined compression and three-point bending tests [Janouchová et al., 2021].

Furthermore, the methodology was demonstrated to be highly efficient also for strictly deterministic, yet highly complex macroscopic models, such as the damage-plastic model for concrete (CDPM2) [Grassl et al., 2013]. By utilizing experimental data from an innovative confined compression test, the

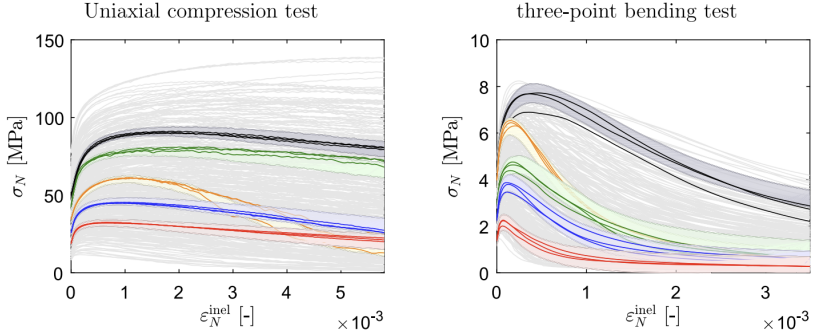


Figure 3.6: Solid lines of the same colour correspond to repeated LDPM simulations for the fixed material parameters reflecting the LDPM's inherent stochasticity due to mesh generation. Areas in colour represent high probability regions corresponding to the identified material parameters. Janouchová et al. [2021]

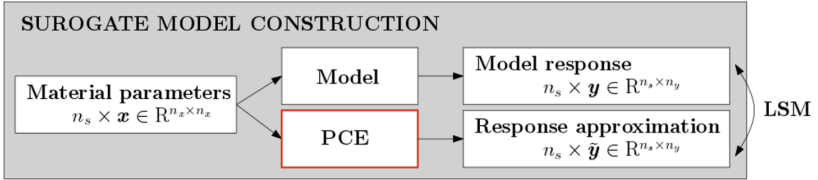


Figure 3.7: Scheme for surrogate model construction using the least-squares method (LSM). Janouchová et al. [2021]

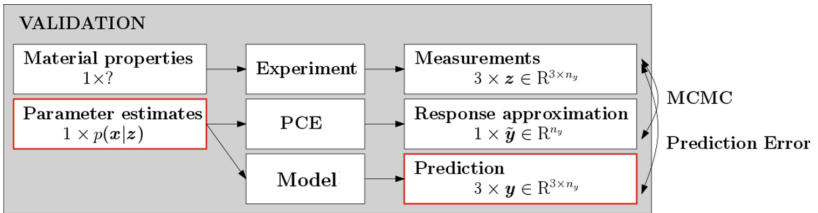


Figure 3.8: Validation scheme for the proposed parameter identification strategy on experimental data. Janouchová et al. [2021]

procedure enabled the simultaneous and stable identification of 15 material parameters, highlighting the immense potential of PCE-accelerated Bayesian inference in the calibration of advanced concrete models [Kučerová et al., 2023]. For an illustration of the identification procedure outcomes, Fig. 3.9 demonstrates the posterior high-fidelity intervals of the posterior parameter

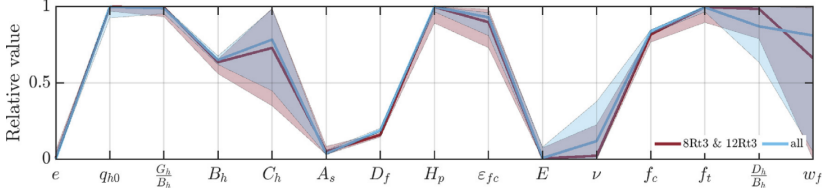


Figure 3.9: Validation scheme for the proposed parameter identification strategy on experimental data. Kučerová et al. [2023]

distributions, considering two and four experimental datasets, and Fig. 3.10 shows the plot of the posterior marginal distributions, revealing the mutual dependence and correlations of the parameter estimates. Finally, Fig. 3.11 shows the best fits of the data obtained for the maximum posterior estimates of the identified parameters along with the high-fidelity predictive regions.

### 3.4 Identification of Random Material Properties

While the previous section discussed the identification of a single deterministic set of effective parameters representing the entire material class, together with the epistemic uncertainty arising from noisy data and model imperfections, this concept can be further extended. For highly heterogeneous materials, it is often more appropriate to assume that each material specimen possesses its own specific parameter value. In such a case, the material properties across an ensemble of specimens can be modeled as random variables drawn from an unknown underlying probability distribution, representing the inherent aleatory uncertainty of the material [Der Kiureghian and Ditlevsen, 2009]. The parameter identification then turns into a stochastic inversion problem, aiming to identify this probability distribution from indirect macroscopic measurements.

To solve this stochastic inversion problem, two fundamentally different approaches were employed in [Kočková and Kučerová, 2026]. The first approach is based on a multilevel setting of Bayesian inference, known as hierarchical Bayesian modeling [Behmanesh et al., 2015, Nagel and Sudret, 2016]. In this formulation, a specific distribution family (e.g., log-normal) is

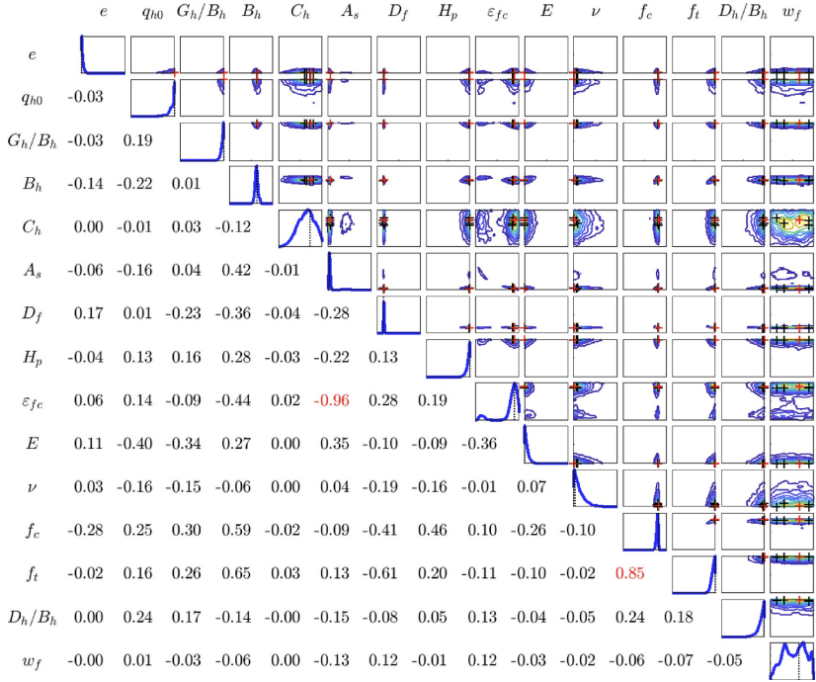


Figure 3.10: 1D and 2D marginal posterior distributions of model parameters accompanied by values of parameter pairwise correlations. Kučerová et al. [2023]

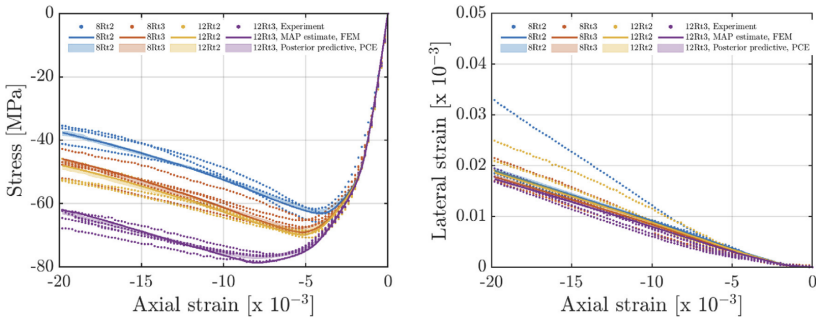


Figure 3.11: Best fits of the experimental data and high-fidelity posterior predictive regions. Kučerová et al. [2023]

prescribed for the material parameters, i.e.

$$\mathbf{x} \sim f_{\mathbf{x}}(\boldsymbol{\theta}), \quad (3.4)$$

where  $f_{\mathbf{x}}$  stands for the unknown distribution family and  $\boldsymbol{\theta}$  for its parameters (e.g. its statistical moments—such as the mean and standard deviation), which are then treated as uncertain hyperparameters to be updated via a Bayesian rule along with the parameter estimates  $\mathbf{x}_i$  corresponding to particular material samples. The Bayes rule thus turns into the following form

$$p(\mathbf{x}_1, \dots, \mathbf{x}_n, \boldsymbol{\theta} | \mathbf{z}_1, \dots, \mathbf{z}_n) \propto \prod_{i=1}^n p(\mathbf{z}_i | \mathbf{x}_i) \prod_{i=1}^n f(\mathbf{x}_i | \boldsymbol{\theta}) p(\boldsymbol{\theta}). \quad (3.5)$$

By updating these hyperparameters via Markov chain Monte Carlo (MCMC) sampling, the method elegantly separates the inherent aleatory variability from the epistemic uncertainty. This framework is particularly beneficial in cases with limited information, such as data obtained from different types of destructive experiments, see also [Šejnoha et al., 2017, Janda et al., 2024] for another applications. However, its major limitation is the necessity to assume a specific type of parameter probability density function a priori, which fundamentally affects the results and can be problematic, namely in the case of phenomenological parameters.

To overcome the requirement of predefining the parameter distribution shape and to improve computational efficiency, a second approach based on the nonlinear transformation of random variables is introduced in [Kočková and Kučerová, 2026]. Instead of updating a prescribed parameter distribution, this method focuses on the joint probability distribution of the experimental data, from which the distribution of the unknown parameters is defined via a nonlinear transformation accelerated by a polynomial chaos-based approximation. The underlying benefit of this formulation is that it reduces assumptions about the unknown parameter distribution structure, allowing for the identification of arbitrary and highly dependent joint distributions. Additionally, the dimension of the searched stochastic space does not change with additional observations, allowing for highly efficient experimental data processing. On the other hand, this approach suffers from quantifying all present uncertainties without distinguishing between the aleatory and epistemic ones. Moreover, it provides less accurate results when information on data correlation is lacking due to the experimental setup. This situation typically occurs when data originates from different types of destructive experiments performed on distinct groups of specimens. Because no single material sample can provide data from all experimental types simultaneously, the inherent statistical dependence between the individual measured quantities cannot be directly estimated. Thus,

in cases with limited data without clear correlation, the hierarchical Bayesian formulation is generally recommended.

### **3.5 Applications to Real-World Structures**

The capabilities of the developed Bayesian framework and its acceleration via Polynomial Chaos Expansion (PCE) were further validated on complex parameter identification tasks provided by the aerospace industry [Janouchová et al., 2016]. In this application, the methodology was deployed to calibrate a highly nonlinear viscoplastic damage model representing the mechanical behavior of a copper alloy used in combustion chambers. By processing experimental data from a series of tensile and cyclic loading tests performed on individual material specimens, the probabilistic approach successfully identified the inherent aleatory uncertainty in the material properties while overcoming the severe computational demands of the underlying finite element simulations.

Beyond well-controlled laboratory tests on material samples, the framework is equally applicable to the monitoring and assessment of existing real-world structures. A prominent example of this scalability is the application of these inverse analysis techniques to the development of a predictive digital twin for the containment of the Temelín nuclear power plant [Šilhánek et al., 2026]. In this context, the probabilistic framework was successfully utilized to systematically identify highly uncertain thermal boundary conditions—such as local ambient temperatures and heat transfer coefficients during reactor shutdown and startup sequences—directly from in-situ temperature monitoring data. Furthermore, the methodology was deployed to calibrate the effective material parameters of a complex concrete creep model based on long-term macroscopic strain measurements collected from sensors embedded within the massive containment wall. Because evaluating the full-scale 3D finite element model simulating the entire lifespan of the structure is computationally prohibitive for standard MCMC sampling, the identification process again successfully relied on fast surrogate models constructed via PCE. Ultimately, this successful deployment demonstrates that the proposed accelerated stochastic tools provide a robust and highly efficient foundation for the long-term aging management of massive heterogeneous structures.

## **4 CONCLUSIONS AND FUTURE WORK**

This overview has presented various approaches to the statistical or probabilistic description of complex heterogeneous materials. These approaches build upon two key and mutually complementary sources of information: direct

images of the material’s microstructure, and macroscopic measurements of its behavioral response—whether obtained from material specimens tested in the laboratory or from data collected directly from existing structures.

Specifically, the extraction of detailed information from direct digital images forms the foundation for robust microstructural characterization, which is the core of Chapter 2. While each proposed methodology effectively addressed a specific descriptive challenge, it simultaneously opened new avenues for future research. To overcome the artificial long-range correlations associated with traditional periodic unit cells, the proposed framework utilizes stochastic Wang tilings to construct strictly aperiodic domains [Novák et al., 2012, 2013]. However, this approach revealed inaccuracies in reproducing short-range details, highlighting the need to incorporate higher-order statistics and to extend the framework to fully three-dimensional microstructures using Wang cubes. To better capture phase connectedness, the computationally demanding lineal-path function was significantly accelerated using GPU programming environments [Havelka et al., 2016]. Nevertheless, although phase connectedness can be improved using the lineal-path function, the optimization of representative cells with specific inclusion shapes often remains inadequate, and despite the GPU acceleration, the reconstruction process continues to be computationally expensive. Nowadays, the application of Convolutional Neural Networks (CNNs) opens promising new possibilities; however, their successful training inherently requires a substantial amount of input data. A potential solution to this problem was proposed in [Das et al., 2026]. Still, persisting ambiguities in detecting the porous phase and peripheral aggregates call for further investigations and the augmentation of the proposed procedure with additional input information, such as granulometric curves. Finally, coupling the extracted statistical features with random field theory and modern deep learning architectures enables the probabilistic representation of the material’s inherent randomness, thereby creating a generator of random and realistic microstructures of the modeled material. However, the remaining bottleneck consists in the highly complex and unknown joint probability distributions of their underlying input variables, which makes accurate and unconditional sampling a significant open challenge for future material modeling [Šilhánek, 2021].

However, direct microscopic images are not always available for the probabilistic description of a material. Even when they are, the material representation can be further updated by utilizing another significant data source: macroscopic measurements of the material or structural behavior. Ultimately, for structural modeling, the key objective is to select the inputs of a computational model such that the model—despite its inherent imperfections—predicts the behavior of the given structure or material specimen as accurately as pos-

sible. At the same time, however, it is crucial to adequately account for the underlying uncertainty in situations where experimental data remain scarce. The inverse analysis of material properties from such limited and noisy data based on Bayesian inference is the focus of Chapter 3.

While the Bayesian framework elegantly regularizes this ill-posed problem and rigorously quantifies uncertainties, the identification procedures presented in Sections 3.1 and 3.3 proved to be methodologically highly successful. Specifically, they enabled the robust identification of the spatial distribution of transport properties parameterized by random fields [Kučerová and Sýkora, 2013, Havelka et al., 2019], as well as the simultaneous estimation of high-dimensional sets of effective material parameters for complex nonlinear constitutive models, such as the LDPM [Janouchová et al., 2021] and CDPM2 [Kučerová et al., 2023]. However, the critical bottleneck in both applications remains the severe computational burden associated with the Markov chain Monte Carlo (MCMC) sampling. Although Section 3.2 attempted to resolve this issue by introducing a sampling-free linear Bayesian update [Rosic et al., 2013], this alternative still does not provide sufficiently accurate results for highly nonlinear material models. Consequently, the MCMC-based inference must still be employed. In the case of random fields, this computational challenge is further exacerbated by the high dimensionality of the inverse problem, even when mitigated by the Karhunen-Loève Expansion [Havelka et al., 2019]. Conversely, the identification of effective properties simplifies the task by suppressing the inherent randomness of the heterogeneous material, meaning that its true aleatory uncertainty is de facto not adequately captured in a probabilistic manner [Janouchová et al., 2021, Kučerová et al., 2023]. This unresolved variability is addressed in Section 3.4, which focuses on the identification of the underlying aleatory uncertainty of random material properties through a hierarchical formulation of Bayes' rule or nonlinear variable transformation [Kočková and Kučerová, 2026]. However, even these methods have their limitations, and the identification of the inherent randomness of material properties without strong assumptions about the type of their distribution remains a subject for further research.

Despite these methodological challenges, the developed probabilistic framework and its acceleration via polynomial chaos expansion have demonstrated significant potential in practical engineering. Beyond laboratory tests, the methodology was successfully deployed in the aerospace industry to calibrate a complex viscoplastic damage model [Janouchová et al., 2016]. Moreover, its scalability was proven on large-scale infrastructure, notably in developing a predictive digital twin for the containment of the Temelín nuclear power plant from long-term in-situ monitoring data [Šilhánek et al., 2026]. These successful deployments confirm that the proposed stochastic tools already

provide a robust foundation for the long-term aging management of massive heterogeneous structures.

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# Curriculum vitae

doc. Ing. Anna Kučerová, Ph.D.

## Personal data

Born 11. 3. 1981 in Prague  
Address U kolejí 10, Prague 6, Czech Republic  
WWW <http://mech.fsv.cvut.cz/~anicka>  
E-mail Anna.Kucerova@cvut.cz  
children Anna Berenika (\*2013), Marie Noemi (\*2014),  
Antonie Lea (\*2017), Jan Sebastian (\*2020)

## Education and professional qualifications

2026 - VICE-RECTOR FOR EDUCATION, Czech Technical University in Prague (CTU Prague)

2021 - 2022 FULBRIGHT GRANTEE at the Massachusetts Institute of Technology in the United States (MIT), Department of Aeronautics and Astronautics, in cooperation with Prof. Youssef Marzouk, (01.11.2021-31.07.2022)

2021 - ASSOCIATE PROFESSOR, CTU Prague, Faculty of Civil Engineering (FCE), Department of Mechanics

2008 - 2021 ASSISTANT PROFESSOR, CTU Prague, FCE, Department of Mechanics

2009 One year scientific residency at Technical University of Braunschweig in Germany (TU Braunschweig), Institute of Scientific Computing, in cooperation with Prof. Hermann G. Matthies, (01.01.-31.12.2009)

2007 DOCTOR OF PHILOSOPHY (double degree Ph.D.), Ecole Normale Supérieure de Cachan (ENS Cachan) & CTU Prague, Supervisors: Prof. Adnan Ibrahimbegović & Prof. Zdeněk Bittnar

2004 MASTER OF SCIENCE - Diplôme d'études approfondies - Matériaux, intégrité des Structures dans leur Environnement, Option: Structures, ENS Cachan, France

2004 MASTER OF SCIENCE (Ing.), CTU Prague, Faculty of Civil Engineering, branch of study : Structures and Materials

### **Citation metrics, January 2026:**

- Publons profile (ResearcherID): **A-5136-2010**
- Total number of citations: WOS: **546**; Scopus: **656**; Google Scholar: **1320**
- **H-index**: WOS: **12**; Scopus: **13**; Google Scholar: **17**

### **Scholarships and Awards**

2021	FULBRIGHT stipend for 10 months scientific residency at MIT - 01.11.2021-31.07.2022
2017	L'ORÉAL - UNESCO FOR WOMEN IN SCIENCE Award for project entitled "Inverse problems in probabilistic engineering mechanics"
2009	Scholarship from TU Braunschweig for 12 months of postdoctoral collaboration with Prof. Hermann G. Matthies
2008	MINISTER'S PRIZE, Ministry of Education, Youth and Sports for excellent students
2008	WERNER VON SIEMENS EXCELLENCE AWARD 2008 - for doctoral thesis
2008	PROF. BABUŠKA HONORABLE MENTION for excellent work in computational sciences (for doctoral thesis)
2004 - 2007	Scholarship from French government for joint doctorate (ENS Cachan)
2004	JOSEF HLÁVKA PRIZE for best students
2004	PROF. BABUŠKA HONORABLE MENTION for excellent work in computational sciences (for diploma thesis)
2004	DEAN'S HONORABLE MENTION for unique results of scientific work during studies and exceptional level and defense of diploma thesis
2003	Scholarship from Komerční banka for international educational stay in the ATHENS program
2002/2003	ERASMUS scholarship for one year stay at ENS Cachan in France

### **Academic Supervision:**

- Currently supervising and co-supervising 3 Ph.D. students
- (Co-)supervisor for 2 doctoral and 2 master theses
- Supervisor for 3 bachelor theses, one awarded PROF. BABUŠKA HONORABLE MENTION for excellent work in computational sciences

**Overall scientific results:**

- 1 scientific book (thesis) published by Ecole Normale Supérieure de Cachan, France
- 19 peer-reviewed journal papers indexed in WOS
- 2 non-ISI refereed journal papers
- 1 book chapter
- 25 proceedings papers indexed in WOS
- More than 50 non-indexed proceedings papers
- 5 authorized software programs

**Reviews:**

- 1 review of a research project
- 5 reviews of Ph.D. dissertations
- 37 reviews of indexed journal papers

**Teaching experience:**

[since 09/2001, Department of Mechanics, Faculty of Civil Engineering, CTU in Prague]

- *Programming in C/C++*
- *Structural Mechanics 1*
- *Structural Mechanics 2*
- *Theory of Elasticity*
- *Reliability of Structures*

[since 09/2022, University Elementary School Lvíčata, CTU in Prague]

- *Preparatory course in mathematics for the 5<sup>th</sup> grade students*

**Team leader:**

- 2025-28 Leader of Workpackage 1/3: Diagnostics, testing and modeling of materials within INODIN: Innovative methods of materials diagnostics and monitoring of engineering infrastructure to increase its durability and service life - (project no. CZ.02.01.01/00/23\_020/0008487), European Regional Development Fund, amount granted 100,000,000 CZK ( $\approx$  4,000,000 €)
- 2018-23 Leader of team: Theory - Optimization Methods, Reliability of Complicated Systems, Center of Advanced Applied Sciences (project no. CZ.02.1.01/0.0/0.0/16 019/0000778), European Regional Development Fund

### **Principal investigator:**

- 2026-28 Safety and Durability of Nuclear-Reactor Concrete Containment: Synergy of Multiphysics/Multiscale and Data Driven Models, Technology Agency of the Czech Republic, project no. TQ26000075 in collaboration with Energoprojekt Praha s.r.o. and TU Compiegne, France, amount granted 5,212,500 CZK ( $\approx$  215,000 €)
- 2023-25 Synergy of multiscale Modelling and machine Learning: Strategy for biomedical sciences and battle against cancer, Ministry of Education, Youth and Sports of the Czech Republic, Mobility project no. MEB 101105 solved jointly with the UT Compiegne, France, amount granted 250,000 CZK ( $\approx$  10,000 €)
- 2016-18 Identification of Aleatory Uncertainty in Parameters of Heterogeneous Materials, Czech Science Foundation, project no. 16-11473Y, amount granted 5,590,000 CZK ( $\approx$  207,000 €)
- 2014-16 Reliability Analysis and Life Prediction with Probabilistic Methods, European Space Agency; part of the Future Launcher Preparatory Programme, amount granted 120,000 €
- 2011-14 Artificial neural networks in multi-scale modelling of transport processes in heterogeneous materials, Czech Science Foundation, project no. P105/11/P370, amount granted 1,413,000 CZK ( $\approx$  52,000 €)
- 2012 Multimedia tools for teaching basics in structural mechanics, Ministry of Education, Youth and Sports of the Czech Rep., Pedagogical Proj. No. 2360/2012, amount granted 134,000 CZK ( $\approx$  5,000 €)
- 2011-12 Uncertainty Quantification and Updating in the Description of Heat and Moisture Transport in Heterogeneous Materials, Ministry of Education, Youth and Sports of the Czech Republic, mobility project no. MEB 101105 solved jointly with the Institute of Scientific Computing, TU Braunschweig, amount granted 198,720 CZK ( $\approx$  7,000 €)
- 2011 Programming of engineering computations in C++, Ministry of Education, Youth and Sports of the Czech Rep., Pedagogical Proj. No. 2834/2011, amount granted 149,000 CZK ( $\approx$  5,500 €)

## WOS Journal papers

- [1] E. Kočková and A. Kučerová: Identification of random material properties as stochastic inversion problem. *Acta Polytechnica*, 2026, Accepted for publication.
- [2] A. Kučerová and J. Sýkora and P. Havlásek and D. Jarušková and M. Jirásek: Efficient probabilistic multi-fidelity calibration of a damage-plastic model for confined concrete. *Computer Methods in Applied Mechanics and Engineering*, 412: 116099, 2023.
- [3] J. Havelka and A. Kučerová and J. Sýkora: Efficient inverse solvers for thermal tomography. *Computers & Mathematics with Applications*, 97: 314–328, 2021.
- [4] E. Janouchová, A. Kučerová, J. Sýkora, J. Vorel and R. Wan-Wendner: Robust probabilistic calibration of a stochastic lattice discrete particle model for concrete. *Engineering Structures*, 236: 112000, 2021.
- [5] J. Havelka, A. Kučerová and J. Sýkora: Dimensionality reduction in thermal tomography. *Computers & Mathematics with Applications*, 78 (9): 3077–3089, 2019.
- [6] E. Janouchová, J. Sýkora, and A. Kučerová: Polynomial chaos in evaluating failure probability: A comparative study. *Applications of mathematics*, 63(6):713–737, 2018.
- [7] D. Jarušková and A. Kučerová: Estimation of thermophysical parameters revisited from the point of view of nonlinear regression with random parameters. *International Journal of Heat and Mass Transfer*, 106:135–141, 2017.
- [8] J. Havelka and A. Kučerová and J. Sýkora : Compression and Reconstruction of Random Microstructures using Accelerated Lineal Path Function. *Computational Materials Science*, 122:102–117, 2016.
- [9] T. Mareš and E. Janouchová and A. Kučerová: Artificial neural networks in calibration of nonlinear mechanical models. *Advances in Engineering Software*, 95:68–81, 2016.
- [10] A. Kučerová and M. Lepš: Soft computing-based calibration of micro-plane m4 model parameters: Methodology and validation. *Advances in Engineering Software*, 72:226–235, 2014.

- [11] E. Janouchová and A. Kučerová: Competitive comparison of optimal designs of experiments for sampling-based sensitivity analysis. *Computers & Structures*, 124: 47–60, 2013.
- [12] A. Kučerová and J. Sýkora: Uncertainty updating in the description of coupled heat and moisture transport in heterogeneous materials. *Applied Mathematics and Computation*, 219(13):7252–7261, 2013.
- [13] J. Novák, A. Kučerová, and J. Zeman: Microstructural enrichment functions based on stochastic wang tilings. *Modelling and Simulation in Materials Science and Engineering*, 21(2):025014, 2013.
- [14] B. Rosić, A. Kučerová, J. Sýkora, O. Pajonk, A. Litvinenko and H. G. Matthies: Parameter Identification in a Probabilistic Setting. *Engineering Structures*, 50:179–196, 2013.
- [15] A. Kučerová, J. Sýkora, B. Rosić, and H. G. Matthies: Acceleration of uncertainty updating in the description of transport processes in heterogeneous materials. *Journal of Computational and Applied Mathematics*, 18(236):4862–4872, 2012.
- [16] J. Novák, A. Kučerová, and J. Zeman: Compressing random microstructures via stochastic Wang tilings. *Physical Review E*, 86(4):040104, 2012.
- [17] A. Kučerová, D. Brancherie, A. Ibrahimbegovic, J. Zeman, and Z. Bittnar: Novel anisotropic continuum-discrete damage model capable of representing localized failure of massive structures: Part II: identification from tests under heterogeneous stress field. *Engineering Computations*, 26(1/2):128-144, 2009.
- [18] O. Hrstka and A. Kučerová: Improvements of real coded genetic algorithms based on differential operators preventing the premature convergence. *Advances in Engineering Software*, 35(3–4):237–246, 2004.
- [19] A. Ibrahimbegović, C. Knopf-Lenoir, A. Kučerová, and P. Villon: Optimal design and optimal control of structures undergoing finite rotations and elastic deformations. *International Journal for Numerical Methods in Engineering*, 61(14):2428–2460, 2004.
- [20] O. Hrstka, A. Kučerová, M. Lepš, and J. Zeman: A competitive comparison of different types of evolutionary algorithms. *Computers & Structures*, 81(18–19):1979–1990, 2003.