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STOCHASTIC MODELLING OF HETEROGENEOUS MATERIALS BASED ON IMAGE ANALYSIS

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Abstract: *Macroscopically heterogeneous materials, characterized mostly by comparable heterogeneity lengthscale and structural sizes, can no longer be modelled by deterministic approach. It is convenient to introduce stochastic approach with uncertain material parameters quantified as random fields. Nevertheless, introduction of random fields brings higher demands on quality of input data, especially on inputs of covariance functions representing the spatial randomness. The present contribution is devoted to the construction of random fields based on image analysis utilizing statistical descriptors, which were developed to describe the different morphology of two-phase random material. The whole concept is demonstrated on a simple numerical example of stationary heat conduction where interesting phenomena can be clearly understood.*

Keywords: Stochastic finite element method, Random fields, Two-point probability density function, Covariance function.

1. Introduction

Nowadays, the stochastic finite element method (SFEM) is very popular approach to modelling of heterogeneous materials. SFEM is an extension of the classical deterministic finite element approach to the stochastic framework i.e. to the solution of stochastic (static and dynamic) problems involving finite elements whose properties are random, see (Stefanou, 2009). The Monte Carlo (MC) method is the most widely used technique in simulating of these problems. Unfortunately, MC simulations require thousands or millions samples because of relatively slow convergence rate, thus the total cost of these numerical evaluations quickly becomes prohibitive. To meet this concern, the surrogate models based on the polynomial chaos expansion (PCE), see (Xiu & Karniadakis, 2002), were developed as promising alternative. The PC-based surrogates are constructed by different fully-, semi- or non-intrusive methods based on the stochastic Galerkin method (Ghanem & Spanos, 2012; Matthies 2010), stochastic collocation (SC) method (Babuška et al., 2004; Xiu, 2009) or DoE (design of experiments)-based linear regression (Blatman & Sudret, 2010).

When the input parameters are defined as random fields, the additional mathematical formulations are introduced to describe the spatial randomness. The Karhunen-Loève expansion (KLE) allow for representation of random fields utilising surprisingly few orthogonal modes from spectral decomposition of covariance matrix, see (Adler & Taylor, 2007). Several analytical covariance functions (CF) were created to describe the spatial covariance, but their relevance in describing real material properties remains questionable and poorly justified. Therefore, relatively new concepts of extracting the spatial covariance from images were established, see (Soize, 2006; Jürgens et al., 2012). Here, we propose a novel construction of CF obtained from two-point probability density function, which is calculated from the given image.

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2. Methodology

Due to the lack of space it is impossible to introduce whole methodology. Therefore, we focus here only on the construction of random fields. Other topics, such as implementation of heat conduction problem into the stochastic framework using the stochastic Galerkin are presented elsewhere; see (Kučerová & Matthies, 2010; Kučerová et al., 2012). As a preamble, we utilise KLE for modelling the spatial randomness. Based on the spectral decomposition of covariance function $C(\boldsymbol{x},\boldsymbol{x}')$ and the orthogonality of eigenfunctions ϕ_i, the real-valued random field $\lambda(\boldsymbol{x},\omega)$ truncated after M terms can be written as

$$\lambda(\boldsymbol{x},\omega) \approx \mu_\lambda(\boldsymbol{x}) + \sum_{i=1}^{M} \sqrt{\zeta_i}\xi_i(\omega)\phi_i(\boldsymbol{x}), \tag{1}$$

where $\mu_\lambda(\boldsymbol{x})$ is the mean value, ζ_i are the positive eigenvalues and $\boldsymbol{\xi}(\omega)$ is a set of uncorrelated random variables of zero mean and unit variance. It is obvious that the CF plays a key role in the construction of random field. Therefore, we introduce following relations: The first two belong to classical analytical approaches and third one is a novel strategy utilizing the information from images:

- Gaussian CF in two-dimensional space is given as

$$C(\boldsymbol{x},\boldsymbol{x}') = \sigma_\lambda^2 \exp\left(-\frac{(x-x')^2}{2L_x^2} - \frac{(y-y')^2}{2L_y^2}\right), \tag{2}$$

  where $\boldsymbol{x} = (x,y)$ and $\boldsymbol{x}' = (x',y')$ are arbitrarily chosen two points, σ_λ^2 is the variance of $\lambda(\boldsymbol{x},\omega)$ and $\boldsymbol{L} = (L_x, L_y)$ are the correlation lengths.

- Exponential CF is defined as

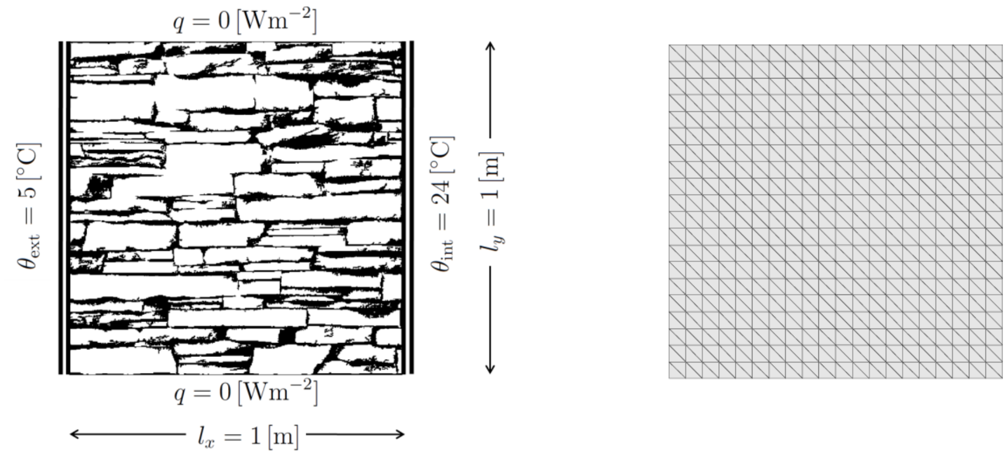
$$C(\boldsymbol{x},\boldsymbol{x}') = \sigma_\lambda^2 \exp\left(-\left|\frac{x-x'}{L_x}\right| - \left|\frac{y-y'}{L_y}\right|\right). \tag{3}$$

  Image-based CF – here we focus in particular on two-point probability function $S_2(\boldsymbol{x},\boldsymbol{x}')$, see (Torquato, 2002), and two-phase medium with constant value $\lambda^{(i)}$ over the domain of the phase (i). According to (Lombardo et al., 2009), the CF is derived as

$$C(\boldsymbol{x},\boldsymbol{x}') = \left(S_2^{(1)}(\boldsymbol{x},\boldsymbol{x}') - \left(c^{(1)}\right)^2\right)\left(\lambda^{(1)} - \lambda^{(2)}\right)^2, \tag{4}$$

  where $c^{(1)}$ is volume fraction of the phase (1).

3. Numerical Example



a) *b)*

Fig. 1: a) Heterogeneous structure with boundary conditions (θ is the temperature [°C], *q is the heat flux* [Wm^{-2}] *and l is the length* [m]*) and b) its finite element discretisation with 441 FE nodes.*

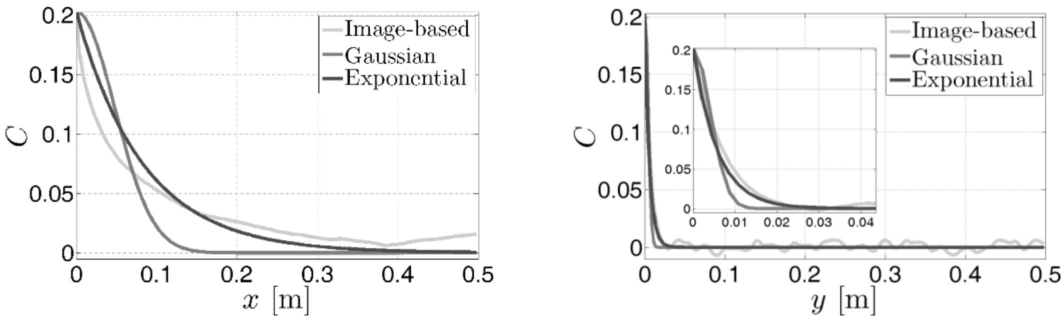
This section supports the proposed methodology through numerical study of heat conduction problem in irregular masonry, where energy balance equation leads to

$$-\nabla\cdot(\lambda(x)\nabla\theta(x)) = f(x), \quad x \in \mathcal{G} \subset \mathbb{R}^2, \tag{5}$$

$$\theta(x) = g(x), \quad x \in \partial\mathcal{G}, \tag{6}$$

where θ is a temperature, f stands for a head source or sink and g is a prescribed boundary conditions. Thermal conductivity is assumed to be $\lambda^{(1)} = 1.9\,\mathrm{Wm^{-1}K^{-1}}$ for bricks (white phase) and $\lambda^{(2)} = 0.9\,\mathrm{Wm^{-1}K^{-1}}$ for mortar (black phase). We consider the geometry obtained from a photograph of irregular masonry. Its black-and-white variant together with the loading conditions is depicted in Fig. 1a, while the employed finite element discretisation is given in Fig. 1b.

While the image-based CF is fully defined by the image and conductivity in particular phases, the Gaussian and exponential CFs need a calibration of correlation lengths L_x and L_y and variance σ_λ^2. Moreover, the expansion of the field in Eq. (1) also requires mean value μ_λ. The latter two moments can be obtained simply as mean and variance of conductivity values $\lambda^{(1)}$ and $\lambda^{(2)}$ prescribed to both phases weighted by their corresponding volume fractions $c^{(1)}$ and $c^{(2)}$. Determination of correlation lengths is, however, not trivial and commonly requires some expert knowledge about the modelled material. Here we exploit our knowledge about image-based CF and optimise the values of correlation lenghts so as to fit the analytical CFs to the one obtained from image. The optimisation process resulted in $L_x = 47.6$ mm and $L_y = 4.07$ mm in case of Gaussian CF and $L_x = 83.3$ mm and $L_y = 5.69$ mm in case of exponential CF. The shape of resulting CFs is shown in Fig. 2, where inadequacy of Gaussian or exponential approximation of image-based CF is clearly visible.



a) *b)*

Fig. 2: CFs corresponding to given microstructure: a) Cut along the axis x; b) Cut along the axis y.

The impact on the shape of random field is given by shape of particular eigenfunctions, which are depicted in Fig. 3. One can see the low oscillation of first eigenfunctions obtained from Gaussian and exponential CFs, while the image-based eigenfunctions clearly describe higher frequencies.

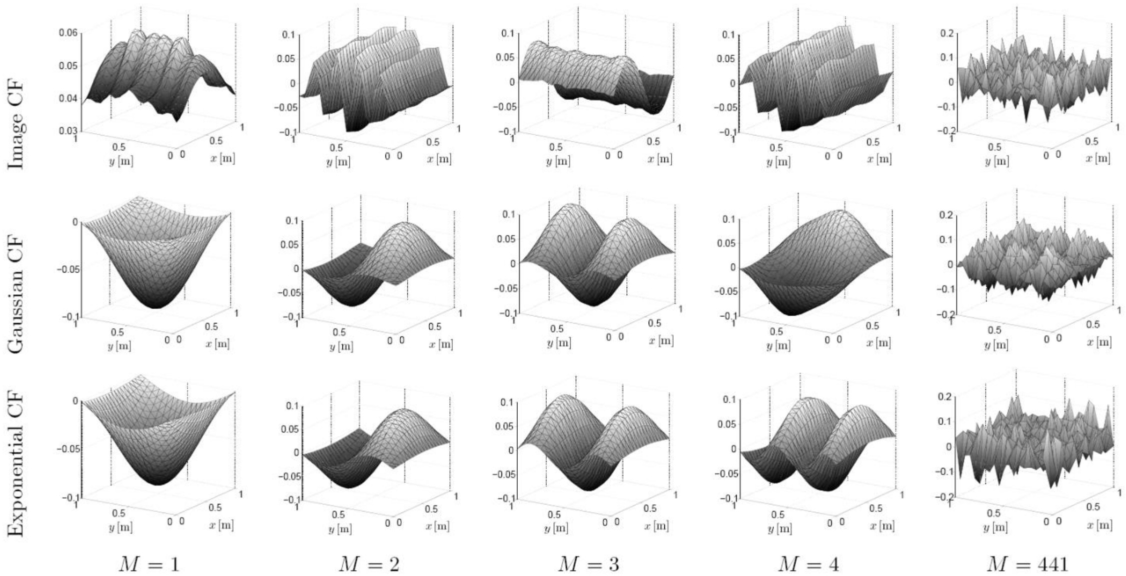


Fig. 2: KL modes (M = 1, M = 2, M = 3, M = 4, M = 441) for given CFs.

Finally, we computed the relative error of temperature fields defined as

$$\epsilon(\theta) = \frac{\left\|\theta_M - \theta_{441}^{\mathrm{image}}\right\|_{l^2(\mathcal{g}\times\Omega)}}{\left\|\theta_{441}^{\mathrm{image}}\right\|_{l^2(\mathcal{g}\times\Omega)}}, \tag{7}$$

where θ_M denotes the temperature field obtained using a given CF described by M modes, $\theta_{441}^{\text{image}}$ denotes the temperature field obtained using image-based CF and all 441 modes, and l^2 is the Euclidean norm computed over the spatial domain $\mathcal{G}$ and stochastic domain Ω discretized into 1000 randomly generated realisations of random variables $\boldsymbol{\xi}(\omega)$. The evolution of resulting errors is shown in Fig. 4 with remarkable divergence of errors obtained using Gaussian and exponential CFs.

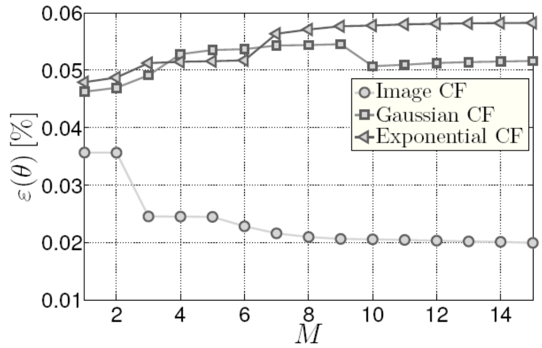


Fig. 3: Relative error of temperature.

4. Conclusions

In this contribution, we present different strategies for construction of random fields. A comparison of classical approach based on the analytical CFs and a novel methodology based on image analysis was shown to assess the quality and accuracy of obtained random fields. The whole concept was demonstrated on the stationary heat conduction problem with spatial random material parameters.

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