Bayesian Calibration of Lattice Discrete Particle Model for Concrete

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Abstract: In lattice or particle formulations of models for quasi-brittle materials, a medium is discretized "a priori" according to an idealization of its internal structure. Geometrical parameters of particles or lattice equip these type of formulations with inherent characteristic lengths and they have the intrinsic ability of simulating the geometrical features of material internal structure. This allows the accurate simulation of damage initiation and crack propagation at various length scales, however, at increased computational costs. Here we employ the so-called Lattice Discrete Particle Model (LDPM) recently proposed by (Cusatis et al., 2011). LDPM was calibrated, and validated against a large variety of loading conditions in both quasi-static and dynamic loading conditions and it was demonstrated to possess superior predictive capability, see (Cusatis et al., 2011b). Nevertheless, the utilized calibration procedure was based on a hand-fitting, which complicates further practical applications of the model. Here we present a Bayesian inference of model parameters from experimental data obtained from notched three-point-bending tests and cube compression tests. The Bayesian inference allows to solve the inverse problem as well-possed and to quantify posterior uncertainty in parameters by combining a prior knowledge about the realistic parameter values and uncertainty contained in measurement errors. In particular, we obtain the posterior distributions by robust the Markov chain Monte Carlo sampling, where the computational burden, arising from repeated model simulations, is overcome by using a polynomial chaos-based surrogate of the LDPM.

Keywords: lattice discrete particle model, concrete, notched three point bending test, cube compression test, Bayesian inference, Markov chain Monte Carlo, polynomial chaos.

1. Introduction

In order to predict the behaviour of the structural system under the loading in a computational way, the corresponding numerical model has to be properly calibrated. In other words, parameters of the mathematical model of the system have to be estimated as accurately as possible to obtain realistic predictions, e.g. for usage in an appropriate reliability analysis or structural design optimisation. In this paper, the Lattice Discrete Particle Model (LDPM) is employed to accurately describe the macroscopic behaviour of concrete in elastic, fracturing, softening, and hardening regimes (Cusatis et al., 2011b; Cusatis et al., 2011a). To infer the model parameters from indirect experimental measurements one can proceed in two principally different ways. The traditional approach is deter-

ministic, while advances in surrogate modelling and increasing computational capacity of modern computers permitted many researches to focus on parameter identification in probabilistic setting.

The most common method of parameter estimation is based on fitting the response of the numerical model to the experimental data. This deterministic approach leads to optimising parameters so as to minimise the difference between the data and the model response. The optimisation problem is, however, often ill-posed and thus requires the employment of robust optimisation algorithms. The result of such optimisation process is only the single-point estimate of parameter values, as you can see in Figure 1b, thus any information beyond the mean values of parameters is omitted. Consequently, this deterministic inversion method does not provide any quantification of the uncertainty in parameter estimates which in fact exists and is caused by e.g. an insufficient number of observations and measurement errors. This contribution focuses on identification of epistemic (reducible, subjective, cognitive) uncertainty arising from our lack of knowledge (Oberkampf et al., 2002) which is supposed to be reduced by any new measurement according to the coherence of learning (Mantovan and Todini, 2006; Beven et al., 2007).

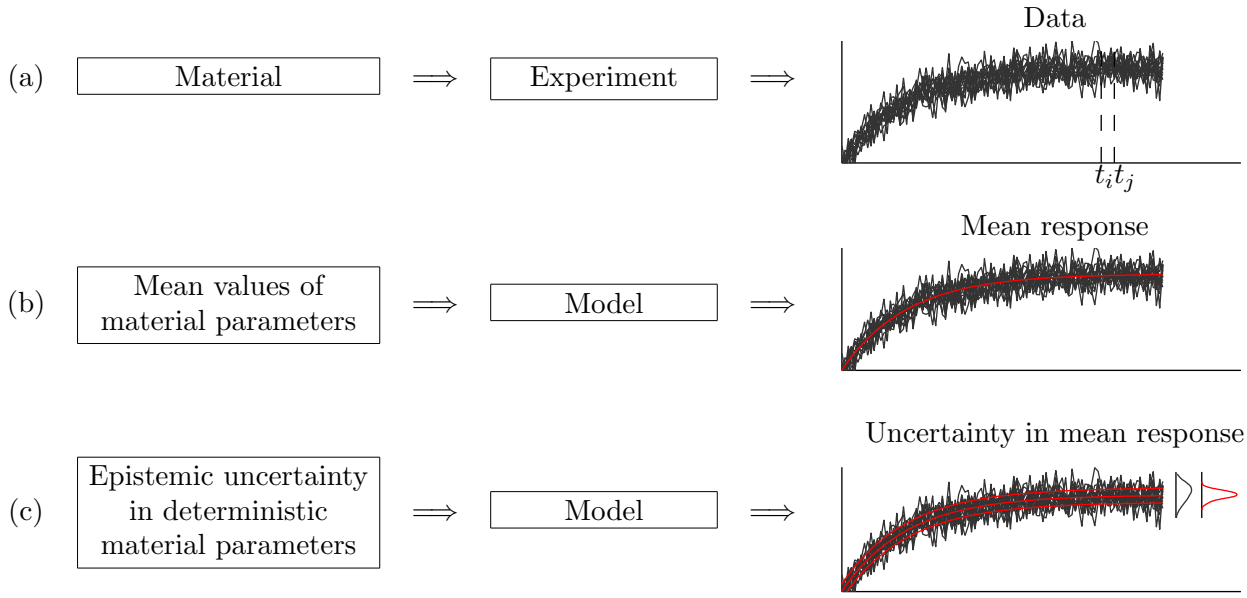

Figure 1. Scheme of an experiment and different approaches to parameter identification.

In the last decades probabilistic methods for stochastic modelling of uncertainties have become applicable thanks to a growing computational capacity of modern computers. The probabilistic approach restates the inverse problem as well-posed in an expanded stochastic space by modelling the parameters as well as the observations as random variables with their probability distributions (Kaipio and Somersalo, 2005). Several methods for the uncertainty quantification in probabilistic settings have been proposed in the literature. The last decade witnessed an intense development in the field of Bayesian updating of epistemic uncertainty (Figure 1c) in description of deterministic material or structural parameters, see e.g. (Marzouk et al., 2007). Here, a likelihood function is

established to quantify our confidence in observed data, with the goal to update our prior knowledge on model parameters (Gelman et al., 2004). The increasing popularity of Bayesian methods is motivated by developments in the field of spectral stochastic finite element method, which allows to alleviate the computational burden by surrogate models such as polynomial chaos expansions (Marzouk and Najm, 2009). The most commonly referred techniques of Bayesian inference in literature are based on the Markov chain Monte Carlo method (Marzouk et al., 2007), the Kalman filter (Rosić et al., 2013) or optimal transport maps (El Moselhy and Marzouk, 2012).

2. Bayesian Inference

Consider a stochastic problem

$$\boldsymbol{z}(\boldsymbol{x},\omega) = \boldsymbol{y}(\boldsymbol{x}) + \varepsilon(\omega), \tag{1}$$

with uncertain model parameters $\boldsymbol{x}$ and random observable data $\boldsymbol{z}$, which can be predicted by a model response $\boldsymbol{y}(\boldsymbol{x})$ besides a measurement error ε. In Bayesian statistics, probability represents a degree of belief about the parameter values (Tarantola, 2005). Combining the initial knowledge in the form of the prior distribution $p(\boldsymbol{x})$ and the experimental data as the likelihood function $p(\boldsymbol{z}|\boldsymbol{x})$ according to Bayes rule

$$p(\boldsymbol{x}|\boldsymbol{z}) = \frac{p(\boldsymbol{z}|\boldsymbol{x})p(\boldsymbol{x})}{p(\boldsymbol{z})} = \frac{p(\boldsymbol{z}|\boldsymbol{x})p(\boldsymbol{x})}{\int_{\boldsymbol{x}} p(\boldsymbol{z}|\boldsymbol{x})p(\boldsymbol{x})\mathrm{d}\boldsymbol{x}}, \tag{2}$$

we obtain the posterior distribution of the parameters. The mean values of the updated distribution are equal to the best guess of the parameters values with the uncertainty represented by the corresponding variance. However the posterior statistical moments cannot be generally computed analytically, because the identified distribution including the whole numerical model is too complicated.

To overcome this obstacle, we use Markov chain Monte Carlo sampling (MCMC) of the posterior distribution, which is a method based on a creation of an ergodic Markov chain of required stationary distribution equal to the posterior (Gilks et al., 2005; Geyer, 2011). There are different algorithms for constructing this chain (Spall, 2003), e.g. Gibbs sampler or Metropolis-Hastings algorithm, which avoids calculating of the normalisation constant in Eq. (2) by evaluating only ratios of target probabilities. Suitable setting of the proposal distribution for a random walk is important and can be evaluated on the basis of acceptance rate (Rosenthal, 2011) or autocorrelation, which is required to be minimal. The convergence speed of the procedure depends also on the appropriate choice of the starting point (Geyer, 2011). The essential advantage of this method is its versatility for usage with nonlinear models, when for an infinite number of samples it gives the exact solution. The disadvantage of this method is its high computational effort resulting from necessity of a high number of model simulations. In order to accelerate this sampling procedure in the identification process, the evaluations of a numerical model can be replaced by evaluations of a computationally efficient model surrogate.

2.1. Polynomial chaos expansion

In this contribution, we employ polynomial chaos expansion (PCE) for the approximation of the model response in the stochastic space (Marzouk et al., 2007), which has the following form:

$$\tilde{\boldsymbol{y}}(\boldsymbol{x}(\boldsymbol{\xi})) = \sum_{\alpha} \boldsymbol{\beta}_{\alpha} \psi_{\alpha}(\boldsymbol{\xi}), \tag{3}$$

where $\boldsymbol{\beta}_{\alpha}$ is a vector of PCE coefficients $\beta_{\alpha,i}$ corresponding to a particular component of the system response y_i. $\psi_{\alpha}(\boldsymbol{\xi})$ are multivariate polynomials. The expansion (Eq. (3)) is usually truncated to the limited number of terms n_{β}, which is very often related to the number of random variables $n_{\boldsymbol{x}}$ and to the maximal degree of polynomials n_{p} according to the relation

$$n_{\beta} = \frac{(n_{\mathrm{p}} + n_{\boldsymbol{x}})!}{n_{\mathrm{p}}! n_{\boldsymbol{x}}!}. \tag{4}$$

PCE can be used to approximate the response with respect to the probability distribution of the random variables $\boldsymbol{\xi}$. The convergence of the approximation error with the increasing number of polynomial terms is optimal in case of orthogonal polynomials of a special type corresponding to the probability distribution of the underlying variables (Xiu and Karniadakis, 2002). In particular, we employ Legendre polynomials associated with the uniform distribution.

The efficiency of this technique depends on computational requirements of the PCE construction and its consequent accuracy. In this contribution, the PCE coefficients are computed with help of linear regression (Blatman and Sudret, 2010a), which is based on a set of model simulations. The samples are drawn according to a stratified procedure called design of experiments (DoE), in particular well-known Latin hypercube sampling (LHS), which is able to respect the prescribed probability distributions (Janouchová and Kučerová, 2013).

2.2. Sensitivity analysis

Global sensitivity analysis (SA) is an important tool for investigating properties of complex systems. It is a valuable part of solution of an inverse problem such as a parameter identification, where the aim of SA can be estimating the influence of the identified parameters to the model response. SA provides some information about the relationship between the system outputs/model response and the system inputs/model parameters on their whole domain. Several approaches to SA have been developed, see e.g. (Saltelli et al., 2000) for an extensive review. The presented contribution is focused on Sobol sensitivity indices expressing an influence of chosen parameters on the response variance. Sobol indices can be analytically computed from the PCE coefficients (Blatman and Sudret, 2010b) according to the following relation

$$S^{\mathrm{PCE}}_{i_1,\ldots,i_s} = \frac{\sum_{\alpha \in \mathcal{I}_{i_1,\ldots,i_s}} \beta_{\alpha}^2 \mathbb{E}[\psi_{\alpha}^2(\boldsymbol{\xi})]}{\sum_{\alpha=1}^{n_{\beta}} \beta_{\alpha}^2 \mathbb{E}[\psi_{\alpha}^2(\boldsymbol{\xi})]}, \tag{5}$$

where $\mathbb{E}[\psi_{\alpha}^2(\boldsymbol{\xi})]$ is computed specifically for Legendre polynomials as

$$\mathbb{E}[\psi_{\alpha}^2(\boldsymbol{\xi})] = \int \psi_{\alpha}^2(\boldsymbol{\xi}) \mathrm{d}\mathbb{P}\psi(\boldsymbol{\xi}) = \int \cdots \int_{n_{\xi}} \prod_{j=1}^{n_{\xi}} (\psi_{\alpha,j}^2(\xi_j)) \mathrm{d}\mathbb{P}\psi(\xi_1) \cdots \mathrm{d}\mathbb{P}\psi(\xi_{n_{\xi}}) = \prod_{j=1}^{n_{\xi}} \frac{2}{2\alpha_{\xi_j} + 1}, \tag{6}$$

where α_{ξ_j} is a degree of ξ_j in a polynomial term ψ_α. $\mathcal{I}_{i_1,...,i_s}$ defines the polynomial terms depending only on $(\xi_{i_1}, ..., \xi_{i_s})$, i.e.

$$\mathcal{I}_{i_1,...,i_s} = \{\alpha_k = 0 \Longleftrightarrow k \notin (i_1, \ldots, i_s), \forall k = 1, \ldots, n_\xi\}. \tag{7}$$

3. Calibrated Material Model

In this section, the examined material model, used for the calibration, is briefly described. The material model, often employed to simulate quasi-brittle materials, is chosen to demonstrate the capability of aforementioned approach. This model is based on lattice or particle formulations in which materials are discretized "a priori" according to an idealization of their internal structure. Particle size and size of the contact area among particles, for particle models, as well as lattice spacing and cross sectional area, for lattice models, equip these type of formulations with inherent characteristic lengths and they have the intrinsic ability of simulating the geometrical features of material internal structure. This allows the accurate simulation of damage initiation and crack propagation at various length scales at the cost, however, of increased computational costs.

Earlier attempts to formulate particle and lattice models for fracture are reported in (Cusatis et al., 2003; Cusatis et al., 2006; Cusatis, 2011; Bažant et al., 1990; Yip et al., 2006) while the most recent developments were published in a Cement Concrete Composites special issue (Cusatis and Nakamura, 2011). A comprehensive discrete formulation for concrete was recently proposed by Cusatis and coworkers (Cusatis et al., 2011b; Cusatis et al., 2011a) who formulated the so-called Lattice Discrete Particle Model (LDPM). LDPM was calibrated, and validated against a large variety of loading conditions in both quasi-static and dynamic loading conditions and it was demonstrated to possess superior predictive capability.

In the present study the basic material properties of the tested concrete mix are kept constant for all simulations. Note that these parameters influence the generation of concrete meso-structure, see Table I. However, the seed number, governing the sampling of cumulative distribution func-

Table I. Values of parameters governing the generation of concrete meso-structure.

material property		unit	value
minimum particle size	d_0	mm	4
maximum particle size	d_a	mm	16
cement content	c	kg/m^3	240
water to cement ratio	w/c	-	0.83
aggregate to cement	a/c	-	8.83
Fuller coefficient	n_F	-	0.5
concrete density	ρ	kg/m^3	2400

tion of concrete granulometric distributions by a random number generator, is kept random. The distribution of particles influences the material response and is assumed to act as a noise in the response.

The parameters of the mathematical model which are kept constant or calibrated by the procedure described above are summarised in Table II.

Table II. Values of material model parameters used in the numerical simulations.

material property		unit	value (range)
normal modulus	E_0	MPa	$20000 - 70000$
shear-normal coupling	α	-	$0.2 - 0.3$
tensile strength	σ_t	MPa	$1.5 - 5$
tensile characteristic length	l_t	mm	$50 - 300$
softening exponent	n_t	-	$0.1 - 1$
shear/strength ratio	σ_s/σ_t	-	$1.5 - 8$
initial friction	μ_0	-	$0.001 - 0.5$
compressive strength	σ_{c0}	MPa	$\sigma_{c0} = 40\sigma_t$
transitional stress	σ_{N0}	MPa	$\sigma_{N0} = 240\sigma_t$
initial hardening modulus ratio	$H_{c0}/E0$	-	0.4
transitional strain ratio	κ_{c0}	-	4
deviatoric strain threshold ratio	κ_{c1}	-	1.0
deviatoric damage parameter	κ_{c2}	-	5.0
asymptotic friction	μ_∞	-	0.0
densification ratio	E_d/E_0	-	1.0
volumetric-deviatoric coupling	β	-	0

4. Results

The identification of the seven material model parameters for concrete is based on two types of experiments, specifically a uniaxial compression test and a notched three-point-bending test. The first experiment was repeated three times while the second one four times. For convenience and readability, data are presented in terms of nominal stress $_N$ and nominal strain ε_N. The most traditional tests to characterise concrete is the compression test performed on cubes of 150 mm side length. The nominal values are defined as

$$\sigma_N = \frac{F}{a^2} \quad \text{and} \quad \varepsilon_N = \frac{u}{a} \tag{8}$$

where F is the applied load, u denotes the load point displacement and a is the side length. The fracture properties of concrete are characterised by means of the notched three-point-bending test. The nominal stress and strain are

$$\sigma_N = \frac{3Fl}{dh^2} \quad \text{and} \quad \varepsilon_N = \frac{CMOD}{h} \tag{9}$$

where l stands for the beam span, h, d are the beam height and width, respectively. $CMOD$ is the crack mouth opening displacement measured over the notch.

Moreover, to eliminate the error in measurement caused by the testing machine stiffness, the inelastic part of the strain is used for the model calibration

$$\varepsilon_N^{\text{inel}} = \varepsilon_N - \sigma_N \left(1/K\right) \tag{10}$$

where K is the corresponding elastic stiffness. To capture the elastic properties of the model, the initial elastic part of the cube compression test is utilised.

The updated joint probability distribution of the parameters is formulated according to Bayes' formula as a product of prescribed uniform prior distribution with bounds given in Table III and likelihood function arising from the experimental errors, which are supposed to be normally distributed with zero mean values and standard deviations derived from the experimental data. Specifically, in the identification process we consider from the compression test the measured stress σ_N discretized into 250 strain steps with the error $\varepsilon \sim N(0, 8^2)$ and elastic stiffness K with error $\varepsilon \sim N(0, 2880^2)$, from the notched three-point-bending test the measured stress σ_N discretized into 250 strain steps with the error $\varepsilon \sim N(0, 2^2)$.

Table III. Prior bounds and identified statistical moments of parameters' distribution.

	E_0 [MPa]	α [-]	σ_t [MPa]	l_t [mm]	n_t [-]	σ_s/σ_t [-]	μ_0 [-]
			Prior				
MIN	20000	0.200	1.500	50.0	0.100	1.500	0.001
MAX	70000	0.300	5.000	300.0	1.000	8.000	0.500
			Identification				
MEAN	31183	0.297	2.236	166.6	0.910	3.192	0.063
STD	1998	0.003	0.193	17.8	0.037	0.338	0.051

The corresponding posterior distribution of the model parameters is obtained by MCMC sampling. Because the full numerical model simulation is computationally intensive (approx. 4 hours for the compression test and 10 hours for the bending test), the surrogate model has to be used. In this case of the stochastic model, the approximation can also serve for a purpose of eliminating the noise of the material model response caused by the random distribution of particles. We employ PCE in a form of Legendre polynomials of the third degree constructed by linear regression based on 200 simulations of the full model for prior parameter samples. Thanks to this approximation we obtain

500, 000 posterior samples in only few hours. The identified mean values of the parameters together with the corresponding epistemic uncertainties expressed by the posterior standard deviations are given in Table III. The updated univariate and bivariate marginal probability distributions are shown in Figure 2.

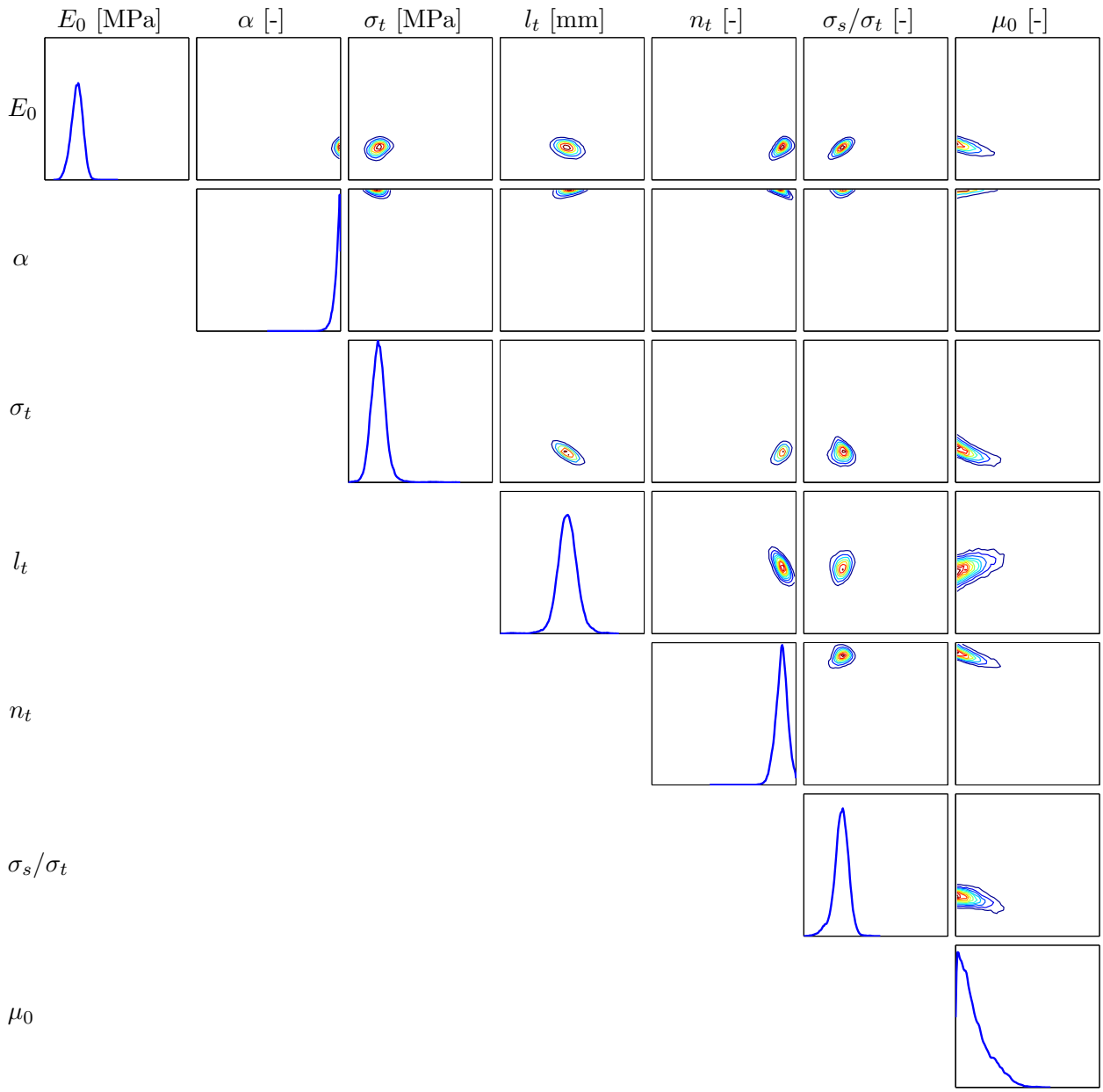

Figure 2. Identified 1D and 2D marginal pdfs of model parameters.

In order to validate the accuracy of the identification process, we compare the experimental data with the model response corresponding to the identified mean values of the model parameters which is shown in Figures 3 and 4. There are plotted five full stochastic model simulations and also the PCE-based response. As one can see, the PCE-based response fits the experimental data very well in the both experimental tests while the full numerical model response differs slightly in the case of the three-point-bending test and more significantly in the case of uniaxial compression test. It means that the used model approximation is not accurate enough. One reason can be a low degree of the polynomials or the training samples are not chosen properly. In Figures 3 and 4, there are also plotted the full numerical model simulations used for the approximation training. From these graphs the training curves seem to be appropriate because the experimental data do not lie outside the covered region.

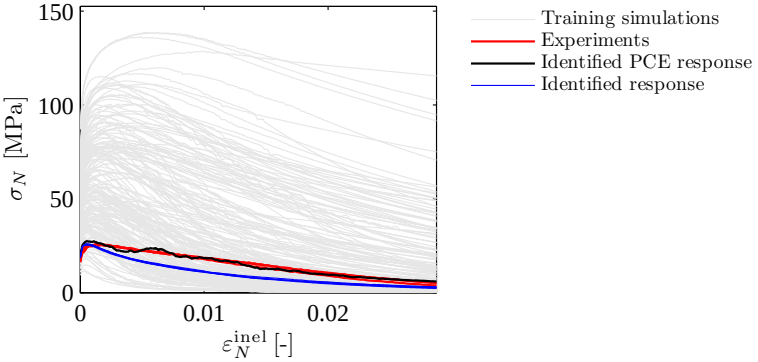

Figure 3. Comparison of experimental data and model response corresponding to the identified parameters for the uniaxial compression test.

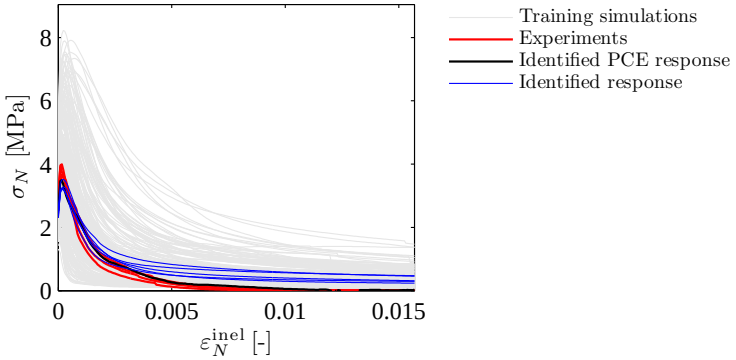

Figure 4. Comparison of experimental data and model response corresponding to the identified parameters for the notched three-point-bending test.

While the increasing part of the stress-strain diagrams is fitted satisfactorily, the approximation error is mainly related to their decreasing part. The problem can be explained with help of Figure 5 which shows a scatter diagram with maximal nominal stress σ_N on the vertical axis and area

below the considered stress-strain curve $A = \int \sigma \mathrm{d}\varepsilon$ on the horizontal axis. From this point of view, the experimental data lie outside the training simulations and the model approximation is forced to extrapolate.

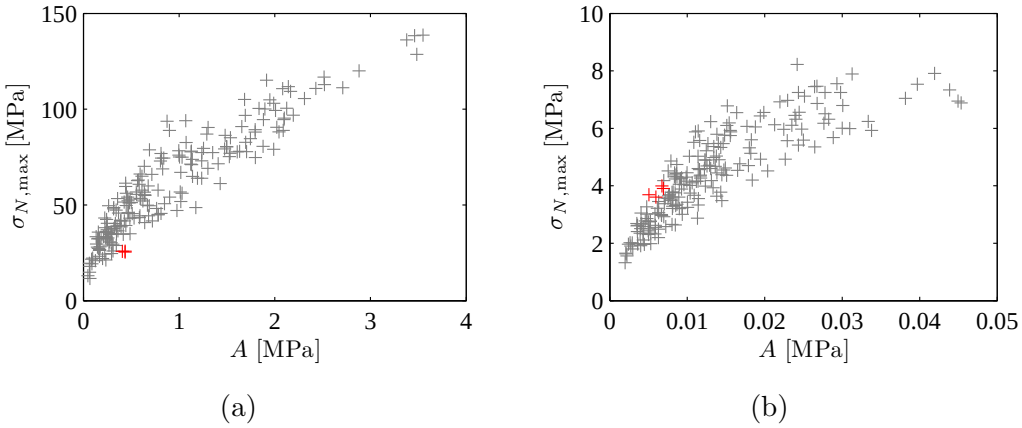

Figure 5. Comparison of integrals of training and experimental curves for uniaxial compression test (a) and three-point-bending test (b).

The unsuccessful calibration of the full model is apparently caused by the inappropriate prior parameters' distribution. The results of sensitivity analysis shown in Figure 6 can help us to estimate the model parameters, which are already identified well and which the decreasing part of the stress-strain curves is sensitive to so they probably cause the problematic approximation error.

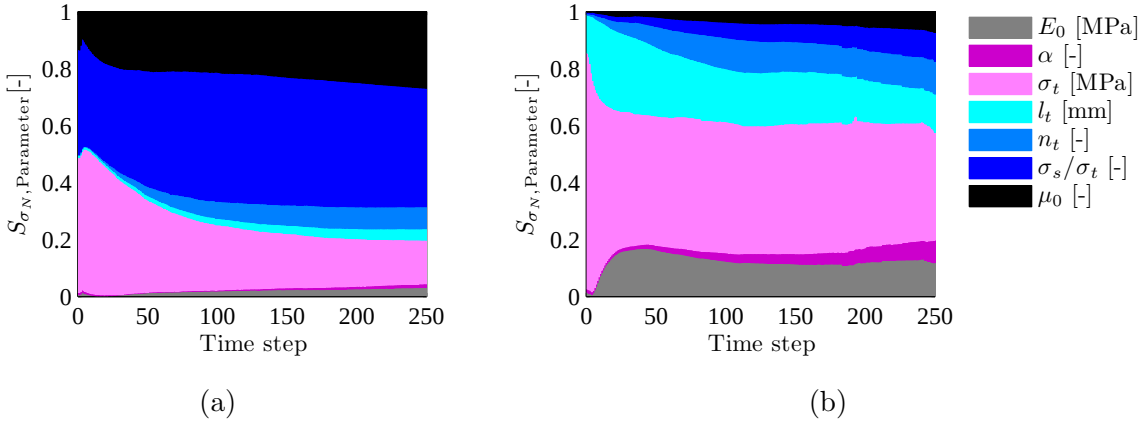

Figure 6. Sensitivity analysis for uniaxial compression test (a) and three-point-bending test (b) based on Sobol indices computed from PCE approximation.

We estimate that tensile strength σ_t and shear/strength ratio σ_s/σ_t can be identified well while softening exponent n_t, shear-normal coupling α and initial friction μ_0 can be the problematic parameters. The posterior mean values of the latter two are also very near to the upper bound of the prior uniform distribution which supports our assumption. Unfortunately, to this day we do not

have the necessary additional simulations to confirm this and provide an appropriate calibration of the examined material model.

5. Conclusions

The employed identification procedure is an efficient tool for calibration of nonlinear models allowing to take into account epistemic uncertainties caused by e.g. experimental errors or a small number of experimental data. Usage of PCE-based model approximation enables to handle the computational requirements of Markov chain Monte Carlo sampling of the posterior distribution. In this contribution, the calibration of the lattice discrete particle model for concrete does not succeed properly because of the inappropriate choice of prior range of the parameters values, which leads to the inaccurate approximation of the model response. In other words, the obtained parameters' distribution is correct with respect to the PCE-based model approximation, which however significantly differs from the full numerical model. This inaccuracy can be overcome by prescribing a new prior ranges for the evaluated parameters to obtain the necessary information for constructing the accurate model approximation.

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