Modelling of polymorphic uncertainty in the mesoscopic scale of reinforced concrete structures

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ABSTRACT: The realistic modelling of structures is essential for their numerical simulations and is mainly characterized by the mechanical model and the consideration of the available data at hand by an adequate uncertainty model. The key idea in this contribution is the consideration of polymorphic uncertainty at the numerical structural analysis and the mechanical modelling for reinforced concrete structures, which are characterized by a combination of heterogeneous concrete and different types of reinforcement (e.g. steel bars or carbon fibres mats). Typically, the reinforcement is denoted by another length scale, compared to the overall structure size. The formulation and development of a computational homogenization approach, considering the different homogeneous and heterogeneous characteristics of a macroscopic structure, is essential for a precise numerical computation. In recent years, focal point of research was on structural analysis considering uncertain material or geometry parameters. Probabilistic approaches are dominating the uncertainty consideration currently, although they are connected with certain disadvantages and limits. In this contribution, a generalized uncertainty model is utilized in order to take variability, impression and incompleteness in to account. That allows a separated evaluation of the influence for each uncertainty source on the results. Therefore, polymorphic uncertainty models are applied and developed by combining and extending aleatoric and epistemic uncertainty, resulting e.g. in the formulation of the uncertainty model "fuzzy p-box" or "fuzzy probability based randomness". The information of the different length scales is considered to be uncertain, e.g. the geometry or the material properties of a representative volume element (RVE) at the mesoscale. Subsequently, the uncertainty of the behaviour of a macro structure is derived from uncertain results on the meso structure. Since the computational effort of such investigations is tremendous, highly developed meta-models (recurrent neural networks) are applied in order to replace the uncertain RVE responses.

1. Introduction

In the numerical simulation of structures in general and reinforced concrete structures in particular, the consideration of uncertain material as well as geometric parameters are crucial for a comprehensive evaluation of the structural performance. In order to distinguish different types of uncertainty, it is common to characterize between aleatoric and epistemic uncertainty models. Both types cover different uncertainties mostly defined by characteristic deficits of data or data quality, consequently merged uncertainty models are referred to as polymorphic uncertainty. Aleatoric uncertainty originates in the natural variablity of a certain quantity, and it is therefore legitimate to assume probability theory as uncertainty model. The possibilities to consider stochastic quantities in structural analysis engineering applications are versatile, as is shown in e.g. Götz et al. (2015). The application of stochastic analysis is partially common in research (see Jenkel et al. (2015)), whereas epistemic and furthermore polymorphic uncertainty models are not equally widespread yet. An profound overview of applicable methods is provided by Möller and Beer (2004). Unlike the stochastic approach, epistemic models describe uncertainty due to e.g. lack of knowledge or incompleteness. Fuzzy sets (see Viertl (1995)) or e.g. interval variables are suitable uncertainty models for epistemic uncertainty, whereas fuzzy probability based random variables or *p*-boxes are representative imprecise probability models.

In case of heterogeneous materials or composites in general, homogenization methods are applied in continuum mechanics. This approach is motivated by large length scale differences of composite structures between their meso (or micro) and macro structure. Thus, the link is denoted between structural investigations at a large length scale and the material behaviour at a small length scale as pointed out in Fleischhauer et al. (2016). Multiple approaches such as e.g. FE^2-method are described e.g. in Hashin (1983); Smit et al. (1998); Miehe et al. (1999); Moulinec and Suquet (1998); Feyel and Chaboche (2000); Kouznetsova (2002). Depending of the considered size of the inclusions, e.g. aggregates or reinforcement in concretes, the smaller scale is named meso scale, whereas the larger length scale is referred to as macro scale. The core idea of the FE^2-method is the assumption of an homogeneous material on the macro scale, whose behaviour is identified from boundary value problems (BVPs) on the meso scale. These mesoscopic BVPs are performed on certain subsection of the material of interest, which is assumed to contain all characteristic features of the material's meso structure. This subsection is named representative volume element (RVE), as introduced in e.g. Hill (1963). The described FE^2-approach is still computationally very demanding, but it can also be used to perform virtual numerical tests on materials (see Terada et al. (2013)). For this purpose very simple macroscopic problems are subjected, e.g. plain tension or shear tests. In these cases, only one quadrature point is necessary and a single stress-strain curve of the heterogeneous material is obtained. This information may be used to deduct homogenized properties of the material, which can be used in a more sophisticated material law on the macro scale.

The contribution is structured as follows. Uncertainty concepts such as interval, fuzzy and fuzzy probability based random variables are introduced. A simplified concept of homogenization, considering small strains is presented and utilized in one example structured. Therefore, the mesoscopic model of concrete is described and further investigated with respect to the evaluation of the uncertain stiffness tensor, which is latter considered in an uncertain macroscopic structural example. The resulting uncertain stresses are exemplarily evaluated.

2. UNCERTAINTY

It is common to distinguish between two general concepts of uncertainty, namely aleatoric and epistemic uncertainties. Where aleatoric uncertainty models, such as randomness, incorporates the variability of data or measurements, epistemic uncertainty considers e.g. incompleteness due to lack of knowledge or a small amount of available data. In the following section general uncertainty models are presented.

2.1. *Uncertainty Models*

Interval variables can be utilized in cases of e.g. few to none data samples or if no realistic assessment of certain data points is possible or reasonable. In contrast to deterministic values, the characteristic function of an interval variable (see Viertl (1995); Götz et al. (2015); Götz (2017)) is defined as

$$\chi_I : \mathbb{R} \mapsto \{0,1\}, x \mapsto \begin{cases} 1, & x \in I \\ 0, & x \notin I \end{cases} . \tag{1}$$

(2)

Subsequently an interval variable can be defined by its boundaries

$$I = [x_l, x_r] = x^{\mathrm{I}},\; x_l, x_r \in \mathbb{R} \wedge x_l < x_r\,. \tag{3}$$

If it seems suitable to asses weightings (e.g. due to expert knowledge) to certain parameter ranges, an interval variable can be extended to a fuzzy-variable, where the corresponding membership function (characteristic function) according to Götz (2017); Möller and Beer (2004) is stated as

$$\mu : \mathbb{R} \mapsto [0,1] \tag{4}$$

holding the property

$$\exists\, x \mid \mu(x) = 1 \; . \tag{5}$$

A resulting fuzzy set (or fuzzy variable, introduced by Zadeh (1965)) can be represented by discrete α-levels

$$A^{\mathrm{f}}_{\alpha} = \{x \in \mathbb{R} \mid \mu_{A^{\mathrm{f}}} \geq \alpha\} \text{ with } \alpha \in]0,1] \; , \tag{6}$$

whereas, in case of an one-dimensional fuzzy variable, each α-level shall be expressed as an interval variable (see Eq. (3))

$$A^{\mathrm{f}}_{\alpha} \subseteq \mathbb{R},\, A^{\mathrm{f}}_{\alpha} = [x_l, x_r]_{\alpha} = (A^{\mathrm{I}})_{\alpha} \; . \tag{7}$$

A convex fuzzy variable is therefore composed by multiple discretized α-levels

$$A^{\mathrm{f}} = \left(A^{\mathrm{f}}_{\alpha}\right)_{\alpha \in]0,1]} \; . \tag{8}$$

If one adheres to the idea of interval-based representation of α-levels, it becomes obvious that an interval analysis as uncertainty quantification method could be extend to a fuzzy analysis, simply by repetitive utilization and previous possibility assessment. A combination with probabilistic approaches towards polymorphic uncertainty methods is extensively discussed in e.g. Möller and Beer (2004); Pannier et al. (2013); Götz et al. (2015).

The definition of fuzzy probability based random variables (*fp-r*) is founded on the assumption that the probability distribution of a random variable X cannot be described exactly due to a lack of information, see e.g. Götz et al. (2015); Pannier et al. (2013). Thus, a fuzzy probability distribution and a fuzzy probability space $(\Omega, \Sigma, \hat{P})$ can be introduced. The fuzzy probability $\hat{P}$ is represented as family of α-cuts

$$\hat{P} = (P_{\alpha})_{\alpha \in (0;1]} \; . \tag{9}$$

Each event $A \in \Sigma$ is related by P_{α} to an interval $[P_{\alpha,l}(A); P_{\alpha,r}(A)]$ for all $\alpha \in (0,1]$ such that the following condition is fulfilled

$$0 \leq P_{\alpha,l}(A) \leq P_{\alpha,r}(A) \leq 1 \; . \tag{10}$$

A fuzzy probability based random variable X is defined by the mapping of the fuzzy probability space onto the observation space $X : \Omega \rightarrow \mathbb{R}$. The fuzzy probability distribution $\hat{P}_X$ is formulated as family of mappings $\hat{P}_X = ((P_X)_{\alpha})_{\alpha \in (0;1]}$, with

$$\begin{aligned} (P_X)_{\alpha} &: \mathscr{B}(\mathbb{R}) \rightarrow \{[l,r] \mid 0 \leq l \leq r \leq 1\} : \\ & I \mapsto P_{\alpha}(X^{-1}(I)) \\ & \quad = [P_{\alpha,l}(X^{-1}(I)), P_{\alpha,r}(X^{-1}(I))] \; . \end{aligned} \tag{11}$$

The fuzzy probability distribution might be represented by a fuzzy cumulative distribution function $\hat{F}_X$, which is again defined as family of α-cuts

$$\hat{F}_X = ((F_X)_{\alpha})_{\alpha \in (0,1]} \tag{12}$$

with an arbitrary cumulative distribution function $F(x)$. The applied cumulative distribution function is usually defined by distribution parameters θ in terms of $F(x,\theta)$. Then, the fuzzy cumulative distribution function $\hat{F}_X$ can be described with fuzzy distribution parameters $\tilde{\theta}_i = (\theta_{i,\alpha})_{\alpha \in (0,1]}$. For example, a two parametric distribution function with parameters θ_1 and θ_2 yields

$$\hat{F}_X = (\{F_{\theta_1 \times \theta_2} \mid \theta_1 \in \tilde{\theta}_{1,\alpha}, \theta_2 \in \tilde{\theta}_{2,\alpha}\})_{\alpha \in (0,1]} \; . \tag{13}$$

This formulation is referred to as bunch parameter representation, since the fuzzy cumulative distribution and the fuzzy probability density function can be considered as assessed bunches of functions which are described by bunch parameters $\tilde{\theta}_i$.

2.2. *Uncertainty Analysis*

3. HOMOGENIZATION SCHEME

Assuming that concrete (without any reinforcement elements) could be considered as an isotropic material or particulate composite, where particles of phase are randomly distributed in a second matrix phase, a comparably simple homogenization scheme is used to represent the uncertainty propagation over the different length scales. For reasons of computability Hooks law is assumed as constitutive law on both length scales.

The effective properties at macro-scale are determined by the volume average of the corresponding quantity at meso-scale. Which yields to

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij}\mathrm{d}V \qquad \text{and} \quad \bar{\varepsilon}_{kl} = \frac{1}{V}\int_V \varepsilon_{kl}\mathrm{d}V\,. \tag{14}$$

Further details are presented e.g. by Hashin (1983). The effective stiffness is determined analogously, such that

$$\frac{\partial\bar{\sigma}_{ij}}{\partial\bar{\varepsilon}_{kl}} = \bar{\mathbb{C}}_{ijkl} = \frac{1}{V}\int_V \frac{\partial\sigma_{ij}}{\partial\varepsilon_{mn}} : \frac{\partial\varepsilon_{mn}}{\partial\bar{\varepsilon}_{kl}}\mathrm{d}V \tag{15}$$

$$\bar{\mathbb{C}}_{ijkl} = \frac{1}{V}\int_V \mathbb{C}_{ijmn} : \mathbb{I}_{mnkl}\mathrm{d}V \tag{16}$$

$$\bar{\mathbb{C}}_{ijkl} = \frac{1}{V}\int_V \mathbb{C}_{ijkl}\mathrm{d}V\,. \tag{17}$$

Alternatively a numerical material test (see Ostoja-Starzewski (2006)) is utilisable in order to determine the coefficients of the effective stiffness tensor. By introducing the Hill-Mandel condition Hill (1963) (in case of small strains)

$$\overline{\boldsymbol{\sigma}:\boldsymbol{\varepsilon}} = \overline{\boldsymbol{\sigma}}:\overline{\boldsymbol{\varepsilon}}\,, \tag{18}$$

boundary conditions, such as e.g. linear displacement boundary conditions could be derived

$$\boldsymbol{u}(\boldsymbol{x}) = \varepsilon_0\boldsymbol{x} \quad \forall\boldsymbol{x}\in\partial\mathscr{B}\,. \tag{19}$$

Uniform traction boundary conditions as well as periodic boundary conditions are applicable as well, whereas it is notable that the interchanging of boundary conditions yields a change in effective stiffness values.

Under the previous constitutive assumptions on the meso-scale, the uncertainty of an interval (or fuzzy) valued effective stiffness influences macroscopic stresses as follows

$$\bar{\sigma}^{\mathrm{I}} = \bar{\mathbb{C}}^{\mathrm{I}} : \varepsilon \tag{20}$$

$$= \left(\bar{\mathbb{C}}_m \pm \frac{\bar{\mathbb{C}}_\Delta}{2}\right) : \varepsilon = \bar{\sigma}_m \pm \frac{\bar{\sigma}_\Delta}{2} \tag{21}$$

$$\bar{\mathbb{C}}^{\mathrm{I}} = [\bar{\mathbb{C}}_l, \bar{\mathbb{C}}_r] = \bar{\mathbb{C}}_m \pm \frac{\bar{\mathbb{C}}_\Delta}{2} \quad , \bar{\mathbb{C}}_\Delta = \bar{\mathbb{C}}_r - \bar{\mathbb{C}}_l\,. \tag{22}$$

4. MESOSCOPIC MODEL OF CONCRETE

One approach in multi scale analysis of concrete structures is the separation into two length scales (macro and meso), whereas the macro scale defines the overall homogeneous macroscopic structure and the meso scale the heterogeneity by means of an representative volume element (RVE) containing aggregates, pores, cement phase and optionally different types of reinforcements. Despite the reinforcement, the accurate modelling of aggregates seems crucial in order to determine the representative material parameters of the composite structure. In civil engineering the grading curve defines the distribution of different size aggregates within one concrete mixture.

Based on Unger (2009), the aggregates are simplified by three dimensional ellipsoids where the principle radii are determined with respect to the medium radius r_2

$$r_1 = \left(1 + u_1\frac{m-1}{m+1}\right) r_2 \tag{23}$$

$$r_3 = \left(1 - u_3\frac{m-1}{m+1}\right) r_2 \text{ with } r_1 \geq r_2 \geq r_3\,, \tag{24}$$

and two realisations u_1, u_3 of uniformly distributed random variables. The flatness of the ellipsoids is defined by the parameter m. Conclusively the volume of one aggregate is denoted as

$$V = \frac{4}{3}\pi^3 r_2^3\left[1 - \left(\frac{m-1}{2(m+1)}\right)^2\right]\,. \tag{25}$$

The grading curve contains the volume-percentage of aggregates passing through a sieve of a predefined size. Due to the sequential decrease of the sieve diameters the grading curve represents the mass or volume percentage of a certain mineral size classes k (defined by minimal $d_{\mathrm{min},k}$ and maximal diameter $d_{\mathrm{max},k}$) in the entire aggregate volume. On basis of logarithmic size distribution, the principle diameter $d_{2,k}$ for each mineral size classes is defined as

$$d_{2,k} = \frac{d_{\mathrm{max},k}\, d_{\mathrm{min},k}}{\sqrt{u_2 d^3_{\mathrm{min},k} + (1-u_2) + d^3_{\mathrm{max},k}}}\,. \tag{26}$$

A sampling scheme is carried out for each mineral size class in a decreasing order, where each aggregate is evaluated in order to avoid intersections with existing aggregates, pores or reinforcement elements. In Fig. 1 a resulting numerical model is depicted, which is utilized for the computation of the effective stiffness.

4.1. Uncertain quantities

In the following example, the impact of mesoscopic uncertain material parameters as well as geometric properties are investigated. All uncertain quantities are assumed as interval variables. The bounds of the Young's moduli for mortar E_c and aggregates E_a are determined by a tolerance of $\pm 10\%$ related to a mean value, resulting in

$$E_\mathrm{c}^\mathrm{I} = [27000, 33000] \text{ MPa} \tag{27}$$

$$E_\mathrm{a}^\mathrm{I} = [47148, 57625] \text{ MPa}\,. \tag{28}$$

Additionally the volume fraction of the cement phase to aggregates is bounded by $v_\mathrm{f}^\mathrm{I} = [0.3, 0.4]$. It is obvious that it is hardly possible to maintain a deterministic grading curve in production process. Therefore an upper and lower boundary for the grading curve is assumed as depicted in Fig. 2. The corresponding intervals for the volume percentage passing the different sieve sizes are listed in Tab. 1 regarding the second principle diameter for the largest three mineral size classes.

An interval analysis yields the extremal boundaries of the single coefficient of the effective (see.

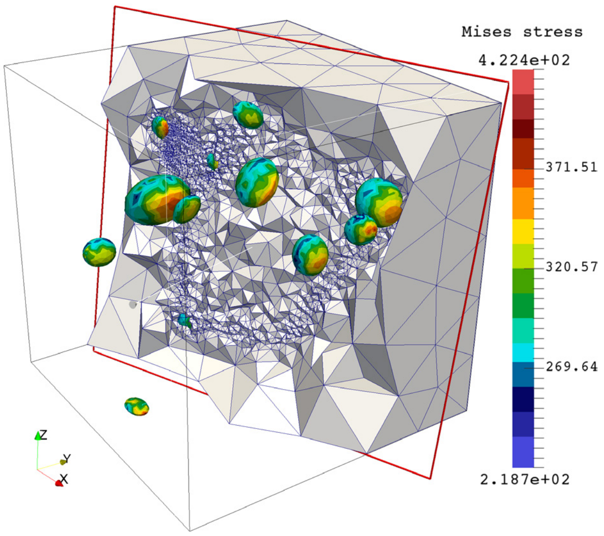


Figure 1: Mesoscopic structural model of concrete (RVE)

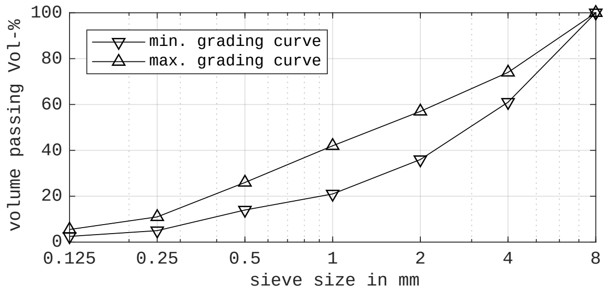


Figure 2: Interval valued grading curve of aggregates

d_2 in mm	Vol-%
2	$[36, 57]$
4	$[61, 74]$
8	$[100, 100]$

Table 1: Interval valued volume of passing aggregates for each principle diameter d_2

Eq. (17)) stiffness values $[\bar{\mathbb{C}}_l, \bar{\mathbb{C}}_r]_{ijkl}$. The representation in Voigt-notation and by its mean values $(\cdot)_m$ and element wise deviation $(\cdot)_\Delta$ yields to

$$\bar{\mathbb{C}}_m = \begin{bmatrix} 66961.9 & 16740.4 & 16740.4 & 0.0 & 0.0 & 0.0 \\ 16740.4 & 66961.9 & 16740.4 & 0.0 & 0.0 & 0.0 \\ 16740.4 & 16740.4 & 66961.9 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 25110.7 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 25110.7 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 25110.7 \end{bmatrix}^\mathrm{V}, \tag{29}$$

$$\bar{\mathbb{C}}_\Delta = \begin{bmatrix} 20140.9 & 5035.2 & 5035.2 & 0.0 & 0.0 & 0.0 \\ 5035.2 & 20140.9 & 5035.2 & 0.0 & 0.0 & 0.0 \\ 5035.2 & 5035.2 & 20140.9 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 7552.8 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 7552.8 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 7552.8 \end{bmatrix}^\mathrm{V}. \tag{30}$$

It shall be mentioned, that the overall stiffness is overestimated due to the edge size of the RVE (40 mm). However, a size study of the RVE revealed convergence to a more realistic level with increasing RVE edge size. Since a RVE of greater volume comes with more aggregates, the mesh could contain more then 10^6 nodes, which leads, even with utilization of parallel computing within the interval analysis, to a unserviceable computation time. Therefore the presented values should be interpreted as an exemplary proof of concept for the computational algorithm in order to consider uncertainty within the numerical simulation.

5. MACRO SCALE EXAMPLE

The influence of a uncertain stiffness matrix is demonstrated at a macro structure. For reasons of simplification a Hookean-material is assumed, where the values of the elasticity tensor are taken from the RVE (see Eqs. (29),(30)).

The exemplary macro structure is a beam, where both ends are restrained (see. Fig 3). As depicted, a horizontal as well as vertical load $F = 4\,\text{kN}$ is applied in the middle cross section. The numerical

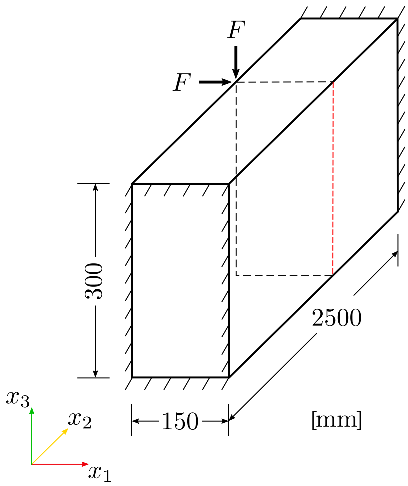
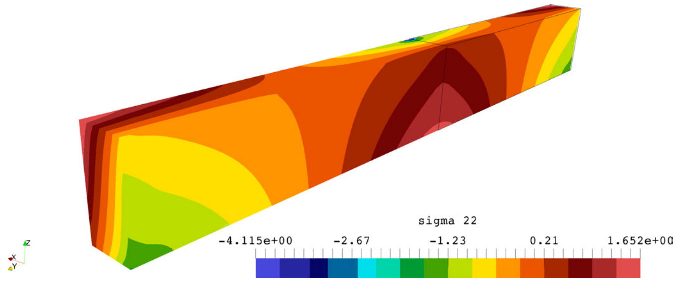
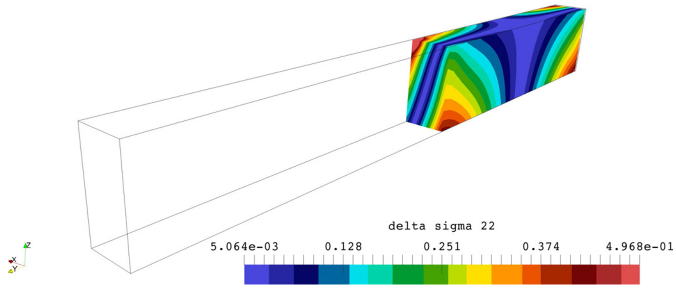


Figure 3: Macroscopic structure example

simulation of the stress mean values and the deviation is performed according to Eq. (20). Stress σ_{22} is depicted in Fig. 4a and related deviations $\sigma_{\Delta,22}$ in Fig. 4b. The dashed red line is indicating the edge where the uncertain stresses are evaluated. As it can be seen, the uncertainty is proportional to the stress value itself, which indeed is plausible due to



(a) Stress σ_{22} at macroscopic structure



(b) Stress deviation $\sigma_{\Delta,22}$ at macroscopic structure

Figure 4: Stress distribution due to uncertain structural analysis

linear elasticity. The resulting uncertainty can be interpreted as inherent material property deviations, since the actual numerical analysis is a purely deterministic computation. If one would additionally assume e.g. uncertain loading conditions the stress deviation would turn out to be greater, at least in case of the Hookean material.

With respect to the outlook of a non-linear material model the prediction of the uncertain results is not as obvious as in the presented case, due to e.g. local damage occurrence. Nevertheless, the proposed process from meso-scale uncertainty to uncertain macroscopic mechanical properties remains equal and can be adopted to more advanced material models on RVE-level.

6. SUMMARY & OUTLOOK

In this contribution, a procedure for structural analysis incorporating polymorphic uncertain material parameters on different length scales is presented. Namely interval, fuzzy and fuzzy probability based random variables are introduced, and proposed as suitable uncertainty models for material properties due to consideration of e.g. variability, imprecision, lack of knowledge or incompleteness. In order to embed the uncertain analysis into a multi scale struc-

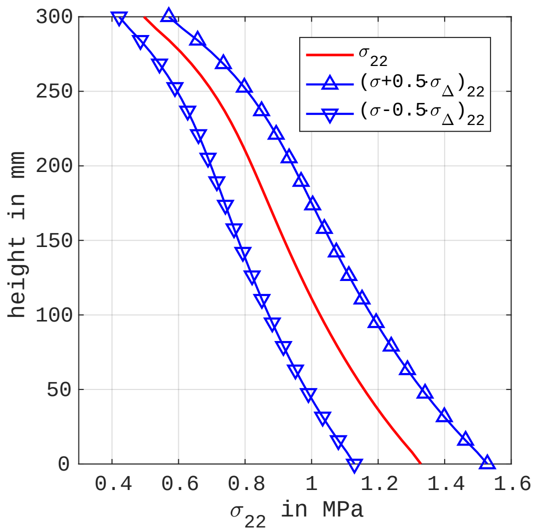


Figure 5: Ucnertainty in macroscopic stress σ_{22} due to uncertainty on meso-scale

tural analysis, separate uncertainty analyses for each length scale are proposed, which concludes in an overall staggered computational procedure. This concepts implies the transition of uncertainty by its representation with representative and uncertainty quantifying measures enabling an deterministic description of the uncertain quantities. Separating the individual uncertainty analysis comprises the possibility to investigate the influence of input uncertainty to effective properties on the particular length scale.

An representative volume element for concrete is presented in this contribution utilized in a numerical structural analysis. The numerical modelling as well as sampling scheme for the individual components of concrete are point out. Subsequently a exemplary evaluation of the uncertain effective stiffness based on micro scale interval uncertainty for concrete is evaluated and utilized in a structural analysis on macro scale. It is shown that evaluated stress deviation does origin in the quantified uncertainty on meso scale. Hence, no further uncertainty analysis is necessary, if this specific concrete is demanded in an structural analysis. Nevertheless, computational multi scale analyses are computational expensive regardless the consideration of uncertainty, which is additionally increasing the computational costs. Therefore surrogate models are under investigation as surrogate model for the constitutive law. The current focal point is on the utilization of recurrent neural networks as substitution for the representative effective measures as well as the uncertainty quantifying measures.

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