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A collocation scheme for deep uncertainty treatment

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ABSTRACT: Considering an uncertain correlation length of the input random fields described by a Karhunen-Loève expansion leads to a probability-box approach for the stochastic finite element computation. But, these computations are highly costly. Then, a stochastic collocation method using sparse grids within a Smolyak algorithm is proposed to reduce the computational cost, particularly in the context of non-linear computations. The interest and the development of the Smolyak algorithm for stochastic model with non-linear finite element methods regarding mixed, aleatory and epistemic, uncertain inputs are here introduced. The limitations of Smolyak algorithm are critically discussed and suggestions for improvement are made.

1. INTRODUCTION

Finite element method (FEM) is a powerful tool to solve partial differential equations, which is widely used in engineering application, particularly in the context of solid mechanics problems. In order to consider uncertain input parameters, several techniques have been developed to extend FEM to stochastic finite element method (SFEM). Moreover, the quantification of uncertainties may be distinguished into two kinds: *aleatory* uncertainties, due to the intrinsic randomness of the phenomena, and *epistemic* uncertainties, which are caused by lack of knowledge (der Kiureghian and Ditlevsen, 2009). In practice, however, engineers often face a mixture of both (Beer et al., 2013). For this reason, advanced approaches are required to handle deep uncertainties.

This distinction allows risk-informed decision-making even in the presence of epistemic uncertainty (Dubois and Guyonnet, 2010). Indeed epistemic uncertainties are not describable within the classical probability framework, but require dedicated tools such as interval analysis (Moens and Vandepitte, 2005), fuzzy description (Möller and Beer, 2004) or imprecise probabilities (Beer et al., 2013). In the context of finite element analysis, these approaches face two main challenges. The firs it to include the spatial variability as here, for example, the material properties are described as random fields. The second challenge is to reduce the computational cost of stochastic computations (Moens and Vandepitte, 2005).

In this contribution, random fields containing both kinds of uncertainties are considered as input material parameters. The input random fields are discretised using Karhunen-Loève expansion (KLE), where the random field is approximated by a series expansion around the mean field (Sudret and der Kiureghian, 2000). The variation within the random field is characterised by the correlation length. However, while the stochastic parameters, mean value and variance, can usually be found experimentally, the correlation length is difficult to determine. Therefore, this lack of knowledge is modelled by assuming the correlation length to be interval-valued.

Here, the mechanical applications of interest are non-linear computations to evaluate the risk reliability. Monte Carlo (MC) approaches, which would require a large number of sampling points to describe the mixed uncertainty, would be too time costly. In order to avoid high computational effort, sophisticated numerical approaches are required to evaluate the probability-box in reasonable computational cost. Among these methods, the Stochastic Collocation (SC) method (Xiu and Hesthaven, 2005) is investigated in this work as a more efficient alternative to MC computations of non-linear problems in solid mechanics, particularly.

The paper is structured as follows. The *probability box approach* is reviewed in Section 3. To increase efficiency, the probability box approach is combined with *stochastic collocation method* introduced in Section 4. The resulting algorithm is tested and analysed for non-linear material problems in Section 5.

2. RANDOM FIELD DISCRETISATION

Input parameters are described as random fields if their values vary with the position in the physical domain. Furthermore, for any couple of two points in the domain, their covariance gives a measure of their variance inter-dependency in the random field. For isotropic field, the covariance kernel describes the dependency of the correlation on the distance between two points. In this work, a Gaussian kernel is assumed, such that the covariance of the random field is given by

$$\mathrm{Cov}(x_1,x_2) = \sigma^2 \exp\left[\left(\frac{|x_1-x_2|}{l_c}\right)^2\right], \quad (1)$$

where l_c is the correlation length of the random field and should be identified from experiments. However this is often a difficult task and, here, the correlation length is treated as an epistemic uncertainty and modelled through an interval.

The first step for an improved efficiency in the computation of non-linear structural problems with finite element method is to discretise the random field by series expansion methods, such as the KLE, in order to reduce the number of random variables in the system. Using KLE, the random field is approximated as

$$\mathrm{Cov}(\mathbf{x}_1,\mathbf{x}_2) \simeq \sum_{n=1}^{T} \lambda_n \phi_n(\mathbf{x}_1)\phi_n(\mathbf{x}_2), \quad (2)$$

where T is the order of truncation of the series expansion, and λ_i and ϕ_i are the eigenvalues and eigenfunctions of the Fredholm integral equation

$$\int_\Omega \mathrm{Cov}(\mathbf{x}_1,\mathbf{x}_2)\phi_n(\mathbf{x}_1)d\mathbf{x}_1 = \lambda_n\phi_n(\mathbf{x}_2). \quad (3)$$

The solution of eq. (3) was done by Galerkin projection (Sudret and der Kiureghian, 2000; Ghanen and Spanos, 1991). The random field represented by the KLE may then be approximated as

$$\tilde{H}(\mathbf{x},\theta) = \mathbb{E}(\mathbf{x}) + \sum_{n=1}^{T} \sqrt{\lambda_n}\phi_n(\mathbf{x})\xi(\theta), \quad (4)$$

where $\xi(\theta)$ are standard normal random variables. A system with n_{RV} random fields is therefore reduced to $n_{RV} \times T$ random variables, which are treated as aleatory uncertainty. The normal random variables, ξ_i, may be sampled using MC or chosen by SC methods.

3. Probability box approach

In this work, it is proposed to capture the lack of knowledge of the correlation length by assigning it an interval-value. Then, the model is decomposed into aleatory uncertainty, in terms of the random distribution, e.g. mean, standard deviation, and epistemic uncertainty in terms of the correlation length. By modelling these deep uncertainties, the description of the randomness turns into a probability-box approach (Beer et al., 2013). Instead of assigning one cumulative distribution function $F_X(x)$ to the probability $P(X \leq x)$ of a random variable X, a probability family $\mathscr{P}$ is enveloped by a left bound $\overline{F}_X(x)$ and a right bound $\underline{F}_X(x)$:

$$\mathscr{P} = \{P \,|\, \forall x \in \mathbb{R}, \underline{F}_X(x) \leq F_X(x) \leq \overline{F}_X(x)\}. \quad (5)$$

This so-called probability box (p-box), depicted in Figure 1, $[\overline{F}_X(x), \underline{F}_X(x)]$ is minimally described by these two bounds but can be fed with additional information on the confidence intervals of the mean value m_X and the variance v_X or the distribution family $\mathscr{F}$ defining a quintuple p-box $\langle \overline{F}_X(x), \underline{F}_X(x), m_X, v_X, \mathscr{F} \rangle$ (Beer et al., 2013).

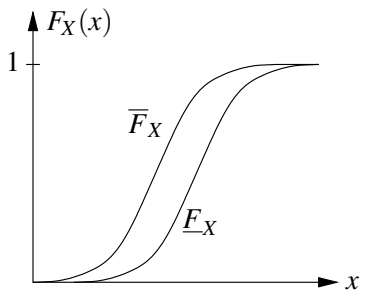


Figure 1: Probability box (p-box) defined by a left bound $\overline{F}_X$ and a right bound $\underline{F}_X$.

Numerically, p-boxes can be handled by sampling or discretisation (Zhang et al., 2010). The numerical complexity is higher than for usual stochastic models. Thus, basic sampling methods such as crude MC method can be not affordable and face the *curse of dimensionality*. This problem becomes more important for non-linear problems, which are already associated with a larger computational effort in deterministic analyses, or for reliability analysis in which unlikely events are of importance.

In order to reduce the number of realisations at a fixed number of random input variables, sophisticated sampling methods are required. Among several advanced Monte Carlo techniques (Stefanou, 2009), SC method has turned out to be a promising approach to improve the stochastic model. One approach based on Smolyak algorithm is introduced and discussed in the following.

4. Stochastic collocation method

Regard within a probability space $(\Omega, \mathscr{F}, P)$ the stochastic partial differential equation (SPDE)

$$\begin{aligned} \mathscr{L}(\omega, x; u) &= f(\omega, x), \quad x \in \mathscr{D} \\ \mathscr{B}(\omega, x; u) &= g(\omega, x), \quad x \in \partial\mathscr{D}, \end{aligned} \quad (6)$$

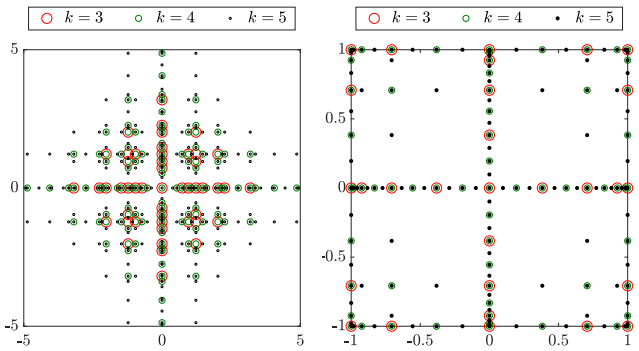
where $\omega \in \Omega$. The differential operator $\mathscr{L}$ and the boundary operator $\mathscr{B}$ as well as the functions f and g may be random. Then, the primary variable u becomes a stochastic function $u(\omega, x) : \Omega \times \mathscr{D} \to \mathbb{R}$ (Xiu and Hesthaven, 2005).

The basic idea of SC is the same as MC, to solve the FE problem in repetitive deterministic simulations. However, the input is not sampled randomly but chosen specifically as so-called *collocation points* (Xiu and Hesthaven, 2005). The set of N-dimensional collocation points $\Theta_N = \{Y_i^N\}_{i=1}^{n_{CP}} \in \Gamma$ in the random space $\Gamma \subset \mathbb{R}^N$, is defined by a grid, here a sparse grid, as illustrated in Figure 2 for the specific cases of Gauss-Hermite and Clenshaw-Curtis grids.

Inserting the collocation points into eq. (6), the SPDE reads

$$\begin{aligned} \mathscr{L}(Y_i^N, x; u) &= f(Y_i^N, x), \quad x \in \mathscr{D} \\ \mathscr{B}(Y_i^N, x; u) &= g(Y_i^N, x), \quad x \in \partial\mathscr{D}, \end{aligned} \quad (7)$$

and can be solved deterministically for each i. Note that Smolyak provides a fast convergence only for problems which are sufficiently smooth within the random space (Xiu and Hesthaven, 2005).



(a) Non-bounded Gauss-Hermite grid *(b) Nested Clenshaw-Curtis grid*

Figure 2: Two-dimensional sparse grids for levels $k = 3$, $k = 4$ and $k = 5$

4.1. Sparse grid construction

Smolyak algorithm defines the set Θ_N by combining the one-dimensional sets Θ^i following

$$\Theta_N = \bigcup_{q-N+1\leq|i|\leq q} \left(\Theta^{i_1} \times \cdots \times \Theta^{i_N}\right), \tag{8}$$

where $i = (i_1, ..., i_N) \in \mathbb{N}^N$ is a multi-index containing the order of interpolation i_j for each stochastic dimension $j = 1, ..., N$ such that $|i| = i_1 + ... + i_N$. Furthermore, q is a parameter defining the bounds and is usually chosen to be $q = N + k$, where $k \in \mathbb{N}$ is called Smolyak level. For a multi-dimensional problem, the number of points in the dimension j described by an interpolation of level i_j equals to

$$m_{i_j}^j = \begin{cases} 1, & \text{if } i_j = 1, \\ 2^{i_j-1}+1, & \text{if } i_j > 1. \end{cases} \tag{9}$$

The points can be chosen following various rules which lead to different kind of grids characterised by their own properties. Most common is the nested *Clenshaw-Curtis grid* defined on $[-1,1]^N$, where the points are chosen as the extrema of the Chebychev polynomials. Alternatively, *Gauss-Hermite grids* are defined on $]-\infty,\infty[^N$, but they are not nested.

After solving the FE problem for every collocation point, the stochastic outcome is obtained as an interpolation following Smolyak algorithm including the input probability distribution.

4.2. Polynomial interpolation of the stochastic moments

Smolyak algorithm defines the N-dimensional interpolant $\mathscr{I}(u)$ as a combination of the one-dimensional interpolants $\mathscr{U}^i(u)$:

$$\mathscr{I}(u) = \sum_{q-N+1\leq|i|\leq q} \eta(|i|) \cdot \left(\mathscr{U}^{i_1} \otimes \cdots \otimes \mathscr{U}^{i_N}\right), \tag{10}$$

$$\mathscr{U}^i(u) = \sum_{k=1}^{m_i} u(Y_k^i) \cdot H_k^i, \tag{11}$$

where the factor $\eta(|i|)$ is defined as

$$\eta(|i|) = (-1)^{q-|i|} \cdot \binom{N-1}{q-|i|}. \tag{12}$$

For the polynomial basis function H_k^i, usually Lagrange polynomials are chosen.

The stochastic moments of the outcome can be estimated by the polynomial interpolation. For instance, the expected value $\mathrm{E}(u)$ is estimated as

$$\mathrm{E}(u) = \sum_{q-N+1\leq|i|\leq q} \eta(|i|) \cdot \sum_{k_1=1}^{m_{i_1}} \cdots \sum_{k_N=1}^{m_{i_N}} u(Y_{k_1}^{i_1}, \ldots, Y_{k_N}^{i_N}) \cdot \mathscr{S}_k(Y), \tag{13}$$

where the integral

$$\mathscr{S}_k(Y) = \int_\Gamma \left(H_{k_1}^{i_1} \otimes \cdots \otimes H_{k_N}^{i_N}\right) f_Y(Y)\,\mathrm{d}Y \tag{14}$$

incorporates the probability density function $f_Y(Y)$ of the input random variables evaluated at the collocation points. Analogously, the variance is determined by

$$\mathrm{Var}(u) = \sum_{q-N+1\leq|i|\leq q} \eta(|i|) \cdot \sum_{k_1=1}^{m_{i_1}} \cdots \sum_{k_N=1}^{m_{i_N}} \left[u(Y_{k_1}^{i_1}, \ldots, Y_{k_N}^{i_N}) - \mathrm{E}(u)\right]^2 \cdot \mathscr{S}_k(Y). \tag{15}$$

The numerical integration of $\mathscr{S}_k(Y)$ can become computationally costly for high stochastic dimensions.

Here, describing the input random fields using KLE as described in Section 2, the stochastic dimension is given by

$$N = \sum_{i=1}^{n_{RF}} T_i + n_{RV}, \tag{16}$$

where n_{RF} is the number of input random fields i truncated at order T_i and n_{RV} is the number of random variables. It can be noted that the problem becomes easily high-dimensional when random fields are involved.

5. An elasto-plastic test problem

Early work using SFEM considered mainly linear materials (Sudret and der Kiureghian, 2000). However, most of the mechanical failure involve some non-linear behaviour, which requires sophisticated numerical tools as the computational cost is largely increased. Here, a non-linear test problem with an elasto-plastic material behaviour is investigated.

The p-box approach is combined with the stochastic collocation method as follows. First, in an outer loop, the interval-valued correlation length is considered. Then, within an inner loop, the corresponding random field $X(x,\omega)$ is discretised by KLE and instead of sampling the standard normal variable, ξ_i, the coordinates of a Gauss-Hermite sparse grind are used (Jablonski, 2014).

5.1. Model description

The algorithm is tested on a two-dimensional test problem depicted in Figure 3. The 1 m $\times$ 1 m-square is discretised by 10×10 elements and compressed on its right side by a constant line load $q_0 = 300\ \frac{\mathrm{kN}}{\mathrm{mm}}$.

An elasto-plastic material model including linear kinematic hardening is considered. The yield stress σ_y is defined as a Gaussian random field discretised by KLE. The expected value is $\mathrm{E}(\sigma_y) =$ 240 MPa, the standard deviation $\mathrm{Std}(\sigma_y)$ is chosen to be $5\%\,\mathrm{E}(\sigma_y)$. The interval-valued correlation length is $l_c \in [0.5,\ 5.0]$ m . The series expansion of the random field is truncated at order T. For each term of the series expansion one dimension of random space is added. Hence, the stochastic dimension of the sparse grid (here Gauss-Hermite) needs to be equal to the order of truncation T. The outcome of interest is the equivalent plastic strain defined by

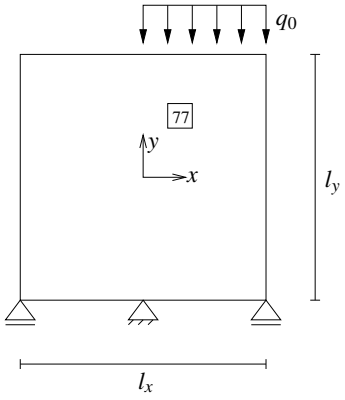


Figure 3: Plate compressed on its right side by a constant line load

$$\bar{\varepsilon}_p = \int_0^t \sqrt{\frac{2}{3}\dot{\varepsilon}_p : \dot{\varepsilon}_p}\,\mathrm{d}t. \tag{17}$$

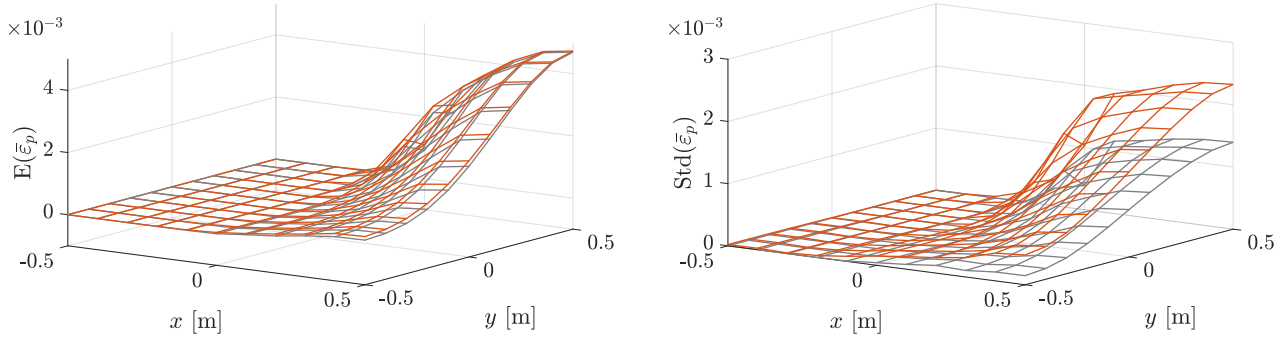
where $\dot{\varepsilon}_p$ is the rate of plastic strain, assuming infinitesimal deformation.

5.2. Results

The simulation is performed using a Smolyak level $k = 4$ and a truncation order of $T = 5$, which means $n_{\mathrm{SC}} = 1471$ realisations. The expected value $\mathrm{E}(\bar{\varepsilon}_p)$ is interpolated by eq. (13) from the set of all realisations. The expected value of the output random field is depicted in Figure 4a for the left and right bounds of the interval-valued correlation length. It seems apparent that the results of the expected value do not differ significantly, so the correlation length does not influence the expected value for the random field of interest.

However, the correlation length highly influences the standard deviation $\mathrm{Std}(\bar{\varepsilon}_p)$ defined as the square root of eq. (15), which is depicted in Figure 4b for the left and right bounds of the correlation length interval. The effect on the standard deviation is significant in the context of engineering applications as it affects the tails of the distribution function, which is the key information for reliability analysis.

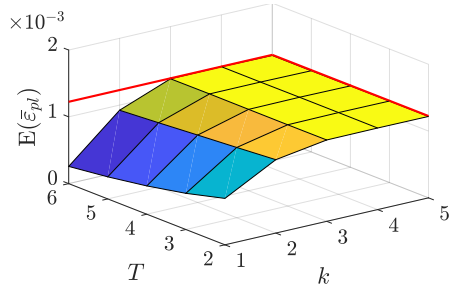
The number n_{SC} of collocation points depends on the Smolyak level k and the stochastic dimension N which here is equal to the truncation order T. To



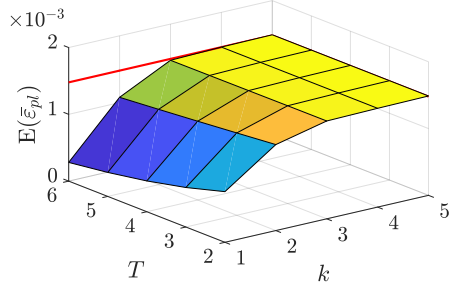
(a) Expected value $\mathrm{E}(\bar{\varepsilon}_p)$ *(b) Standard deviation* $\mathrm{Std}(\bar{\varepsilon}_p)$

Figure 4: Stochastic moments of the equivalent plastic strain for the bounds of the correlation length interval (left bound in grey, right bound in brown, $k = 4$*,* $T = 5$*)*

judge on the accuracy of the stochastic collocation results, a parameter study on k and T is performed and compared to the results of a converged Monte Carlo simulation using $n_{\mathrm{MC}} = 10^5$ samples. The results are analysed regarding element 77, which is marked in Figure 3.



(a) Left bound $l_c/l = 0.5$



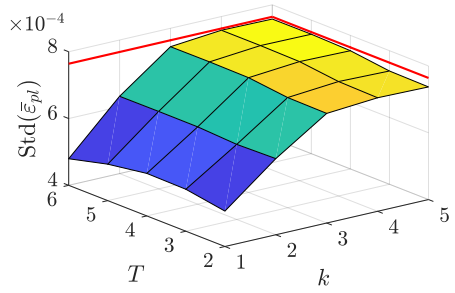
(b) Right bound $l_c/l = 5$

Figure 5: Expected value $\mathrm{E}(\bar{\varepsilon}_p)$ *of the equivalent plastic strain* $\bar{\varepsilon}_p$ *for different Smolyak levels k and orders of truncation T (stochastic dimension* $N = T$*) as well as MC reference solution (red line) with* $n_{MC} = 10^5$ *samples at element 77.*

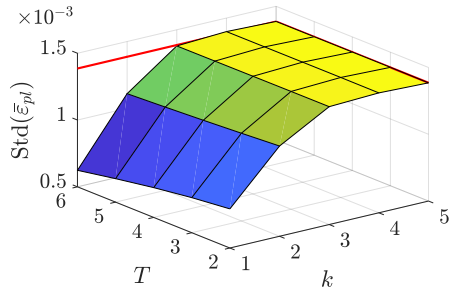
The convergence of the expected value $\mathrm{E}(\bar{\varepsilon}_p)$ towards the Monte Carlo reference solution (red line) is depicted in Figure 5 for the left and right bounds of the interval-valued correlation length. Here, the quality of the results is mainly depending on the Smolyak level k and to a lesser extent on the truncation order. However, the influence of T is still not negligible as it causes an error in the input random field affecting mainly its standard deviation. From the convergence plots it can be concluded that the chosen Smolyak level $k = 4$ is sufficient for the problem of interest.

In Figure 6, the convergence of the standard deviation at element 77 is shown. In the case of the left bound, the influence of the truncation order is noticeable, while the right bound also shows a good convergence for increasing k even for small T. This is due to the fact that for decreasing correlation lengths the truncation error increases when T is fixed. Still, an acceptable convergence is reached by Smolyak level $k = 4$.

The p-box $[\overline{F}_\varepsilon, \underline{F}_\varepsilon]^{\mathrm{el.77}}$ of the equivalent plastic strain $\bar{\varepsilon}_p$ at element 77 is depicted in Figure 7. It can be highlighted that here just a rough approximation of the distributions are given, as the sampling for post-processing has been avoided for this representation. However, this approximation allows one to observe that there is a significant difference between the two bounds of the p-box, which is in agreement with the difference in terms of standard deviation.



(a) Left bound $l_c/l = 0.5$



(b) Right bound $l_c/l = 5$

Figure 6: Standard deviation $\mathrm{Std}(\bar{\varepsilon}_p)$ *of the equivalent plastic strain* $\bar{\varepsilon}_p$ *for different Smolyak levels k and orders of truncation T (stochastic dimension* $N = T$*) as well as MC reference solution (red line) with* $n_{MC} = 10^5$ *samples at element 77.*

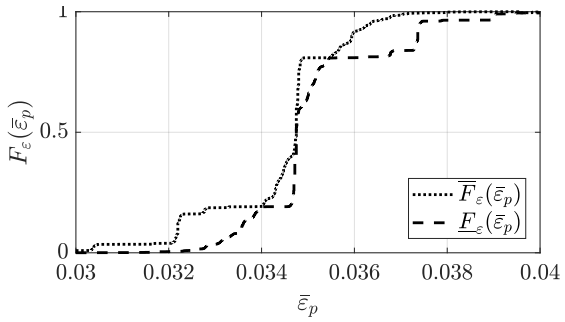


Figure 7: P-box of the equivalent plastic strain $\bar{\varepsilon}_p$ *at element 77*

It is to be noted that negative stochastic moments can occur for increased Smolyak level k. This is due to negative weights that are defined by the Smolyak algorithm (ven den Bos et al., 2017). For instance, in case of non-linear problems which are non-smooth enough, such as damage simulations, initial studies have shown that this problem may occur for some test cases. The convergence of the stochastic collocation method requires high Smolyak level, which leads to negative stochastic moments. However, this requires further investigation.

6. CONCLUSIONS

This paper dealt with stochastic finite element method considering random field input parameters, which are mixed, i.e. epistemic and aleatory, uncertain. To capture such deep uncertainty, a probability box approach has been suggested. For an efficient stochastic analysis, the approach has been combined with stochastic collocation method using sparse grids within a Smolyak algorithm.

The algorithm has been tested for non-linear material problems and compared to the results gained by a Monte Carlo simulation. Using an elasto-plastic material, sufficient convergence of expected value and standard deviation is reached using a Smolyak level $k = 4$ and a KLE truncation order of $T = 5$. Regarding the number of collocation points $n_{\mathrm{SC}} = 1471$ the time saved compared to the Monte Carlo simulation using $n_{\mathrm{MC}} = 10^5$ samples is significant. Higher stochastic moments will probably demand for more truncation terms. For this purpose, fast integration methods for high dimensions are required.

It has been found that an interval-valued correlation length mainly affects the standard deviation. This emphasizes the need for considering epistemic correlation lengths as long as there is no reliable information on its exact value.

The developed approach for including deep uncertainty in the FEM computation of non-linear problems in solid mechanics, may still lead to large computational cost for larger problems. One possibility to improve the efficiency of the algorithm is to use a hierarchical approach with nested sparse grids, e.g. by using Leja points. This would reduce the number of deterministic computations needed for higher levels of collocation points. In the case of three-dimensional models, the deterministic computation cost may also be reduced by combining the approach with model order reduction techniques.

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