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POLYUQ: A SOFTWARE TOOL FOR THE SIMULTANEOUS CONSIDERATION OF ALEATORY AND EPISTEMIC UNCERTAINTIES IN ENGINEERING PROBLEMS

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Abstract. *The adequate consideration of uncertain parameters in engineering applications is essential for a realistic prediction of state variables, such as displacements or stresses. Uncertainty is omnipresent and polymorphic. The source of the uncertainty and the quality of available information determine whether the uncertainty is aleatory, epistemic or a combination of both.*

Aleatory uncertainty is inherent, unavoidable, and irreducible. Sufficient statistical information is available for the corresponding parameters, enabling them to be modeled and quantified using stochastic variables within the framework of probability theory. Epistemic uncertainty, on the other hand, is avoidable, as it can generally be reduced by better models or additional data. Various uncertainty quantification approaches exist, such as Bayesian inference, random sets, p-boxes, or representations using non-stochastic variables based on possibility theory.

We present a software tool that allows the simultaneous definition of stochastic variables, interval variables, fuzzy variables, and mixed forms as input variables. Different input dependencies can also be considered before samples are automatically generated based on user-defined solution methods. For a given computational model, the desired output variables are then determined and graphically displayed using different evaluation methods in each uncertainty space. The influence of the uncertainty description on the results will be investigated on an academic example first. Then, results from studies on various engineering problems will be presented, followed by an outlook on further development steps.

Keywords: Polymorphic Uncertainty Modeling, Aleatory Uncertainty, Epistemic Uncertainty, Fuzzy-Stochastic Variables, MATLAB.

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1 INTRODUCTION

The numerical investigation of real-world problems always requires modeling. Good numerical models are as accurate as possible, but as complex as necessary, so an optimal balance between the opposing aspects of efficiency and accuracy should be found. Based on models that are as realistic as possible, reliable predictions can then be made. The efficiency and accuracy of these predictions depend, on the one hand, on the underlying structural model and, on the other hand, on the input variables to be considered. The model is always an approximation of reality, based on simplifications and subjective decisions in the modeling process, which result in unavoidable model uncertainties. Some input variables cannot be represented in the model or are deliberately neglected, leading to additional model uncertainty. Other input variables are integrated (simplified) taking into account their existing data uncertainty [10].

The influence of uncertainty has been studied for decades in various fields of application, such as weather and climate forecasting [20], geosciences [13], and nuclear energy [2]. In structural engineering, uncertainty quantification is mainly related to the design and optimization problems [3, 14], geotechnics [15] or system and parameter identification [21]. As part of the SPP 1886, funded by the DFG, several scientists across Germany have worked on various engineering questions regarding polymorphic (*πολύμορφος* (Greek) = multifaceted) uncertainty modeling in recent years [5, 19]. The foundation is that uncertainty is omnipresent and diverse. A classification into aleatory (*alea* (Latin) = chance, risk, randomness) and epistemic (*επιστήμη* (Greek) = science, knowledge, insight) uncertainty is common, depending on the existing source of uncertainty, as shown in Fig. 1.

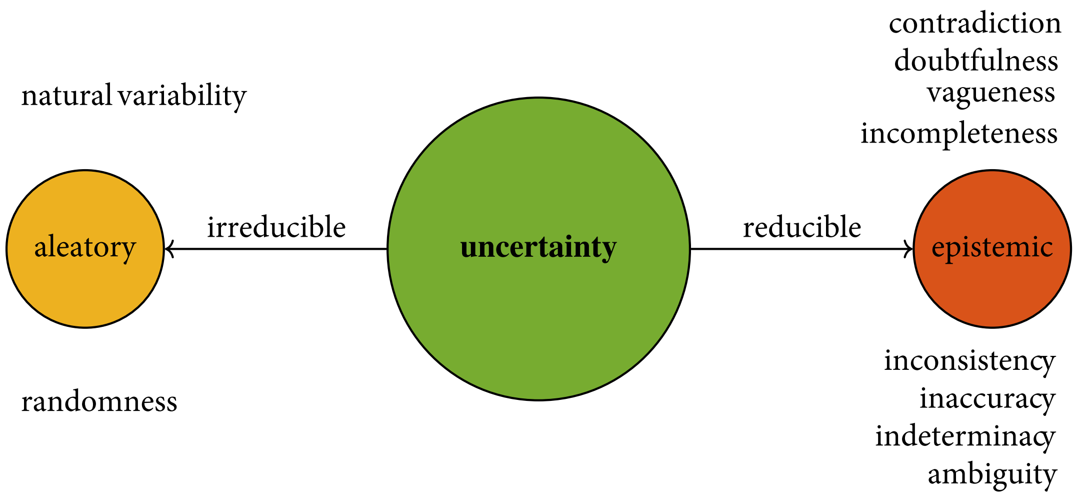


Figure 1: Uncertainty types and sources.

Aleatory uncertainty is an inherent uncertainty, as it is based on randomness and natural variability. Objectively speaking, aleatory uncertainty is therefore unavoidable and irreducible. Its treatment using probabilistic methods based on probability theory is scientifically established, as substantial statistical information, such as in the form of a histogram, is available [17, 18]. The experience with this modeling approach is already reflected in design codes of practice [4]. The probability density function (pdf) $f_X(x, \boldsymbol{\lambda})$ and the cumulative distribution function (cdf)

$F_X(x, \boldsymbol{\lambda})$ with shape parameters $\boldsymbol{\lambda}$ are connected through the indefinit integral:

$$P(X \leqslant x) = F_X(x, \boldsymbol{\lambda}) = \int_{-\infty}^{x} f_X(t, \boldsymbol{\lambda})\, \mathrm{d}t \tag{1}$$

As an example of many possible distributions, consider the normal distribution $x \sim \mathcal{N}(\mu, \sigma^2)$ in Fig. 2 with $f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$ as pdf and $\mu = \mathrm{E}(X)$ and $\sigma^2 = \mathrm{E}\left((X-\mu)^2\right)$ as shape parameters.

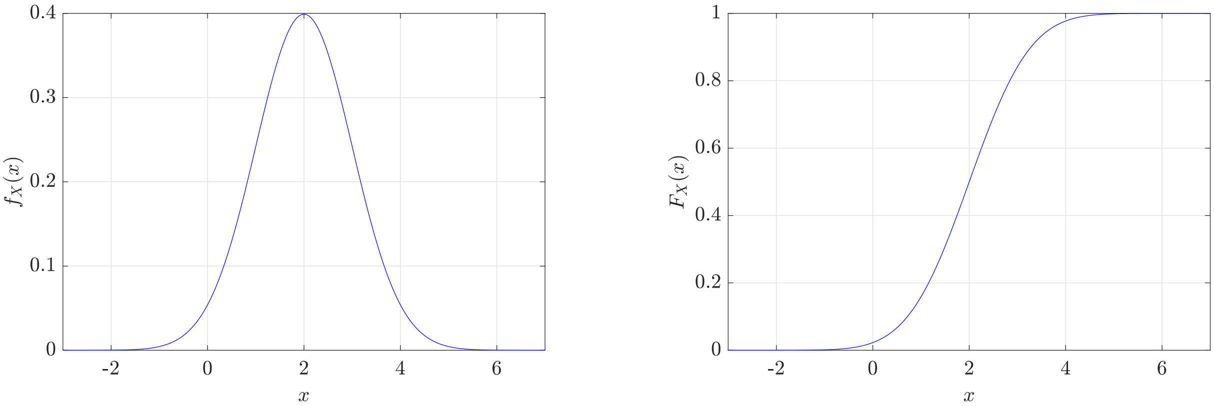


Figure 2: Modeling of aleatory uncertainty using probabilistic methods, e. g. the normal distribution $x \sim \mathcal{N}(2, 1)$. Left: Probability density function (pdf). Right: Cumulative distribution function (cdf).

Epistemic uncertainty is based on limited, inaccurate, or inconsistent data, which can result from expert knowledge, subjectivity, and model simplifications As a result, epistemic uncertainty is reducible, provided more information becomes available and/or model improvements are made. Therefore, modeling within the framework of classical probability theory is no longer recommended, and alternative approaches should be chosen, such as Bayesian inference, random sets, p-boxes, or representations using non-stochastic variables based on possibility theory [1]. If only limits or linguistic expressions are available for a parameter, a set-theoretic approach based on possibility theory [11, 23] can be chosen, where the possibility of a value is quantifie using a possibility distribution function, also called a membership function. The simplest form describes membership through the Boolean expressions $\{\mathrm{true}, \mathrm{false}\}$, meaning full membership with the value one or no membership with the value zero. These two events are disjoint sets, and operations can be performed based on classical set theory. If limits are provided for an epistemically uncertain value, quantificatio using an interval variable $\bar{X} = [x_\mathrm{l}, x_\mathrm{r}] = \{\bar{x} \in \mathbb{R} | x_\mathrm{l} \leqslant \bar{x} \leqslant x_\mathrm{r}\}$ is sensible. If an interval variable is considered too restrictive, a gradual, non-Boolean extension of classical set theory is appropriate, from which fuzzy set theory [22] developed. The membership function $\mu(\tilde{x})$ is usually normalized so that a real-valued fuzzy variable $\tilde{x}$ can be described on the fuzzy set $\tilde{X} = \{(\tilde{x}, \mu(\tilde{x})) \,|\, \tilde{x} \in \mathbb{R}, 0 \leqslant \mu(\tilde{x}) \leqslant 1\}$. In Fig. 3, an interval variable and a triangular symmetric membership function of a fuzzy number ($\mathrm{TFN}\langle x_\mathrm{l}, x_\mathrm{m}, x_\mathrm{r}\rangle$ = triangular fuzzy number) are exemplarily shown.

It is also possible for an input variable to be both aleatorically and epistemically uncertain at the same time. In this case, the combination of monomorphic uncertainty models leads to a polymorphic uncertainty model. Furthermore, polymorphic uncertainty may only become visible in the output variables when different aleatory and epistemic uncertainties have been

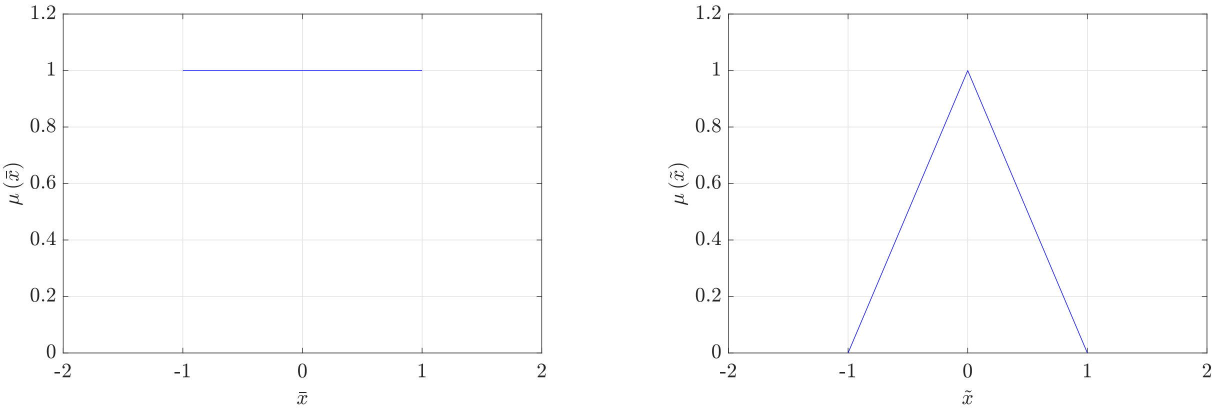


Figure 3: Modeling of epistemic uncertainty using non-probabilistic methods. Left: Interval variable $\bar{x} = [-1, 1]$. Right: Fuzzy variable $\tilde{x} = \mathrm{TFN}\langle -1, 0, 1\rangle$.

integrated into the model. Regardless, in general, the calculation of an underlying model considering various uncertainties is necessary. This leads to the embedding of the computational model in a multi-layered uncertainty space, as shown in Fig. 4.

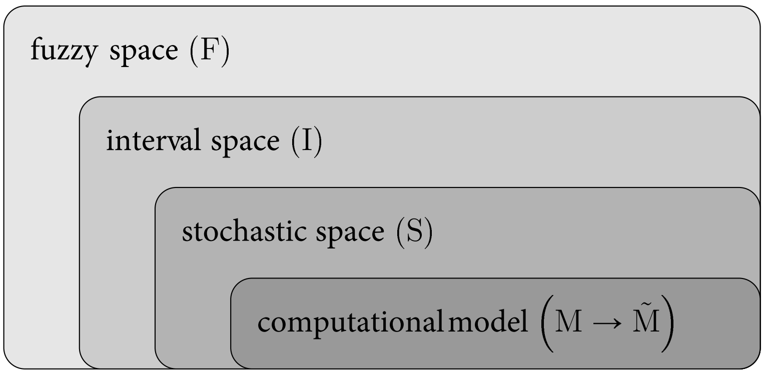


Figure 4: Scheme of a multi-layered uncertainty space with an embedded computational model.

The software tool PolyUQ, developed for the resulting nested analysis, is introduced in Section 2. An academic example is presented in Section 3. Section 4 includes various engineering applications. Section 5 finall provides the conclusions and offers an outlook on further development steps.

2 POLYUQ

The software tool PolyUQ has been developed to solve various problems under polymorphic uncertainty. Thereby, a computational model is embedded in the uncertainty space. First, the existing uncertainties are data-driven modeled and quantified Then by choosing appropriate solution methods, efficien uncertainty propagation is possible. Finally, evaluation methods are applied to the uncertain output variables. The user will have the results in both tabular and graphical form. A general workfl w is shown in Fig. 5.

The following provides a general overview of the user inputs and the functionalities. A detailed description can be found in [6]. All file can be downloaded from here.

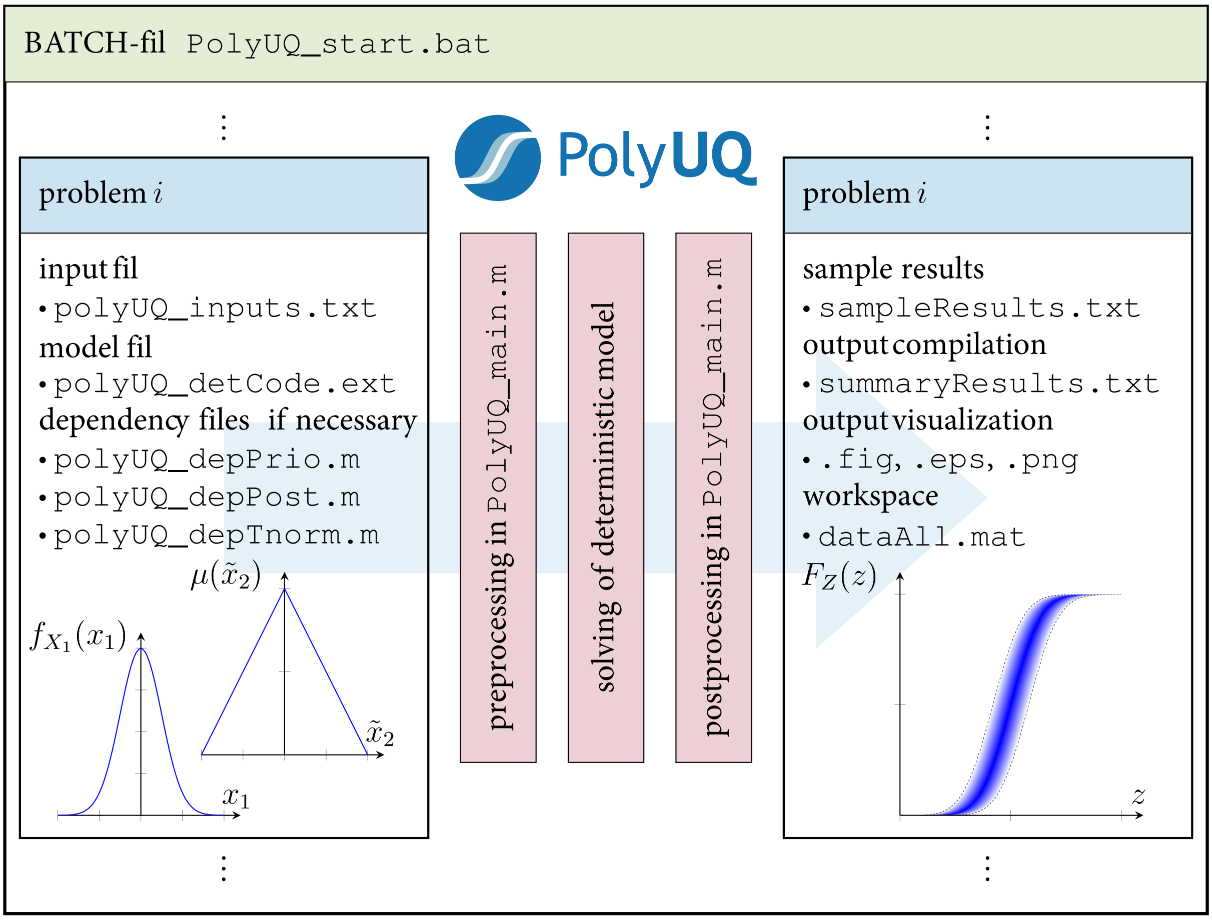


Figure 5: PolyUQ workfl w [6].

2.1 User input

The user can defin multiple problems, each consisting of an input file a model fil and input dependency files if input dependencies are present. The BATCH fil `PolyUQ_start.bat` controls the computation. The MATLAB main fil is called `PolyUQ_main.m`. The MATLAB functions are saved in the folder `PolyUQ_functions`. All three components have to be saved in the same directory.

2.1.1 BATCH-file

The BATCH-fil `PolyUQ_start.bat` controls the computation of multiple models. The user must defin a model path `pathModel[i]` and a solver `solver[i]` for each model. If the computational model is not directly define in MATLAB, additional information must be provided for the solver, such as the exe-fil or the license. After that, the user inputs are automatically controlled. If all inputs are correctly defined the models are serially solved. For each model, the start time and the end time is displayed in the command window for the user.

2.1.2 Input file

In the input fil `polyUQ_inputs.txt` created in `pathModel[i]` for the i-th model, the definitio of the uncertain input variables, the solution methods, the output variables, the output evaluation methods and the output evaluation is necessary.

Uncertain input variables Uncertain input variables can be quantifie either as stochastic, interval, fuzzy, interval-stochastic or fuzzy-stochastic variables. For each variable, a unique name and a unit have to be defined

- Stochastic variables require a distribution type, the associated distribution parameter(s) and, if desired, truncation limits.
- Interval variables are define by a lower and an upper bound.
- Fuzzy variables require a fuzzy type and corresponding parameters.
- Interval-stochastic and fuzzy-stochastic variables are combinations of the single parts.

Solution methods The need of the definitio of solution methods depends on the uncertain input variables which have been defined It is further possible to defin mutliple solution methods which are combined line by line. Thus, the influenc of different solution methods on the result can be examined.

Output variables Multiple output variables can be defined For each variable, a unique name and a unit have to be defined

Output evaluation methods The need of the definitio of output evaluation methods depends on the uncertain input variables which have been defined It is further possible to defin mutliple output evaluation methods which are combined line by line. Thus, the influenc of different output evaluation methods on the result can be examined.

Output evaluation It can be specifie whether the results on all evaluated points or only the evaluated result(s) in the individual space are at disposal for the user.

2.1.3 Model file

In the model fil created in `pathModel[i]` for the i-th model, the user has to defin the deterministic model. The model fil has to be named `polyUQ_detCode` with the associated extension for the desired solver.

2.1.4 Input dependency files

Dependencies of the uncertain input variables can be define either as a-priori dependencies (`polyUQ_depPrio.m`) or a-posteriori dependencies (`polyUQ_depPost.m`). Between fuzzy variables, also a fuzzy t-norm (`polyUQ_depTnorm.m`) is possible. No dependencies are present, if the dependency file are not define by the user.

2.1.5 Preprocessing

After the subfolders `0_automation`, `1_preprocessing`, `2_solving` and `3_postprocessing` are automatically created in the model path `pathModel[i]` for the i-th model, the input file the model fil and, if present, the input dependency file are checked. Furthermore, the user input in the input fil is read in and saved in appropriate variables. If errors are present in the files they are displayed in the command window to indicate necessary corrections. A formally corrected, optimal input is also displayed.

Uncertain input variables The define uncertain input variables are displayed and saved in the subfolder `1_preprocessing`. In addition, a tabular compilation is saved in the fil `summaryInputs.txt` in the same subfolder.

Solution methods The solution methods are summarized in the fil `summarySoluMethods.txt` in the subfolder `2_solving`.

Output variables and evaluation methods The output variables and evaluation methods are summarized in the fil `summaryResults.txt` in the subfolder `3_postprocessing`.

2.2 Solving

The solution phase is subdivided into two steps. First, all evaluation points in all non-empty uncertainty spaces are generated based on the define input variables, input dependencies and solution methods. The procedure is conducted top-down referring to Fig. 4. Then, the deterministic model is solved on each evaluation point depending on the applied solver.

2.3 Postprocessing

The fil `sampleResults.txt` is automatically created in the subfolder `3_postprocessing`. The results on all sampling points of all output variables by all solution method combinations are summarized. Based on these values, the output evaluation is conducted which depends on the define input variables and the output evaluation methods. The results on the sampling points are evaluated bottom-up referring to Fig. 4, whereby an empty space is skipped. In addition to the text file the output variables are displayed and saved in the same subfolder. Finally, the workspace is saved as `dataAll.mat` in the subfolder `0_automation`. A summary of the PolyUQ workfl w is saved as `PolyUQ_output.txt` in the same subfolder.

3 ACADEMIC EXAMPLE

The complete PolyUQ workfl w is presented in the following using an academic example. It concerns a two-dimensional frame structure in the x-z plane with a system length L and a system height H, as shown in Fig. 6. The girder is subjected to a horizontal point load λF_{H} and a vertical point load λF_{V} applied at the center. The rectangular cross-sections have a width b and a height h. The frame is built of steel S 235.

The input variables are define partially as deterministic and partially as uncertain, using different uncertainty models, as shown in Tab. 1. The characteristic value of the yield stress is $f_{\mathrm{yk}} = 235\,\mathrm{N/mm^2}$, that is the $5\,\%$ quantile value of the statistical distribution. According to the Probabilistic Model Code [16], lognormal distributions are recommended to be applied with a coefficien of variation of $3\,\%$ for the Young's modulus E and with a coefficien of variation of $7\,\%$ for the yield stress f_{y}. The vertical point load F_{V} is also integrated as a stochastic variable into the model, this time as a right-sided truncated normal distribution with a coefficien of variation of $10\,\%$. The cross-sectional parameters b and h may exhibit deviations from a target value due to manufacturing tolerances. However, quality management ensures minimal and

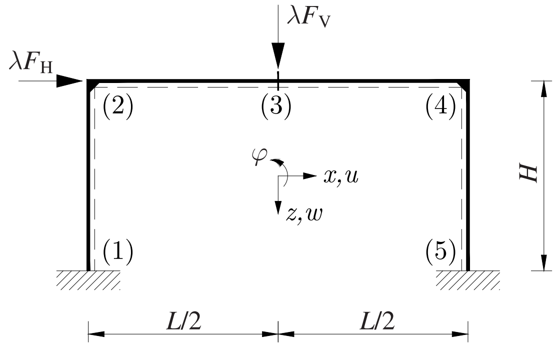


Figure 6: Frame structure.

maximal possible values $5\,\%$ around the target value. The modeling is done here using fuzzy variables with a triangular membership function.

Table 1: Input variables.

variable	unit	deterministic	stochastic	fuzzy
L	[m]	10		
H	[m]	5		
E	[N/mm^2]		$\mathcal{LN}(210000, 6300)$	
f_{y}	[N/mm^2]		$\mathcal{LN}(264.27, 18.50)$	
F_{H}	[N]	5000		
F_{V}	[N]		$\mathcal{TN}(6000, 600, -\infty, 7000)$	
b	[mm]			$\mathrm{TFN}\langle 114, 120, 126\rangle$
h	[mm]			$\mathrm{TFN}\langle 95, 100, 105\rangle$

The computational model M is directly generated in MATLAB. The solution methods chosen are the Monte Carlo simulation with 1000 samples in the stochastic space and the reduced transformation method with eleven equidistantly distributed α-cuts in the fuzzy space. For the output evaluation, the mean (μ) in the stochastic space and the center of gravity (COG) in the fuzzy space are calculated.

3.1 Determination of internal forces and displacements

In the firs step, the maximum bending moment $M_{y,\max}$ [kNm] and the horizontal girder displacement u_{G} [mm] are considered as output variables for a load factor of $\lambda = 1.0$. In Fig. 7, the bending moments and the system displacements are shown as examples for the sample with mean and core values. The maximum bending moment $M_{y,\max}^{\det} = 10.81\,\mathrm{kNm}$ is located here at the support of the right column. The horizontal beam displacement is $u_{\mathrm{G}}^{\det} = 21.7\,\mathrm{mm}$.

Due to the existing uncertainties, the use of PolyUQ results in an uncertain output, as shown in Fig. 8.

It is evident that the maximum bending moment does not exhibit epistemic uncertainty, and is thus independent of the fuzzy input parameters b and h. The uncertainty regarding the stochastic input parameters (here, only with respect to F_{V}) is present. Values between $10.0\,\mathrm{kNm}$ and $11.4\,\mathrm{kNm}$ are probable. Due to the skewed pdf of F_{V}, the mean $M_{y,\max}^{\mu} = 10.78\,\mathrm{kNm}$ is

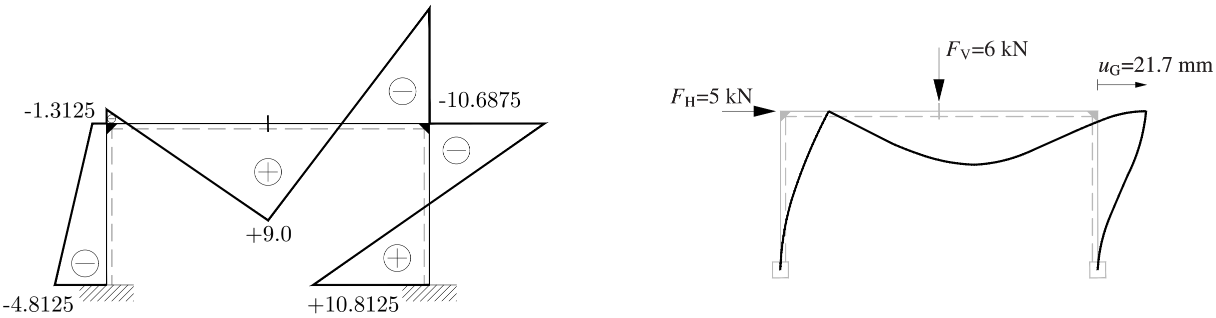


Figure 7: Deterministic results with mean and core values. Left: Bending moments. Right: Displacements.

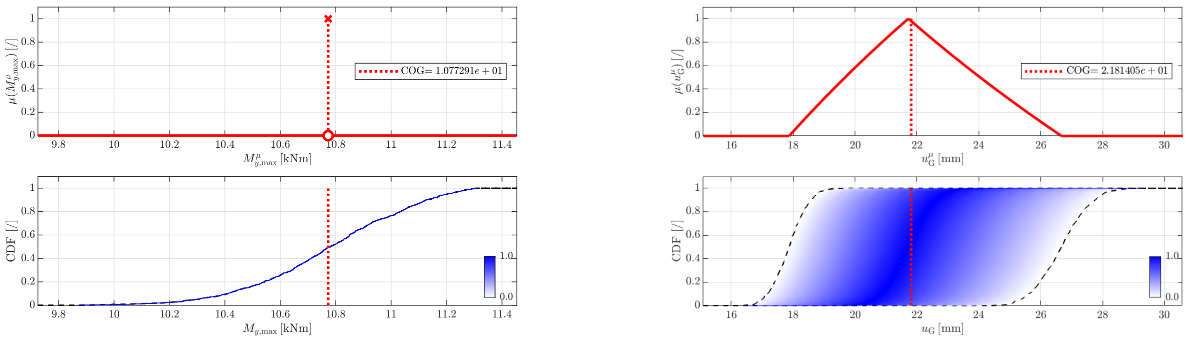


Figure 8: Uncertain outputs caused by present aleatory and epistemic uncertainties. Left: Maximum bending moment $M_{y,\max}$ [kNm]. Right: Horizontal girder displacement u_{G} [mm].

slightly smaller than the deterministic value $M_{y,\max}^{\mathrm{det}} = 10.81\,\mathrm{kNm}$. In the horizontal girder displacement, both the influence of the aleatory and epistemic uncertain parameters are visible. On the support ($\mu = 0$), values between $16.0\,\mathrm{mm}$ and $28.0\,\mathrm{mm}$ are probable, with the mean $u_{\mathrm{G}}^{\mathrm{supp}(\mu)} = [17.8, 26.6]\,\mathrm{mm}$. On the core ($\mu = 0$), values between $20.0\,\mathrm{mm}$ and $24.0\,\mathrm{mm}$ are probable, with a mean of $u_{\mathrm{G}}^{\mathrm{core}(\mu)} = 21.7\,\mathrm{mm}$. The defuzzifie value $u_{\mathrm{G}}^{\mathrm{COG}(\mu)}$ is also $21.7\,\mathrm{mm}$. Based on the evaluation of the uncertain results, decisions can be made in the next step, taking the uncertainty into account.

3.2 Determination of the load-deformation curve

The problem is extended to account for physically nonlinear effects. The load-deformation curve is sought, which is derived using cross-section and system reserves with the first-orde yield line theory. Again, the uncertainties in the input variables are propagated through the model and influenc the output. In Fig. 9, the fina solution with mean and core values is illustrated on the left, having an ultimate load factor of $\lambda_{\max} = 8.65$. With the results automatically saved in `sampleResults.txt`, the load-displacement diagram on the right could be created. The mean values are shown in blue and the $5\,\%$ and $95\,\%$ fractile values on the support with dashed lines.

The deterministic solution is enveloped by the solution that takes the uncertainty in the input parameters into account. It is clearly evident that there is a strong dependence of the curve on the uncertain input parameters, both in the u_{G}- and λ-direction. As an example, the ultimate load factor $\lambda_{\max}$ is analyzed. The mean on the support range between 7.48 and 10.10, with the $5\,\%$ and $95\,\%$ fractile values even ranging from 6.53 to 11.60. The mean on the core is quite

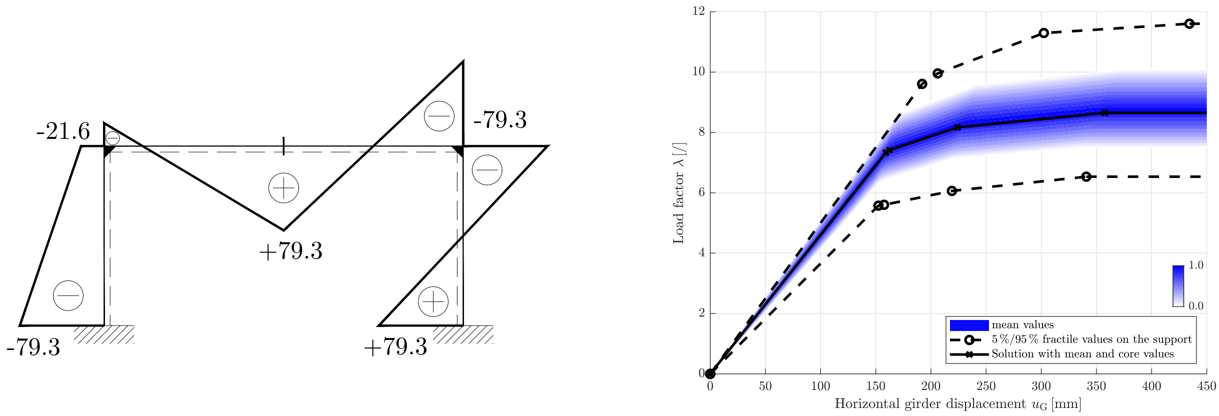


Figure 9: Consideration of physically nonlinear effects. Left: Final bending moments $M_y(\lambda_{\max})$ [kNm] with mean and core values. Right: Uncertain load-displacement diagram.

similar to the defuzzifie value of 8.74. It is worth mentioning that qualitative differences in system behavior may also occur which have to be analyzed in further studies.

4 ENGINEERING APPLICATIONS

The computational model (M) is fully interchangeable, and this does not affect the definitio of the (multi-layered) uncertainty space. Thus, the application to various engineering problems and beyond is possible, as shown in the following sections.

4.1 Surrogate modeling

In [8], a structure made of carbon fibe -reinforced plastic (CFRP) with an Ω-shaped cross-section was subjected to a three-point bending test until nonlinear stability failure. The focus was on the tilted webs, which have a reduced thickness compared to the flanges, and therefore, lower load-bearing capacity. Relevant uncertain input variables were modeled using both stochastic and non-stochastic approaches and integrated into the model. The underlying computational model (M) is a finit element model, which leads to a high computational effort in the context of a nonlinear analysis. Therefore, a surrogate model ($\tilde{\mathrm{M}}$) based on artificia neural networks (ANN) was used. The numerical predictions of local strains and the entire displacement fiel were compared with experimentally obtained data, as shown in Fig. 10.

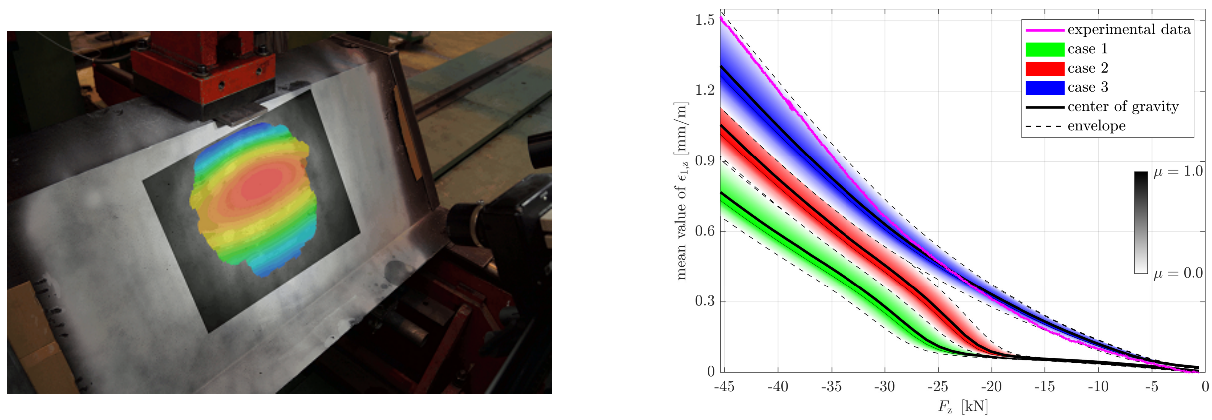
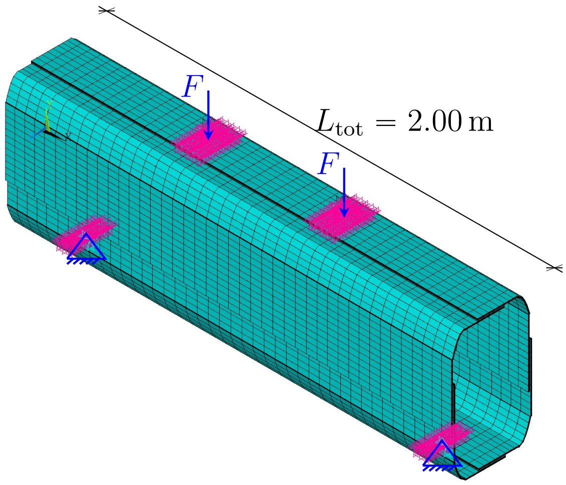


Figure 10: Numerical and experimental results using a surrogate model ($\tilde{\mathrm{M}}$). Left: Displacement fiel $\boldsymbol{u}_{\mathrm{norm}}(\boldsymbol{x})$. Right: Local horizontal strain $\epsilon_{1,z}$.

4.2 Multicriteria optimization

In [7], a beam made of glass fibe -reinforced plastic (GFRP) with bonds made of epoxy resin (EP) has been investigated in a four-point bending test. The structure was optimized in terms of cost minimization and compliance minimization, for which an embedding of the PolyUQ framework into an optimization routine was carried out [12]. Different topologies regarding the number of bonding layers were examined, and constraints concerning structural failure and maximum deformations were defined Uncertain cross-sectional and material parameters were integrated into the model. The Pareto optimal points for a topology with four bonds are exemplarily shown in Fig. 11.



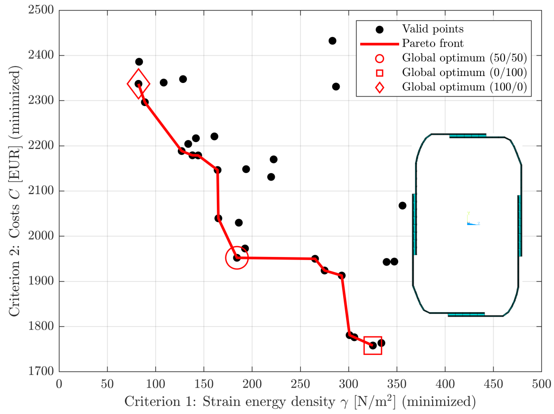


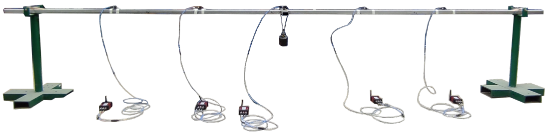
Figure 11: MuScaBlaDes beam. Left: Isometric view with boundary conditions. Right: Pareto optimal points after fina optimization step of beam with four bonds.

4.3 Data assimilation

In [9], the focus was on considering numerical predictions and real measurement data of system responses, as well as the simultaneous estimation of unknown model parameters under the presence of aleatory and epistemic uncertainty. The data assimilation approach was used, with the EnKF (ensemble Kalman filter being employed, which, in its extended form, can simultaneously estimate state variables $\boldsymbol{x}$ and unknown model parameters $\boldsymbol{b}$. For this purpose, the EnKF was directly embedded into the stochastic space generated within the PolyUQ framework. The real test structure was a stainless steel beam with a hollow box cross-section, on which vertical accelerations were experimentally determined during oscillation tests using five accelerometers, as shown in Fig. 12.

5 CONCLUSIONS AND OUTLOOK

PolyUQ is a software tool that was developed in-house and is made available for download to everyone. A detailed documentation can be found in [6]. It is used to solve problems involving aleatory and epistemic uncertainty, which are modeled using stochastic and non-stochastic variables. Although various application examples from engineering have been presented in this paper, extensions to the current version are necessary, particularly with regard to input options, user-friendliness, solution methods, and interfaces to external solvers. For any questions, further ideas or interest in cooperation, please contact the corresponding author via e-mail.



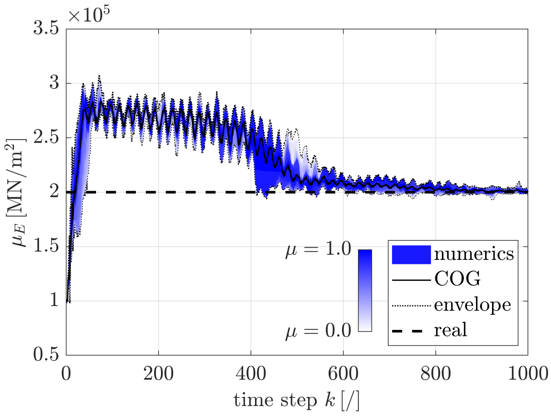


Figure 12: Application of the EnKF. Left: Real structure with five accelerometers. Right: Prediction of the mean of Young's modulus $\mu_E(t)$.

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