Small-sample simulation for uncertainties modelling in engineering: Theory, software and applications

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Abstract

The objective of the paper is to present methods for efficient statistical, sensitivity and reliability assessment. The attention is given to the techniques which are developed for an analysis of computationally intensive problems which is typical for a nonlinear FEM analysis. The paper shows the possibility of "randomization" of computationally intensive problems in the sense of the Monte Carlo type simulation. Latin hypercube sampling is used, in order to keep the number of required simulations at an acceptable level. The technique is used for both random variables and random fields levels. Sensitivity analysis is based on nonparametric rank-order correlation coefficients. Statistical correlation is imposed by the stochastic optimization technique – the simulated annealing. The simulation can be used for preparation of virtual training set for artificial neural network used in inverse analysis. The multipurpose software FReET is briefly described.

Keywords: Statistical analysis, sensitivity, reliability, Monte Carlo simulation, Latin hypercube sampling, simulated annealing, inverse analysis.

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1 Introduction

A large number of efficient stochastic analysis methods have been developed during last years. In spite of many theoretical achievements the acceptability and a routine application in industry is still rare. Two main categories of stochastic approaches can be distinguished: Approaches focused on the calculation of statistical moments of response quantities, like estimation of means, variances etc. and approaches aiming at the calculation of estimation of theoretical probability of failure. There are many different methods developed by reliability researchers covering both the approaches. The common feature of all the methods is the fact that they require a repetitive evaluation (simulations) of the response or limit state function. The development of reliability methods is from the historical perspective a struggle to decrease an excessive number of simulations. Some small-sample simulation methods utilized by author and implemented in probabilistic software FReET are described:

- Small-sample simulation of Monte Carlo type Latin hypercube sampling for both random variables and random fields
- Imposing statistical correlation using the simulated annealing approach
- Small number of random variables to represent random fields based on spectral decomposition of covariance matrix
- Sensitivity analysis based on nonparametric rank-order statistical correlation

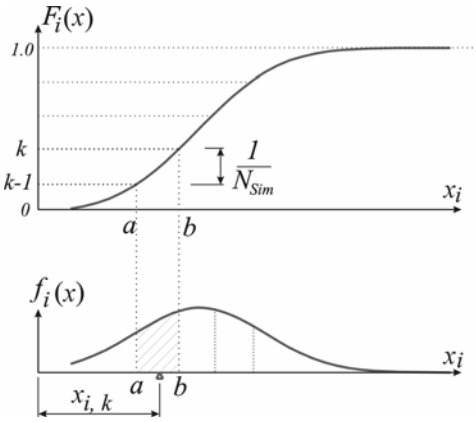
The methods were integrated within the complex software system SARA (Pukl et al. 2003ab, Novák at al. 2002, Bergmeister at al. 2004). The system represents a combination of statistical simulation package FReET (Novák et al. 2003, 2006) and nonlinear mechanics software ATENA (Červenka and Pukl 2005, Červenka 2003). The most interesting applications are referenced.

2 Small-sample simulation of Monte Carlo type – Latin hypercube sampling

For time-intensive calculations, the small-sample simulation techniques based on stratified sampling of Monte Carlo type represent a rational compromise between feasibility and accuracy. Therefore Latin hypercube sampling (LHS) was selected as a key fundamental technique.

The method belongs to the category of stratified simulation methods (e.g. Mc Kay and Conover 1979, Novák et. al 1998). It is a special type of the Monte Carlo simulation which uses the stratification of the theoretical probability distribution function of input random variables. It requires a relatively small number of simulations to estimate statistics of response – repetitive calculations of the structural response (tens or hundreds).

The basic feature of LHS is that the probability distribution functions for all random variables are divided into N_{Sim} equivalent intervals (N_{Sim} is a number of simulations); the values from the intervals are then used in the simulation process (random selection, middle of interval or mean value). This means that the range of



the probability distribution function of each random variable is divided into intervals of equal probability. The samples are chosen directly from the distribution function based on an inverse transformation of distribution function. The representative parameters of variables are selected randomly, being based on random permutations of integers *1, 2, ..., j,* N_{Sim}.

Figure 1: Illustration of LHS.

Every interval of each variable must be used only once during the simulation. Being based on this precondition, a table of random permutations can be used conveniently, each row of such a table belongs to a specific simulation and the column corresponds to one of the input random variables.

It has been proved that best LHS strategy, which simulates the means and variances very well, is the approach suggested by Keramat and Kielbasa (1997) and Huntington and Lyrintzis (1998). The mean of each interval should be chosen as (Fig. 1):

$$x_{i,k} = \frac{\int_{y_{i,k-1}}^{y_{i,k}} x \cdot f_i(x)\,dx}{\int_{y_{i,k-1}}^{y_{i,k}} f_i(x)\,dx} = N_{Sim} \cdot \int_{y_{i,k-1}}^{y_{i,k}} x \cdot f_i(x)\,dx \tag{1}$$

where f_i is the probability density function of variable X_i, and the integration limits are:

$$y_{i,k} = F_i^{-1}\left(\frac{k}{N_{Sim}}\right) \tag{2}$$

The estimated mean value is achieved accurately and the variance of the sample set is much closer to the target one. For some probability density functions (inclusive e.g. Gaussian, Exponential, Laplace, Rayleigh, Logistic, Pareto, etc.) the integral (1) can be solved analytically Vořechovský and Novák (2003).

3 Imposing statistical correlation

Once samples are generated, the correlation structure according to the target correlation matrix must be taken into account. There are generally two problems related to the statistical correlation: First, during sampling an undesired correlation can occur between the random variables. For example, instead of the correlation coefficient zero for the uncorrelated random variables, i.e. an undesired correlation, can be generated. It can happen especially in a case of a very small number of simulations (tens), where the number of interval combination is rather limited. The second task is to introduce the prescribed statistical correlation between the random variables defined by the correlation matrix. The columns in LHS simulation plan should be rearranged in such a way that they may fulfill the following two requirements: to diminish the undesired random correlation and to introduce the prescribed correlation. It can be done by using different techniques published in literature on LHS (e.g. Huntington and Lyrintzis 1998, Iman and Conover, 1982) but we found some serious limitations while using them.

A robust technique to impose statistical correlation based on the stochastic method of optimization called simulated annealing has been proposed recently by Vořechovský and Novák (2003). The imposition of the prescribed correlation matrix into the sampling scheme can be understood as an optimization problem: The difference between the prescribed **K** and the generated **S** correlation matrices should be as small as possible. A suitable measure of quality of the overall statistical properties can be introduced:

$$E_{overall} = \sqrt{\sum_{i=1}^{N_V - 1} \sum_{j=i+1}^{N_V} \left(S_{i,j} - K_{i,j}\right)^2} \tag{3}$$

The norm E has to be minimized from the point of view of the definition of the optimization problem using simulated annealing optimization approach, N_v random variables realizations are related to the ordering in the sampling scheme.

4 Simulation of random fields

A higher level of uncertainties modelling may be in the consideration of the spatial variability of mechanical and geometrical properties of a system and intensity of load. Such quantities should be represented by means of random fields. Because of the discrete nature of the finite element formulation, the random field must also be discretized into random variables. This process is commonly known as random field discretization. The computational effort in reliability problem generally increases with the number of random variables. Therefore it is desirable to use small number of random variables to represent a random field. To achieve this goal, the transformation of the original random variables into a set of uncorrelated random variables can be performed through a well-known eigenvalue orthogonalization procedure. A few of these uncorrelated variables with largest eigenvalues are sufficient for the accurate representation of the field.

Let us consider the fluctuating components of the homogenous random field, which is assumed to model the material property variation around its expected value. Correlation characteristics can be specified in terms of the covariance matrix C_{aa} constructed by discretization using autocorrelation function and geometry of FEM mesh. An eigenvalue orthogonalization procedure will transform variables into uncorrelated space:

$$\mathbf{C}_{XX} = \mathbf{\Phi\Lambda\Phi}^{T} \tag{4}$$

The covariance matrix in the uncorrelated space **Y** is a diagonal matrix $\mathbf{\Lambda}=\mathbf{C}_{YY}$. The vector of uncorrelated Gaussian random variables **Y** can be simulated in the traditional way (Monte Carlo simulation). The transformation back into correlated space yields the vector **X** (discretized random field) using eigenvectors **Φ**:

$$\mathbf{X} = \mathbf{\Phi Y} \tag{5}$$

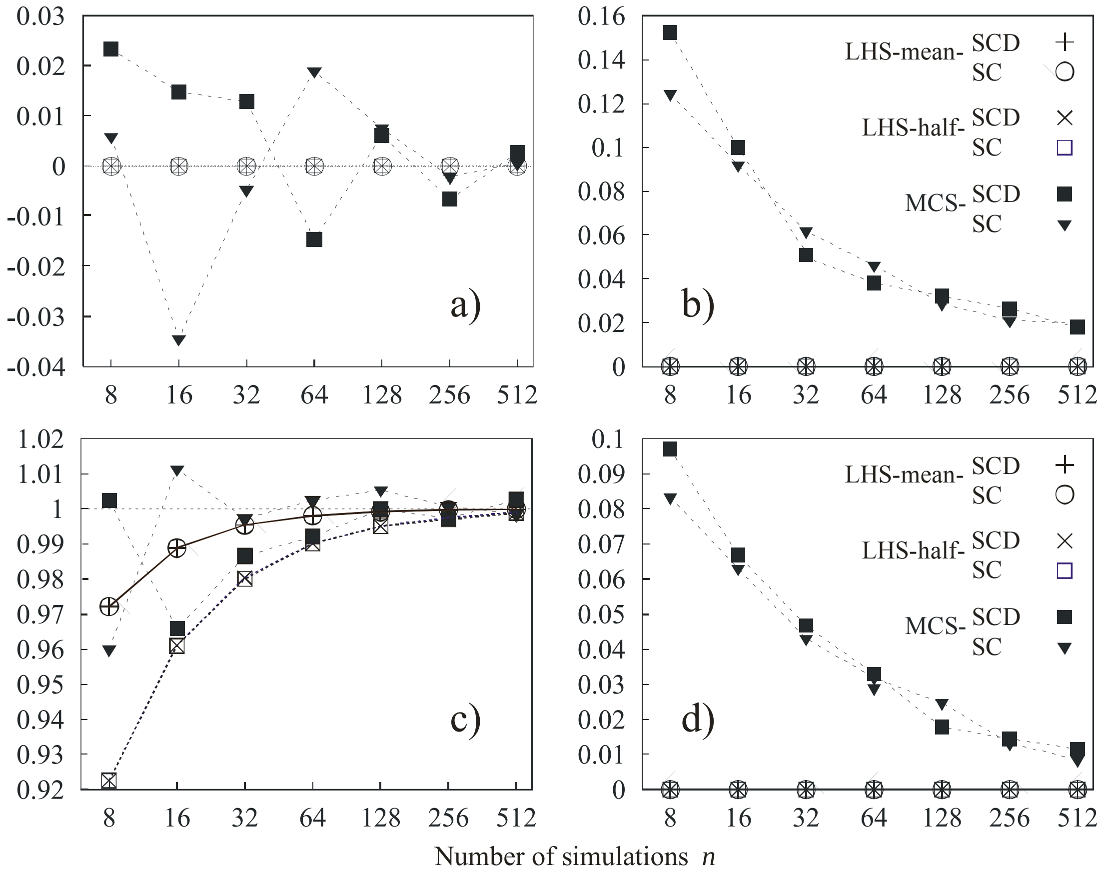


Figure 2: Comparison of convergence to target fields statistics of crude Monte Carlo Sampling and Latin Hypercube Sampling with number of simulations: a) average, b) dispersion of mean value estimation, c) sample standard deviation, d) dispersion of sample standard deviation.

The utilization of LHS method for simulation of Gaussian uncorrelated variables is the new simple idea of improvement of random field simulation using orthogonal transformation of covariance matrix suggested e.g. by Novák et al. (2000). The superiority of this stratified technique remains here also for accurate representation of random field, thus leading to the decrease of number of simulations needed. This was proved numerically by Vořechovský and Novák (2005). In particular, it has been shown that the ability to simulate mean value of random field is excellent in case of LHS, see Figs. 2a) and b). This ability is rather poor in case of MCS, average value of mean fluctuates and standard deviation of mean is high in comparison to LHS. With regard to the second statistical moment, the ability to simulate standard deviation of random field is documented in figures 2c) and d). Again, capturing of this statistics is "random" in case of MCS, standard deviation of sample standard deviation is high in comparison to LHS. In the same study, it has been shown the impact of having the random vector **Y** perfectly uncorrelated. If an attention is paid to spurious correlation between marginals of **Y** (this correlation diminished by a suitable technique) the resulting estimated autocorrelation structure of the field after orthogonal transformation matches perfectly the desired one. Note that the algorithm described briefly in section 3 has proved itself to be very efficient in this regard.

5 Sensitivity and reliability analyses

An important task in the structural reliability analysis is to determine the significance of random variables. With respect to the small-sample simulation techniques described above the straightforward and simple approach uses the non-parametric rank-order statistical correlation between the basic random variables and the structural response variable (Iman and Conover 1980, Novák et al. 2004). The sensitivity analysis is obtained as an additional result of LHS, and no additional computational effort is necessary.

The relative effect of each basic variable on the structural response can be measured using the partial correlation coefficient between each basic input variable and the response variable. The method is based on the assumption that the random variable which influences the response variable most considerably (either in a positive or negative sense) will have a higher correlation coefficient than the other variables. Because the model for the structural response is generally nonlinear, a non-parametric rank-order correlation is used by means of the Spearman correlation coefficient or Kendall tau.

In cases when we are constrained by small number of simulations (tens, hundreds) it can be difficult to estimate the failure probability. The following approaches are therefore utilized here; they are approximately ordered from elementary (extremely small number of simulations, inaccurate) to more advanced techniques:

- Cornell´s reliability index - the calculation of reliability index from the estimation of the statistical characteristics of the safety margin
- The curve fitting approach - based on the selection of the most suitable probability distribution of the safety margin.
- FORM approximation (Hasofer-Lind´s index)
- Importance sampling techniques
- Response surface methods

These approaches are well known in reliability literature and also providing all details is beyond the aim of this paper. In spite of the fact that the calculation of the failure probability (or/and reliability index) using some of these techniques does not always belong to the category of very accurate reliability techniques (first three in the list), they represent a feasible alternative in many practical cases.

6 Inverse analysis

The inverse analysis technique is based on the combination of the statistical simulation method of the Monte Carlo type and the artificial neural network (ANN), Novák and Lehký (2006). The emphasis is mainly on: (1) the efficiency of the training set preparation for the neural network training using small numbers of simulations based on the stochastic technique Latin hypercube sampling; (2) the multipurpose character of the methodology relatively easy to apply. The whole procedure is conceptually simple and can be itemized as follows:

1) The computational model of a particular problem has to be first developed using e.g. the appropriate FEM software. The model has to be calibrated by trial-and-error procedure using model parameters (IP); initial calculation uses a set of the initial computational model parameters resulting in a rough agreement with the experimentally measured data (MD). Note, that an initial guess of IP has to be done based on testing, engineering judgement and virtual computational simulation. Parameters are estimated only roughly and therefore next identification can and should follow. Without any idea about the values of IP proposed methodology cannot guarantee good results. Fortunately, this is not case happening in engineering computational mechanics as there is usually a rough idea on values of parameters.
2) IP of the computational model are considered as random variables described by a probability distribution; the rectangular distribution is a "natural choice" as the lower and upper limits represent the bounded range of the physical existence of IP. However, also other distributions can be used, e.g. the Gaussian one. IP are simulated randomly based on the Monte Carlo type simulation, the small-sample simulation LHS is recommended. The results are random realizations of IP (vector **y**). A statistical correlation between some parameters may be taken into account too. If correlation is known, then it can help to the inverse analysis in consequent stochastic training – keeping the consistency of computational parameters in a computational model.
3) A multiple calculation (simulation) of the deterministic computational model using random realizations **y** of IP is performed, a statistical set of the virtual response **p** is obtained. Note, that the selection of appropriate number of simulations is driven by many factors, mainly by complexity of the problem (computational demand), structure of neural network and variability of IP. No general rule can be therefore suggested.
4) Random realizations **y** (outputs of ANN) and the random responses from the computational model **p** (inputs of ANN) serve as the basis for the training of an appropriate artificial neural network. This key point of the whole procedure is illustratively sketched in Fig. 3 (here for the FEM

model response in the form of a nonlinear load-deflection curve including both pre-peak and post-peak behaviour).

5) The trained neural network is ready to give an answer to the key task: To select the best parameters IP so that the calculation may result in the best agreement with MD, which is performed by means of the network simulation using MD as an input. This results in an optimal set of parameters $\mathbf{y}_{opt}$.
6) The last step is the results verification – the calculation of the computational model using optimal parameters $\mathbf{y}_{opt}$. A comparison with MD will show to what extent the inverse analysis was successful.

Note that the importance of the training sample preparation has be emphasized and tested by Tong and Liu (2004), including LHS scheme. In spite of the fact that these authors concluded that the number-theoretic methods appear as the most efficient, LHS scheme also provided very good results. Moreover, our focus to LHS is also determined by the general applicability of this small-sample simulation technique for practical statistical, sensitivity and reliability analyses in many fields of engineering.

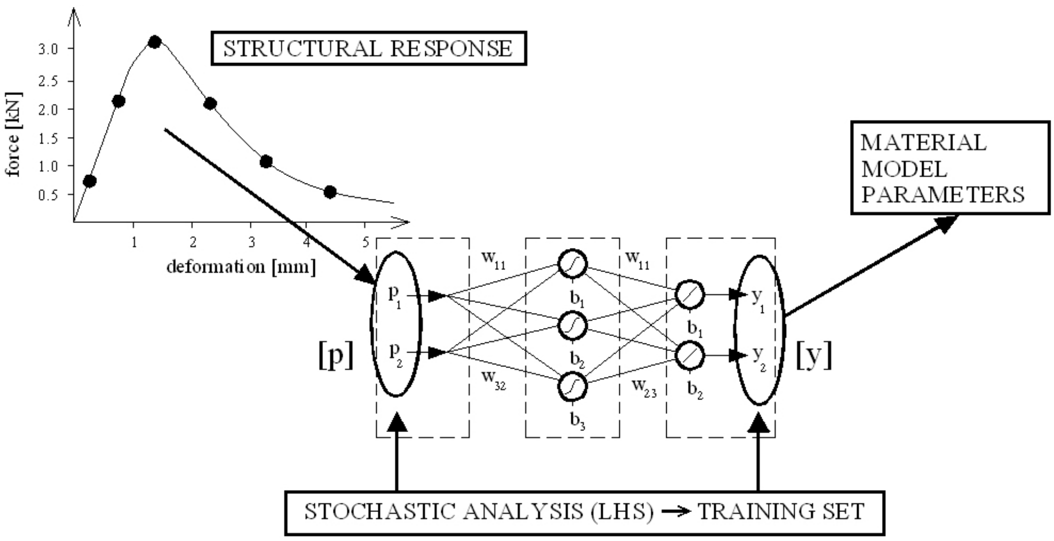


Figure 3: A scheme of stochastic training of the neural network.

7 Software FREET

The multipurpose probabilistic software for statistical, sensitivity and reliability analysis of engineering problems FREET (Novák, et al., 2003, Novák, et al., 2006) is based on efficient reliability techniques described above. There are three basic parts in present version:

The window “Random Variables” (Fig. 4) allows the user-friendly input of basic random variables of analyzed problem. Uncertainties are modeled as random variables described by their probability density functions (PDF). The user can

choose from the set of selected theoretical models like normal, lognormal, Weibull, rectangular, etc. Random variables are described by statistical characteristics (statistical moments): Mean value, standard deviation (or coefficient of variation) and coefficient of skewness, respectively.
The window “Statistical Correlation” serves for the input of correlation matrix, Fig. 5. The user can work at the level of a subset of correlation matrices (each related to a group of random variables) or at the global level (all random variables resulting to a large correlation matrix). The level of correlation during interactive input is highlighted, the positive definiteness is checked. Note, that the Simulated Annealing applied consequently does not require this strong requirement.
Random input parameters are generated according to their PDF using LHS sampling. Samples are reordered by Simulated Annealing approach in order to match required correlation matrix as close as possible, Fig. 6. Generated realizations of random parameters are used as inputs for analyzed function (computational model). The solution is performed *N* times and results (structural response) are saved. At the end of the whole simulation process the resulting set of structural responses is statistically evaluated. The results are: estimations of the mean value, variance, coefficient of skewness and kurtosis, empirical cumulative probability density function estimated by empirical histogram structural response. This basic *statistical assessment* is visualized through the window Histograms. Such a basic statistical analysis is followed by *reliability analysis* based on several approximation techniques: (i) basic estimation of reliability by the Cornell safety index, (ii) curve fitting approach applied to the computed empirical histogram of response variable and (iii) simple estimation of probability of failure based on the ratio of failed trials over the total number of simulations, see Fig. 7.
Additional information to the problem solved is the *sensitivity analysis* of each response function based on its rank-order correlation coefficient. Even though this is actually a byproduct of the simulation not requiring special additional effort, it provides very useful information in many cases. If the correlation coefficient between a certain input and output variables is close to zero, we can conclude that the input variable has (in its simulated range) a small or even negligible effect on the output. This can sometimes help to decrease the probabilistic dimension of the problem because such an input can be considered deterministic.

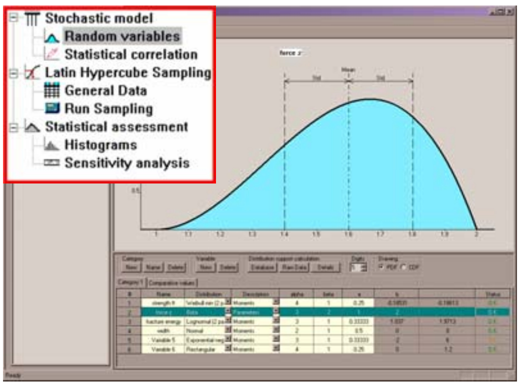


Figure 4: Window “Random variables”.

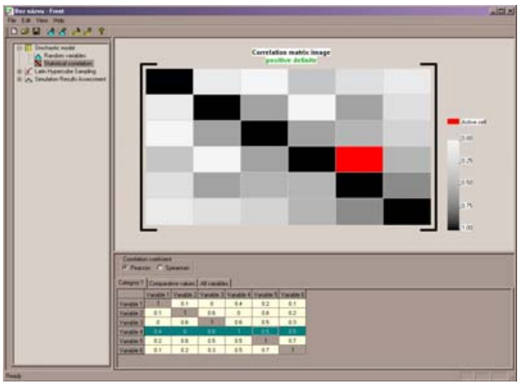


Figure 5: Window “Statistical correlation”.

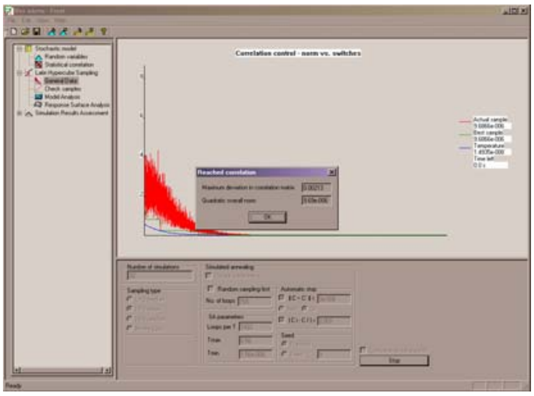


Figure 6: Window showing the progress of imposing the statistical correlation by Simulated Annealing algorithm.

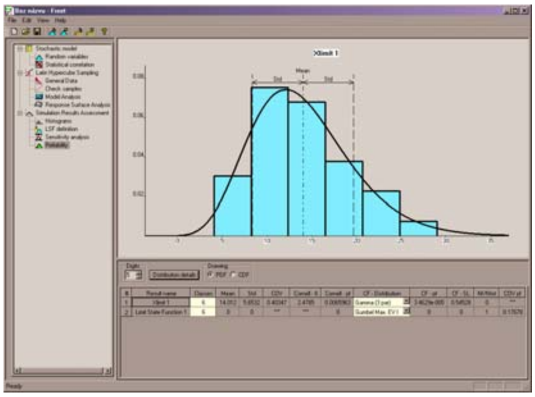


Figure 7: Window "Reliability" with empirical histogram, Curve fitting, Cornell safety index and Monte Carlo sampling estimation.

8 List of selected applications

The applications of software FReET within the framework of complex system SARA belong to the most successful and interesting ones. Dominating topics with published results are listed as follows:

Probabilistic analyses of concrete structures

The presented approach has been used for statistical and probabilistic nonlinear analysis of concrete structures. The main interest is focused on probabilistic bridge assessments, including degradation and retrofitting modeling. References: Pukl and Bergmeister (2005), Bergmeister et al. (2005), Pukl et al. (2005), Bergmeister et al. (2004), Pukl et al. (2003ab)**,** Novák et al. (2002).

Statistical size effect studies

The probabilistic simulation approach was used to capture the statistical size effect obtained from experiments. The probabilistic treatment of nonlinear fracture mechanics in the sense of extreme value statistics has been recently applied for two crack initiation problems which exhibits the Weibull-type statistical size effect. References: Bažant et al. (2005), Vořechovský et al. (2004, 2005), Bažant at al. (2004), Novák et al. (2003), Lehký and Novák (2002).

Identification of computational model parameters

The recently proposed inverse analysis is based on a coupling of the stochastic nonlinear fracture mechanics analysis and the artificial neural network. Such inverse analysis utilizes SARA package. References: Novák and Lehký (2005), Lehký and Novák (2005), Červenka et al. (2005), Strauss et al. (2004ab), Lehký and Novák (2004), Novák and Lehký (2004).

9 Conclusions

The paper briefly describes the small-sample simulation techniques for statistical, sensitivity and reliability analyses of computationally intensive problems implemented in FREET software. Efficient techniques of stochastic simulation methods were combined in order to offer an advanced tool for the probabilistic assessment of the complex problems, like those of nonlinear fracture mechanics modeling (SARA, ATENA). A wide range of applicability both practical and theoretical gives an opportunity for further intensive development – bridging first theory and praxis, and second, reliability and nonlinear computation.

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