Spatial variability of material properties in nonlinear computer simulation

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ABSTRACT: Spatial variability of structural properties is an important phenomenon, which should be accounted for in realistic computer simulation of structural response behavior and damage. Methodology for introducing spatial variability of material properties into a nonlinear finite element program system is presented together with a brief description of selected applications.

1 INTRODUCTION

Randomness and spatial variability of material properties, boundary and initial conditions of mechanical systems, random fluctuations in temperature, humidity, and other environmental factors is commonly recognized. It can considerably affect structural behavior, response and damage.

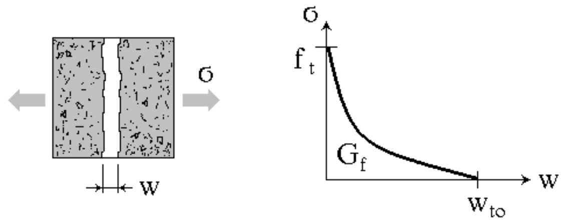
In contradiction to reality these phenomena are usually neglected in computer simulation. The material and other structural and environmental parameters are assumed to be deterministic values. This assumption makes the computer models less realistic and less satisfactory.

Fortunately, the entire object of uncertainty can be solved in a rational and mathematically precise way and the random characteristics of nature can be addressed by computational models. A high level and also very natural (physical) technique of uncertainties modeling is their representation by random fields.

2 NONLINEAR COMPUTER SIMULATION

The nonlinear finite element program ATENA employs advanced constitutive models for concrete based on damage mechanics, nonlinear fracture mechanics (Fig. 1) and plasticity theories with smeared crack approach. It is a proven tool for computer simulation of reinforced structures including failure mechanism and post-peak behavior (Červenka 2000, 2002, Pukl et al. 2005).

The program consists of solution core and user-friendly graphical environment. The graphical user interface serves for creating of structural model and evaluation of results, even already during the analysis. The solution core includes finite element modeling, numerical equation solver, nonlinear solution methods and nonlinear material models.



$$\frac{\sigma}{f_t} = \left(1+c_1\frac{w}{w_{to}}\right)^3 \exp\left(-c_2\frac{w}{w_{to}}\right) - \frac{w}{w_{to}}\left(1+c_1^3\right)\exp(-c_2)$$

$$c_1 = 3, \quad c_2 = 6.93, \quad w_{to} = 5.14\frac{G_f}{f_t}$$

Figure 1. Nonlinear fracture mechanics approach for concrete in tension. Exponential stress – crack-opening law by Hordijk (1991).

For computer simulation of concrete and reinforced concrete structures including its interaction with neighborhood the program offers variety of nonlinear material models for concrete, quasi-brittle materials, soils and metals, namely:

- damage-based material model
- fracture-plastic cementitious material
- microplane material model
- Drucker-Prager plasticity model
- Von Mises plasticity model
- plasticity with hardening for reinforcement
- etc.

All these material models contain number of parameters, which define the numerical model and describe the nonlinear behavior. Typical parameters for concrete are Young’s modulus of elasticity, compressive and tensile strength, fracture energy, Poisson’s ratio etc. In the standard (deterministic) solution these parameters are treated as deterministic values, constant within the structure or its parts.

This assumption allows calculating a response to given actions in terms of mean values. Safety issues at the deterministic level should be addressed by means of global safety factors.

3 RANDOMNESS OF INPUTS

The solution to the variety of complex engineering problems, involving randomness in the mechanical properties and in the excitations they are subjected to, can be found by means of simulation. The Monte Carlo type of simulation is usually used for this purpose.

However, a requirement of large number of samples can be time consuming and thus can be a serious limiting obstacle in practical cases. An efficient solution of this problem is offered in software SARA, which couples the nonlinear finite element analysis with appropriate stochastic methods (Pukl et al. 2003, 2005, Bergmeister et al. 2004, Novák et al. 2005). Part of the SARA package is the software FREET for stochastic functions (Novák et al. 2003). It is used in two stages of analysis:

(i) Generation of random samples, which are passed to the deterministic solver.

(ii) Statistical assessment of random response together with information on dominating and non-dominating variables (sensitivity analysis) and estimation of reliability using reliability index and/or theoretical failure probability.

For time-intensive calculations like nonlinear fracture mechanics of concrete, 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 in FREET as a key fundamental technique.

The method belongs to the category of stratified simulation methods. 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} equiprobable intervals (N_{Sim} is a number of simulations); the values from the intervals are then used in the simulation process (random selection, median of interval or the probabilistic mean value of an interval). This means that the range of the probability distribution function of each random variable is divided into intervals of equal probability (McKay et al. 1979, Iman & Conover 1980). The samples are chosen directly from the distribution function based on an inverse transformation of distribution function, Fig. 2.

The order of representative parameters of variables are selected randomly, being based on random permutations of integers *1, 2, ..., j*, N_{Sim}. 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.

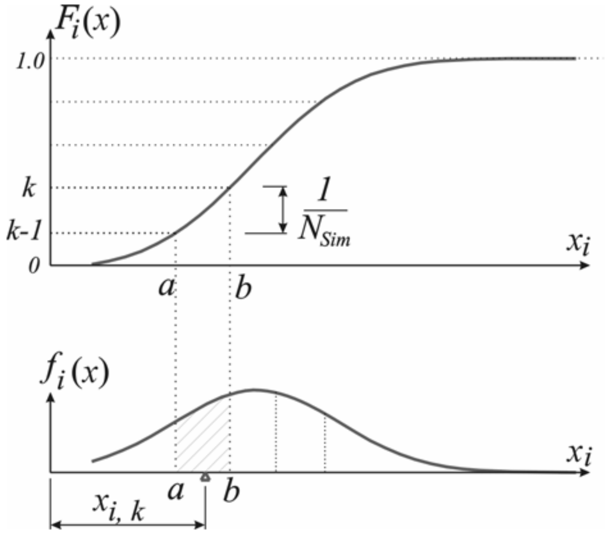


Figure 2. Illustration to Latin hypercube sampling.

Once samples of each input random variable alone 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 an undesired correlation can be generated. It can happen especially in the case of a very small number of simulations (tens), where the number of interval combination is rather limited. Another 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.

A robust technique to impose statistical correlation based on the stochastic method of optimization called simulated annealing has been proposed recently by Vořechovský & 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 and the generated correlation matrices should be as small as possible. In such a way, the optimal sets of input parameters are generated and passed to the solver.

The nonlinear finite element solver, represented in SARA by program ATENA, performs analyses of the structure with generated sets of input variables in order to obtain more realistic structural response. The results are evaluated by stochastic methods according to paragraph (ii). Safety of the structure is assessed directly by built-in reliability methods.

The basic level of introducing randomness into the nonlinear finite element analysis by SARA system is treatment of the input parameters as random variables. Selected parameters are randomized as described above, and their values differ from sample to sample, but inside of a single sample they are constants over the structure or structural part respectively. Thus, the spatial variability of the structural properties is neglected at the level of random variables.

4 SPATIAL VARIABILITY OF STRUCTURAL PROPERTIES

Spatial variability of structural properties, in particular of material properties, is an important phenomenon, which can have substantial influence on the structural damage and failure – e.g. crack initiation and localization in homogeneous stress state region as it occurs in four point bending tests. Therefore, it should be properly accounted in the computer simulation of structures if realistic results are desired.

The ATENA program has been extended in order to be able to account for the spatial variability of material properties. General parameters for the material models are updated according to the predefined values over the structure.

The parameters of material models in the nonlinear finite element analysis are created and stored individually for each integration (material) point, since they can have individual settings and can locally change during the solution (e.g. due to damage processes or stress redistribution). Standard treatment of the local material models can be itemized as follows:

- input of general parameters
- adjustment of local parameters in integration (material) point (e.g. scaling to the finite element size)
- changes of local parameters during nonlinear solution (e.g. reduction of lateral strength and shear stiffness in cracks, increase of compressive strength due to lateral compression etc.)

If the spatial variability should be reflected, the above scheme will change as follows:

- input of general parameters
- substitution of general parameters with predefined local parameters
- adjustment of local parameters in integration points (here comes the association with a random field realization)
- changes of local parameters during solution

Since the number of material models in ATENA is rather high, and the spatial variability should be enabled for all of them, an efficient methodology has been developed for substitution of the general parameters with the local ones by encapsulating the existing material models into an envelope. This envelope provides transfer of the local material parameters from the predefined geometrical matrix to the influenced material model. The value from the nearest geometrical point is adopted for the material point. If the parameter values are defined in the material points (Gaussian integration points), they are directly used for substitution of the general parameters.

The geometrical matrix describing the spatial distribution of the material parameters is stored in an ASCII file with coordinates and corresponding parameter values. It can be created in several ways:

- it can contain the values from (in situ) measurements
- it can be written arbitrary by user – e.g. for introducing of (a local) inhomogeneity
- it can be generated in a scientific and mathematically precise way – by random fields methodology

5 RANDOM FIELDS

The term stochastic or probabilistic finite element method (SFEM or PFEM) is used to refer to a methodology, which accounts for uncertainties in the geometry or material properties of a structure, as well as the applied loads. The representation of spatial variability of structural properties by random fields is a high level of their modeling with a scientific background. Random fields describe the spatial distribution of a structural (material) property over the region representing the structure.

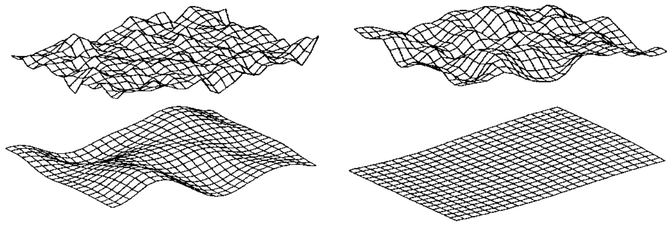


Figure 3. Realizations of 2D random fields with increasing spatial correlation.

The spatial correlation of the generated random fields, defined by correlation length (and the autocorrelation function), is of crucial importance. Randomly selected examples of realizations of 2D random fields over a rectangular support for different correlation lengths are shown in Fig. 3 for illustration.

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. It has been demonstrated that a few of these uncorrelated variables with largest eigenvalues are sufficient for the accurate representation of the random field.

The utilization of the above-described LHS method for simulation of Gaussian uncorrelated variables is a new simple idea for improvement of random field simulation using orthogonal transformation of covariance matrix suggested 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 (Vořechovský & Novák 2005). The approach is based on utilization of stratified sampling technique LHS for simulation of dominating uncorrelated random variables. The result is that only a few random variables and quite small number of simulations is necessary for accurate representation of a random field.

This methodology is implemented in FREET as a level of random fields, which can represent the spatial variability of material properties for the structural analysis in ATENA. The technology of encapsulating existing nonlinear material models and spatial distribution matrix are utilized in SARA system at this level. It enables to model the spatial variability and material inhomogeneities in the nonlinear finite element solution in a highly scientific and systematic way. The results can be therefore directly statistically evaluated and used for statistical assessment of response variables, sensitivity analysis and estimation of structural reliability and failure probability.

6 APPLICATIONS

The use of the SARA system at level of random fields is illustrated on several examples presented by Novák et al. (2005)

Random crack initiation and localization in numerical simulation of four-point bending tests is shown in Fig. 4.

The first (uniformly grey) beam was analyzed with the deterministic strength value, which was constant over the whole structure. Two major symmetrical cracks and symmetrically distributed microcracks appear in this case. In the next four beams the strength is randomly distributed over the structure. The regions with lower concrete strength are dark colored. The localized cracks are depicted by short black lines in the damaged material points; the thicker line the larger crack width.

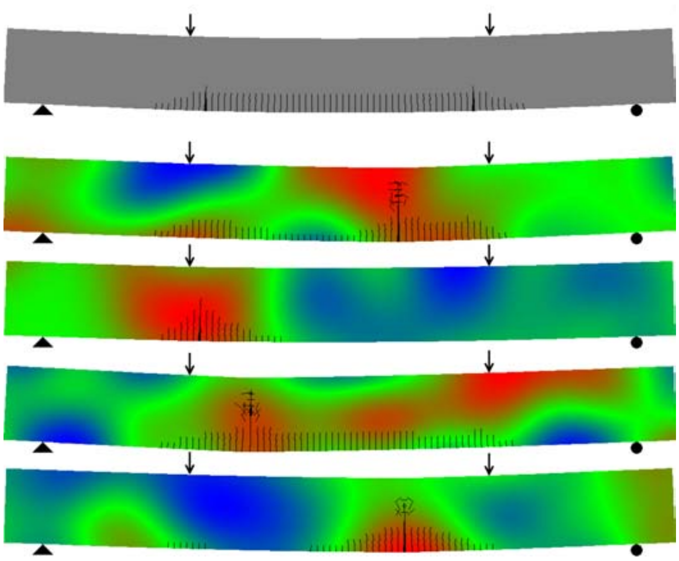


Figure 4. Four-point bending tests - random fields of strength and crack patterns.

A bundle of normalized load-deflection curves from the extensive random-fields simulation of four-point bending beams is presented in Fig. 5. Due to spatial randomness the mean of the peak load decreases comparing to the deterministic capacity.

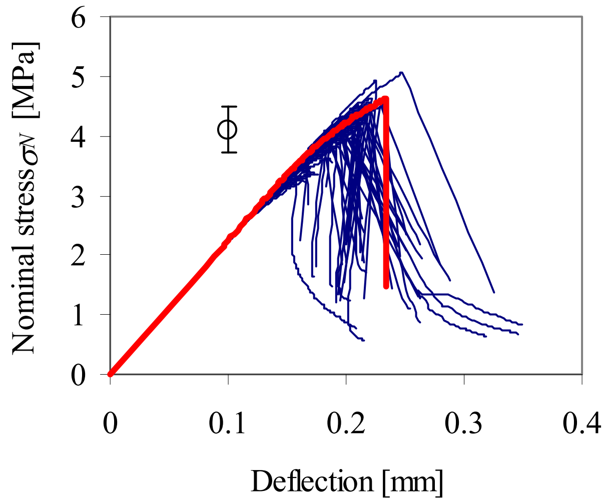


Figure 5. Random stress–deflection curves (the thick curve represents deterministic calculation).

Note that also the average plus one sample standard deviation does not reach the peak deterministic nominal stress. This is an important fact with fatal consequences in rational design and assessment of structures.

The application of random fields is also very suitable for solution of soil-structure interaction tasks. The influence of spatial variation of Young's modulus and material constants of Drucker-Prager failure criterion (based on cohesion and angle of internal friction) was studied. The stability of concrete tunnel tube in complicated geological conditions has been analyzed. The thickness of geological layers was between 10 and 25 m, the diameter of the tunnel tube was 11 m, the typical wall thickness 0.5 m. The whole analyzed part of the soil with tunnel had the dimensions of 50 x 60 m. It was solved in plane strain state and discretized in 5000 finite elements. Drucker-Prager plasticity was used for modeling of soil behavior. The spatial variability was simulated using Gaussian random fields with correlation length of 2 m. A model sample is illustrated in Fig. 6.

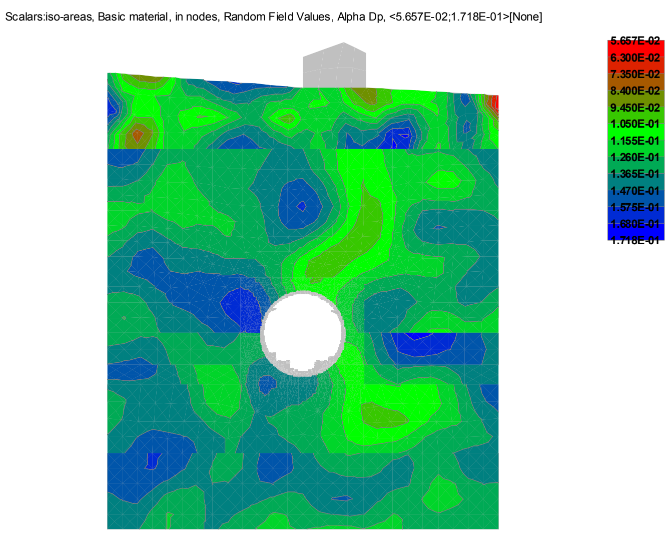


Figure 6. Random field of soil property around concrete tunnel tube.

Another complex example utilizing the random fields methodology is published in a separate paper (Vořechovský & Matesová, 2006). It presents numerical simulation of experimentally obtained size effect in dog-bone shaped concrete specimens under uniaxial tension (illustrative Fig. 7).

In the cited paper it is shown how the statistical size effect can be computationally captured. Since the deterministic model automatically models the energetic size effects caused by stress redistribution, the complex statistical-energetic size effect gets truly modeled by the presented software tools.

7 CONCLUSIONS

An efficient method encapsulating the existing material models has been developed and implemented in order to account for spatial variability of material properties in the nonlinear finite element framework. The variable structural properties used for calculation can be measured in situ or generated by random fields technology.

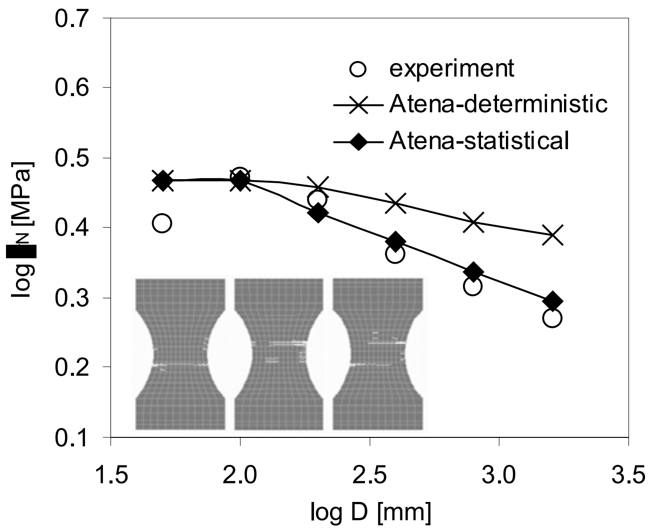


Figure 7. Random crack initiation and size effect curves – experiment vs. simulation.

The presented technology enables to model inhomogeneities in the nonlinear finite element solution, which can simulate random occurrence of structural damage (crack) even in a homogeneous stress state (four-point bending beams), capture complex statistical-energetic size effect etc.

These features are in particular important in materials with high variability and uncertainty of their properties like fiber reinforced concrete or soil.

The numerical results can be directly statistically evaluated and used for structural reliability assessment.

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