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MULTI-OBJECTIVE OPTIMIZATION OF MATERIAL PARAMETERS FOR NANOINDENTATION MODEL

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Summary: *Optimization of input material parameters from a nanoindentation model is discussed in this paper. Nanoindentation allows testing physical properties of materials in the scale of their components. Because this testing is very expensive, it is effective to use numerical models. The target of the optimization is to find input parameters for the model to achieve an agreement between the numerical response and the experiment. As an optimization algorithm, the multi-objective evolutionary algorithm PAES was used. Objective functions are based on a difference between an optimized curve and a result from the model. From the point of view of efficiency and accuracy, the proposed methodology provides a promising alternative to the existing approaches.*

1. Nanoindentation: the method and the model

The experimental method called nanoindentation (Němeček et al., 2006) allows testing the physical properties of materials on the scale of the typical dimension of individual components. The tested material is loaded by a very sharp and rigid point (see Figs. 1 and 2).

Fig. 1. Nanoindenter.

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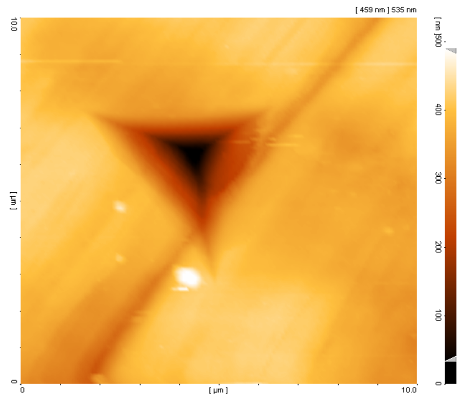

Fig. 1. Picture of indent from atomic force microscope.

In our case properties of the cement paste were tested. Specimens are characterized by a 30 mm diameter and a 4 mm height. The water-cement ratio (w/c) is equal to 0.5; a Portland cement CEMI 52.5 N is used. For indentation, Berkovich's indenter with pyramidal shape is applied. The loading is cyclic and is driven by a force in a short period of time (only several minutes). The whole experiment consists of five loading and unloading periods with a small constant force period aimed at creep development, see Fig. 3.

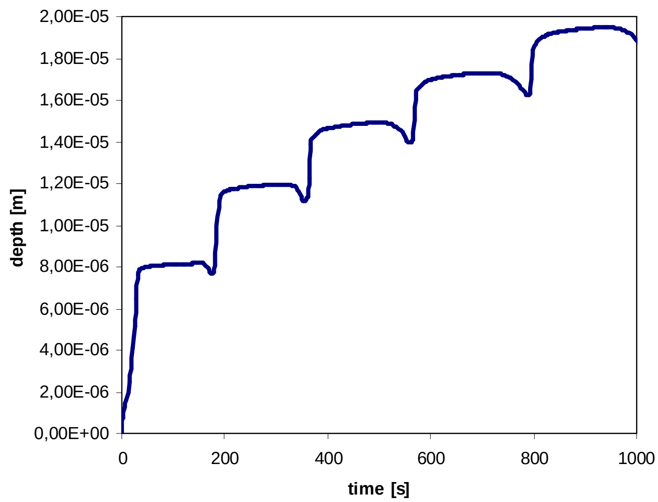

Fig. 3. Typical evaluation of indentation test: depth vs. time curve.

These tests are very expensive; hence it is advantageous to use numerical models instead. The extraction of material parameters from the experiment is far from being straightforward, because the loading imposed by the indenter introduces highly heterogeneous stress and strain fields. In particular, the closed-form relations are available only for the simplest material models (linear elasticity); more realistic constitutive description leads to a large-scale computational simulation based on, e.g., the Finite Element Method. The problem then is to find a set of material parameters for the chosen discrete model to achieve the best agreement between the numerical "response" and the experiment.

The numerical model was created using the ADINA software (Adina, 2005). The spatial problem was considered as planar thanks to axisymmetry (Jůn, 2005). A finite element mesh is decomposed into 1800 isoparametric four-node elements and is refined around the tip. The indenter is ideally rigid and the contact between indenter and paste is updated every iteration.

A combined visco-plastic model was chosen to properly describe the non-linear behavior of the cement paste. The tensor of the total strain is composed of three parts:

$$\varepsilon = \varepsilon^E + \varepsilon^C + \varepsilon^P \tag{1}$$

where ε^E is time independent elastic part,
ε^C is time dependent creep strain and
ε^P is time independent plastic part.

An effective creep strain is described by the power creep law:

$$\varepsilon^C = a_0 \sigma^{a1} t^{a2} \tag{2}$$

where a_0, a_1 and a_2 are free model parameters. Remaining input parameters are Young's modulus E and the yield stress σ_y. Input parameters bounds for the identification are introduced in Tab. 1.

Table 1: Bounds for nanoindentation model parameters.

Parameters	Units	Minimum	Maximum
E	GPa	15	45
σ_y	MPa	20	600
a_0	-	$1.32 \cdot 10^{-19}$	$1.32 \cdot 10^{-14}$
a_1	-	0.49	2.50
a_2	-	0.05	0.55

2. Optimization algorithm

For many optimization tasks the gradient-based methods are considered to be the most computationally efficient algorithms. But analytical determination of sensitivities for the current model is fairly difficult, mainly due the history dependency of the model as well as complex interaction of individual parameters. Hence, techniques of soft-computing can be employed for optimization as an alternative to a standard approach (Hrstka et al., 2003).

Single-objective optimization

Firstly, the single-objective optimization was tested. The methodology consists of the minimization of the least square error function between an experiment and results from the numerical model. The numerical model of nanoindentation is very time consuming, hence it is useful to use its approximation instead of the real model.

The applied methodology is based on the idea of radial basis function networks (RBFN) as proposed e.g. in (Karakasis et al., 2004, Nakayama et al., 2004). This approach comes from the domain of a general approximation, usually called the Response Surface methods (Lee et al., 2001), Diffuse Approximations (Ibrahimbegovic et al., 2004) or Surrogate models (Karakasis et al., 2004). RBFN is based on artificial neural networks, but has some specific properties: the neural net is created only with one layer of neurons, it has a specific type of a transfer function and the training of this net leads to the solution of a linear system of equations. Our particular implementation is based on the variant introduced in (Kučerová et al., 2005).

The main principle of the approach is the replacement of an objective function by a neural network approximation and its subsequent optimization by an evolutionary algorithm. The approximation is adaptively improved by new neurons (points), where values of an objective function are calculated exactly. As an optimization algorithm, the evolutionary algorithm GRADE with its extension called CERAF is used (Hrstka et al., 2004). This extension allows solving the multi-modal problems. The main advantage of this methodology is an inexpensive evaluation of the approximation, which is repeatedly used during a stochastic optimization process. The computationally expensive objective function is evaluated only when new neurons are added to the neural network.

Two objective functions were tested. The first on was the mean square error between the target curve and a simulation:

$$R_j = \sum_{i=1}^{t} \left(\frac{h_{\exp,i} - h_{sim,j,i}}{h_{\exp,i}} \right)^2 \tag{3}$$

where$h_{exp,i}$ is the depth in the *i*-th time step on the target curve and
$h_{sim,j,i}$ is the depth in the *i*-th time step on the *j*-th simulation.

The second objective function was based on the difference between "shapes" of two curves by minimizing the errors among slopes of the given curves:

$$D_j = \sum_{i=1}^{t} \left(\frac{d_{\exp,i} - d_{sim,j,i}}{d_{\exp,i}} \right)^2 , \tag{4}$$

where $d_i = \dfrac{h_i - h_{i+1}}{t_i - t_{i+1}}$,

t_i is the *i*-th time and
$t_{(i+1)}$ is the (i + 1)-th time.

Obtained results were satisfactory only partially, therefore, both objective functions were used in a multi-objective manner.

Multi-objective optimization

Multi-objective optimization is based on simultaneously optimizing several contradicting goals. Therefore, the solution is found as a compromise satisfying partially all of them and the result is usually found as a set of feasible solutions called Pareto set. Hence, the scalar concept of optimality is replaced with Pareto optimality. Pareto optimal solutions present a set, for which cannot be found any solution that makes at least one objective function better without making any other criterion worse.

Multi-objective optimization algorithm was based on an evolutionary algorithm called Pareto Archived Evolution Strategy (PAES) (Knowles et al., 2000). PAES in the simplest version 1+1 was used; this version works only with individuals not with the population of solutions. Each individual in optimization represents a unique set of input parameters. All so far found Pareto optimal solutions are stored in an archive, which represents Pareto set. From genetic operators PAES uses only a mutation and a selection is replaced by updating the archive. The pseudo-code for the algorithm is described in Fig. 4.

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1.The initial individual is created randomly and it is added
   to the archive.
2.A new individual is created by mutation.
3.The parent and the offspring are compared.
   3.a. The offspring is dominated by the parent solution;
        the offspring is rejected.
   3.b. The offspring dominates the parent solution;
        the  parent  is  replaced  by  the  offspring  in  the
        archive.
   3.c. The offspring and the parent are indifferent;
        the offspring is added to the archive.
4.The  archive  is  updated;  all  dominated  solutions  are
   rejected.
5.An individual is chosen from the archive for the mutation.
6.Points 2) to 5) are repeated until some stoping criteria
   is reached.
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Fig. 4. Pseudo-code for PAES.

As was mentioned above, both previously proposed objective functions were tested together. All objectives were to be minimized.

Following figures show the final Pareto set after 100 iterations. We tested three different computer generated curves as a target; therefore we can judge not only the shape of curve (bigger graph) but also the precision of parameter estimation (smaller graph), see Figs 5 - 7.

Apparently, the shape of target curve (the black curve) and shapes of curves from the final Pareto set are very similar, but not all parameters are found with satisfactory precision. The successfulness in parameter estimation corresponds to their sensitivity to the objective functions. For example, the curve I (Fig. 5) has bigger creep deformation than other curves, and therefore final parameters are more accurate in estimation of parameters a_0-a_2, which influence the creep strain.

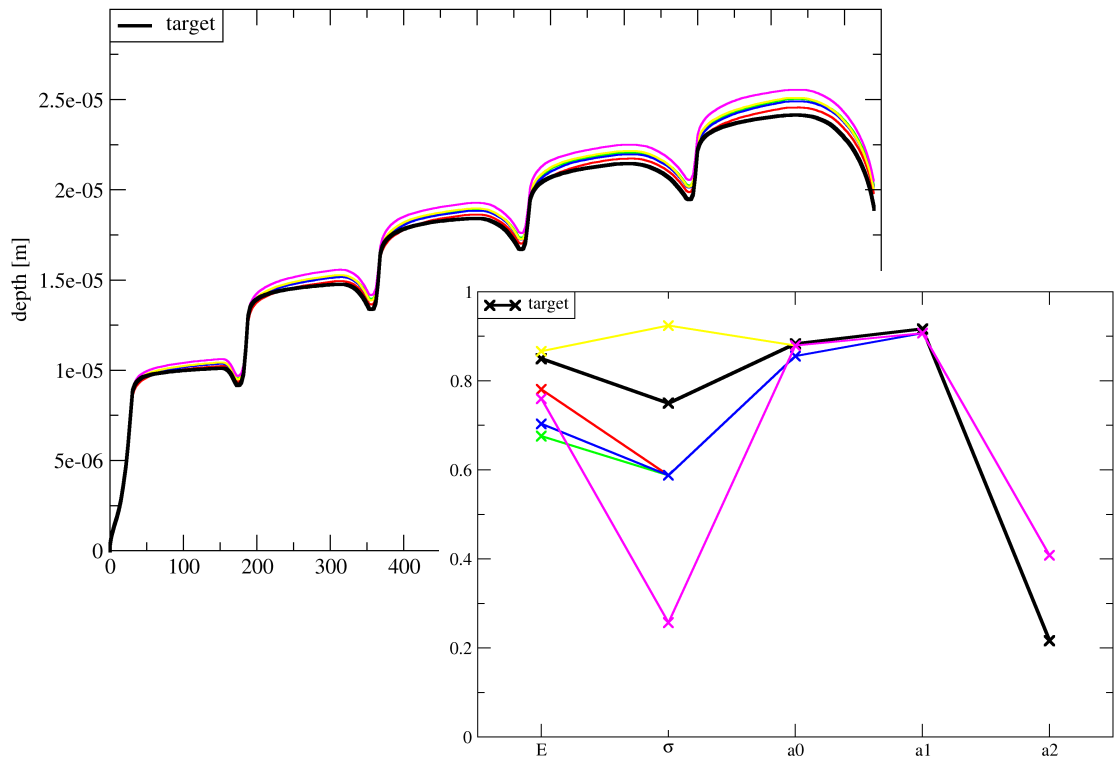

Fig. 5. Final Pareto set for curve I.

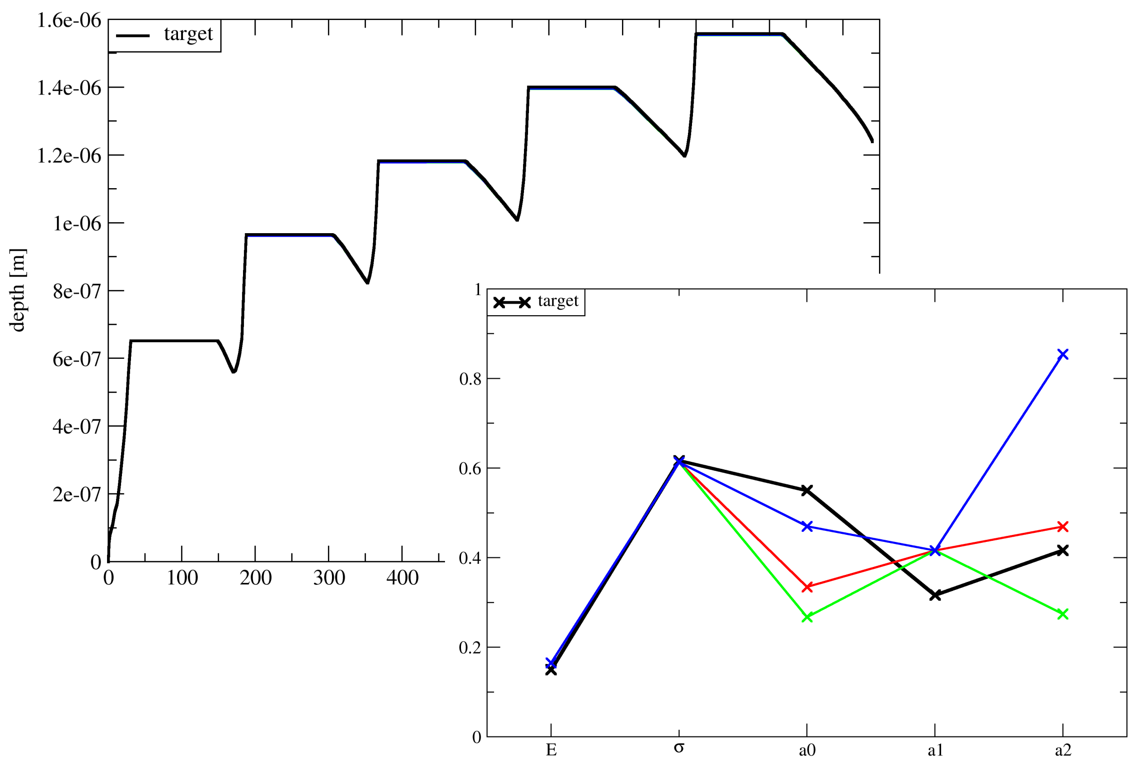

Fig. 6. Final Pareto set for curve II.

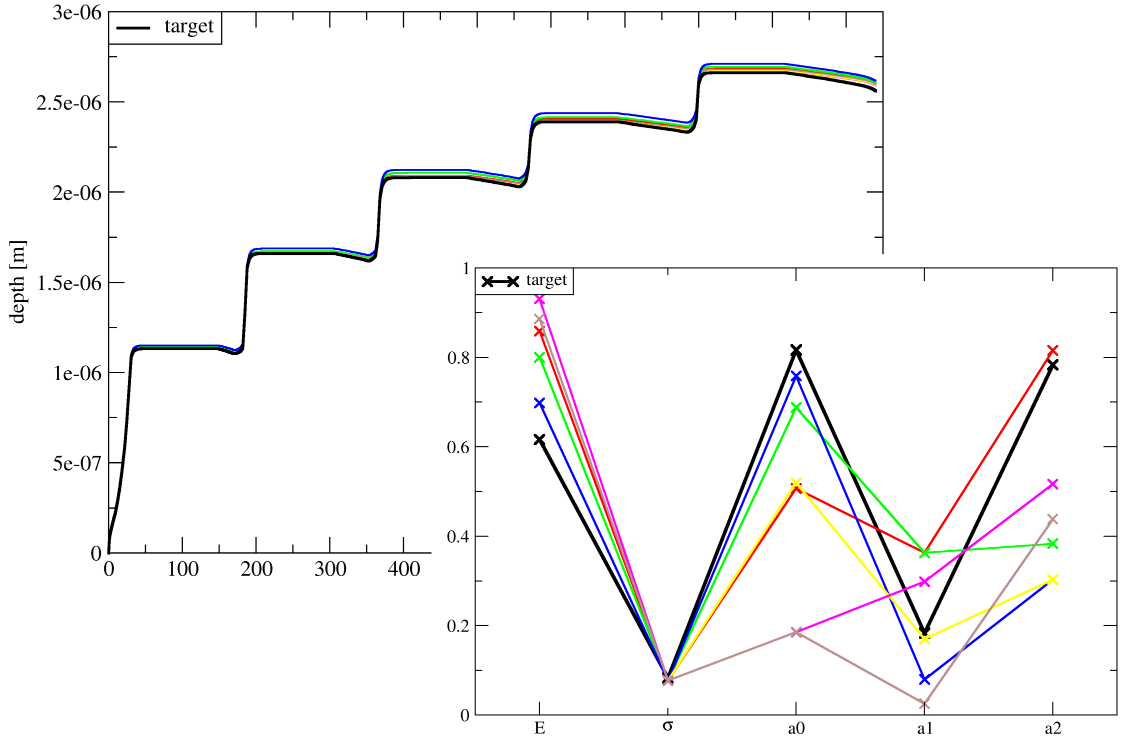

Fig. 7. Final Pareto set for curve III.

3. Conclusions

Multi-objective optimization of input material parameters for nanoindentation model was presented. Multi-objective results indicate the proposed method as very promising. The performance and the successfulness of the optimization could be increased by using PAES in version $\mu+\lambda$. In that case the space of parameters will be searched more thoroughly and the final set will not be so dependent on initial solution. Moreover, the adaptive probability and mutation size will be implemented for finer search near existing solutions.

The next problem in proposed methodology is the inability to deal with the multi-modal problem; this will be solved by an implementation of the above-mentioned algorithm CERAF.

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