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On improved evolutionary algorithms application to the physically based approximation of experimental data

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In this paper an evolutionary algorithms (EA) application to the physically based approximation (PBA) of experimental and/or numerical data is considered. Such an approximation may simultaneously use the whole experimental, theoretical and heuristic knowledge about the analyzed problems. The PBA may be also applied for smoothing discrete data obtained from any rough numerical solution of the boundary value problem, and for solving inverse problems as well, like reconstruction of residual stresses based on experimental data. The PBA presents a very general approach formulated as a large non-linear constrained optimization problem. Its solution is usually complex and troublesome, especially in the case of non-convex problems. Here, considered is a solution approach of such problems based on the EA. However, the standard EA are rather slow methods, especially in the final stage of optimization process. In order to increase their solution efficiency, several acceleration techniques were introduced. Various benchmark problems were analyzed using the improved EA. The intended application of this research is reconstruction of residual stresses in railroads rails and vehicle wheels based on neutronography measurements.

Keywords: evolutionary algorithms, solution efficiency increase, experimental data smoothing, large non-linear constrained optimization problems.

1. Introduction

In this work, we consider analysis of experimental and numerical data using the physically based approximation (PBA) [8, 13] and accelerated evolutionary algorithms (EA). The PBA allows for simultaneous use of all information about the analyzed problems. This approach may take into account all available experimental data obtained by means of various measurement techniques, their statistics as well as all theoretical and/or heuristic knowledge about the considered problems. In general, the PBA is formulated as a constrained optimization problem [8, 13]. Usually such a problem may be large, non-linear and may involve numerous equality and inequality constraints. Its solution is usually complex and troublesome, especially in the case of non-convex problems. So far several attempts of application of the EA to the solution of such problems were made and presented at conferences. Short information about general ideas of considered methods may be found in extended abstracts of those conferences [17, 18]. Here, we are describing general concepts of the PBA approach, the EA acceleration techniques, and chosen results of numerical tests.

The EA are precisely understood here as decimal-coded genetic algorithms consisting of three standard operators: selection, crossover and mutation [3, 10]. In contrast to most deterministic methods, the EA may be successfully applied to non-convex optimization problems. However, general solution efficiency of the standard EA is rather low, especially when approaching to the optimal solution. Therefore, our long-term research [4] is focused, first of all, on a significant acceleration of the optimization process. We have already proposed, and preliminarily tested, several acceleration techniques based on simple concepts [4, 15, 16].

The final objective of our research is development of efficient optimization algorithm for a wide class of large non-linear constrained problems. However, we have also in mind practical, engineering applications, like residual stresses analysis [6, 13] in railroad rails and vehicle wheels. Tensile residual stresses are of great importance in reliable prediction of rail and wheel service life resulting from its fatigue failure [13]. Both theoretical and experimental investigations of residual stresses may be expressed in terms of non-linear constrained optimization problems [8, 12]. Theoretical model of residual stresses analysis in bodies under cyclic loadings is based on shakedown theory and may be found in [13, 14]. This work, however, involves only an inverse approach based on the experimental data measurements and the PBA.

We are presenting here, however, a preliminary approach to application of the improved EA to sample benchmark problems of the PBA. Particularly, considered are analysis of beam deflections and residual stresses reconstruction in the thick-walled cylinder based on pseudo-measured data obtained for cyclic loadings. The purpose of such an analysis of the PBA problems was to investigate practical chances of obtaining efficient solutions in this way for real large complex problems. A variety of tests provided encouraging results. However, this is only the first step of such investigation. Further research is needed.

2. PBA – METHOD FORMULATION

In the PBA all information of the considered problem may be used. The whole available knowledge is introduced in the functional and related constraints, consisting of the experimental and theoretical parts. The problem is posed in the following general way, as a non-linear constrained optimization problem [8]:
find the stationary point of the functional

$$\Phi = \lambda\overline{\Phi}^E + (1-\lambda)\overline{\Phi}^T, \qquad \lambda \in [0,1]\,, \tag{1}$$

satisfying the equality constraints (usually of theoretical nature)

$$A(\sigma) = 0, \tag{2}$$

and the inequality constraints (usually of experimental nature)

$$B(\sigma) \leq e. \tag{3}$$

Here, $\overline{\Phi}^T(\sigma) = \Phi^T(\sigma)/\Phi^T_{ref}$ and $\overline{\Phi}^E(\sigma) = \Phi^E(\sigma)/\Phi^E_{ref}$ are the theoretical and experimental parts of the functional, scaled to be dimensionless quantities, σ is the required solution, and λ is a scalar weighting factor.

Experimental requirements

The experimental part of the functional (1) is defined [8] as the weighted averaged error resulting from discrepancies between the measured data and its approximation, as follows:

$$\Phi^E(\sigma) = \frac{1}{N}\sum_{n=1}^{N} F\left[\frac{f\left(\sigma(r_n)\right) - f_n^{\exp}}{e_n}\right], \tag{4}$$

where σ represents the required unknown field, f is a 'measured' function of σ, $f_n^{\exp}$ is its experimental value at the point r_n, e_n is an admissible experimental error, N is a number of measurements, $F(x) = p(\overline{x}) - p(x-\overline{x})$ is a data scattering function defined by the probability density function $p(x-\overline{x})$, and $\overline{x}$ is the expected value.

The enhanced field $\sigma(r)$ cannot differ too much from experimental data. Thus, the constraints (3) are defined as local requirements:

$$\left|f\left(\sigma(r_n)\right) - f_n\right| \leq e_n, \qquad n = 1, 2, ..., N. \tag{5}$$

It is useful to impose also an averaged global constraint:

$$\sqrt{\Phi^E} \leq e_E. \tag{6}$$

Admissible experimental errors e_E and e_n, $n = 1, 2, ..., N$ should be evaluated taking into account the true statistics of measurements.

Theoretical requirements

The theoretical part of the functional (1) is based on a known theory and/or on a heuristic principle [8]. For instance, in mechanics, $\Phi^T(\sigma)$ can be represented by a well-known energy functional that has to be minimized, e.g., the total complementary energy of statically admissible stresses. On the other hand, as a heuristic principle, e.g., requirement of smoothness may be introduced. In such case, the minimal average curvature κ can be used hence

$$\Phi^T = \frac{1}{\Omega} \int_{\Omega} \kappa^2 d\Omega, \tag{7}$$

where

$$\kappa^2 = \frac{1}{2\pi} \int_0^{2\pi} \left(\frac{\partial^2 f}{\partial \nu^2} \right)^2 d\varphi. \tag{8}$$

Theoretical constraints are usually presented as equality conditions (2).

Specific formulation proposed

One of the main difficulties in the general formulation (1)–(3) is the problem of how to establish the weighting factor λ, i.e., how to determine a reasonable balance between experiment and theory involved. Specific formulations addressing this problem may be found in [8, 13].

3. EA AND ACCELERATION TECHNIQUES

The optimization problem formulated above may involve large number of decision variables and requires efficient solution methods. Acceleration of the EA-based solution approach may be obtained in several ways. General efficiency may be increased by means of an appropriate hardware, software, and algorithm improvements. Hardware acceleration techniques include distribution and parallelization of calculations on various multiprocessor systems, e.g., computer clusters, GP GPUs or FPGA devices. Efficient software implementations dedicated for particular hardware architectures are crucial as well. However, our research is mainly concentrated now on introduction of new algorithms and improvements of certain existing ones. Distributed and parallel computations are used as well, but mostly as a support for new acceleration techniques.

Algorithmic acceleration of the optimization process may be obtained in various ways including: development of new, problem-oriented evolutionary operators, e.g. gradient mutation, development of hybrid methods [2, 5] combining the EA with deterministic techniques, application of standard parallel and distributed calculations [9, 11], choice of the most efficient combination of particular variants of selection, crossover and mutation operators, and evaluation of the best values of the EA parameters. Moreover, we have recently proposed, and preliminarily tested, several acceleration techniques based on simple concepts [4, 15, 16], i.e., solution smoothing and balancing, a'posteriori solution error analysis and related techniques, non-standard use of distributed and parallel calculations and adaptive step-by-step mesh refinement. Some of them are problem- (or class of problems) oriented, other are of more general character. Some of these techniques are addressed to optimization of functionals, where a large set of nodal values of a function is searched. Particular attention has been paid to the application of a'posteriori solution error estimation and related techniques [15]. A brief overview of the proposed solution approach and the state of the art may be found in [4]. They are also briefly discussed below.

3.1. Smoothing and balancing

If additional information about solution smoothness is available, it may be used to improve the optimization process in various ways [4, 16]. For instance, an extra procedure based on an appropriate approximation method, like moving weighted least squares (MWLS) technique [19, 20], or any other equivalent method, may be applied in order to smooth raw results obtained from the standard EA. However, in problems of mechanics each smoothing may result in global equilibrium loss of a considered body. Restoration of equilibrium may be done by artificial balancing of body forces performed directly after smoothing. Information about smoothness may be also used in the selection process [4]. A new criterion based on a mean local solution curvature may be introduced to any selection operator.

3.2. A'posteriori error analysis and related techniques

The EA-based optimization is a stochastic process; therefore solutions obtained from independent populations may differ from each other. The weighted average of the best solutions taken from such populations is expected to be more precise than majority of its particular components. Moreover, the averaged solution may be used as a reference one for a'posteriori error estimation [1, 15]. Calculations may be intensified in large error zones using information about the magnitude and the distribution of local errors. It is done by appropriately modified mutation and crossover operators [15]. Information about estimated global error is used by selection operator. Moreover, representation of the best solutions, collected at the same time from all populations involved, may also be very useful, and improve the solution process [15]. Both solution averaging and error analysis may be well supported by parallel and distributed calculations in addition to other standard advantages provided by multiprocessor systems. All independent populations are calculated simultaneously in a parallel way. Calculations carried out in each population may also be partitioned among processing units. Such an approach essentially improves efficiency of the solution process.

3.3. Adaptive step-by-step mesh refinement

Solution time needed for optimization of functional is in many problems strictly dependent on the number of decision variables used, i.e. on the mesh density in the domain. Therefore, the basic concept of an adaptive step-by-step mesh refinement [4] is to start analysis from a coarse mesh, where solution is obtained much faster than in the fully dense case. However, such a solution for the sought function is usually not precise enough. In order to increase its precision the mesh is refined by inserting new nodes, based on the results of the error analysis. During the whole optimization process the mesh may be refined many times, until sufficient density is reached everywhere. Initial function values at the inserted nodes in each refinement are found by means of an appropriate approximation technique, e.g., MWLS, built upon the coarse mesh nodal values. Furthermore, the mesh refinement strategy may also be useful for the a'posteriori error analysis [4]. Refined and smoothed solutions may be used as the initial reference ones for a'posteriori error evaluation.

4. Benchmark problems

A variety of benchmark problems was chosen in order to evaluate the efficiency of the proposed acceleration techniques and their possible combinations [4]. In particular, we have analyzed theoretical approach for evaluation of residual stresses in an elastic-perfectly plastic bar subject to cyclic bending, and in the thick-walled cylinder made of the same material, and subject to cyclic loadings, like internal pressure, torsion and tension [4]. These problems were analyzed as 1D (taking into account existing symmetries), and as 2D ones as well.

We have also investigated several benchmark tests using simulated pseudo-experimental data and the PBA approach, including smoothing of beam deflections, and reconstruction of residual stresses in the thick-walled elastic-perfectly plastic cylinder subject to cyclic loadings [17, 18].

4.1. Benchmark test 1 – smoothing of beam deflections

Given are free-supported beam displacements $w_j^{\exp}$, measured at points x_j, $j = 1, 2, 3, ..., N-1$. Searched are nodal values of smoothed displacements w. The following, particular PBA problem is considered: find the stationary point of the functional

$$\Phi(w) = \lambda \overline{\Phi}^E(w) + (1-\lambda)\overline{\Phi}^T(w), \qquad \lambda \in [0,1]\,, \tag{9}$$

where

$$\Phi^E(w) = \frac{1}{N-1}\sum_{j=1}^{N-1}\left(\frac{w_j - w_j^{\exp}}{e_j}\right)^2, \tag{10}$$

$$\Phi^T(w) = \frac{1}{L}\int_0^L \kappa^2 dx \approx \frac{1}{L}\int_0^L (w'')^2 dx \approx \frac{1}{N}\sum_{j=0}^{N} (w''_j)^2, \tag{11}$$

satisfying:

$$w_0 = w_N = 0, \qquad \text{(boundary conditions)}, \tag{12}$$

$$\left|w_j - w_j^{\exp}\right| \le e_j, \quad j = 1, 2, 3, ..., N-1, \quad \text{(admissible local error constraints)}, \tag{13}$$

$$\sqrt{\Phi^E(w)} \le e_E, \qquad \text{(admissible global error constraint)}. \tag{14}$$

4.2. Benchmark test 2 – residual stresses reconstruction in the thick walled cylinder

Strains $\varepsilon_i^{\exp}$, experimentally measured in the 2D cross-section of the thick walled cylinder under cyclic internal pressure are given. Find residual stresses $\sigma = \{\sigma_r^r, \sigma_t^r, \sigma_z^r\}$ in the 2D cross-section. The following formulation in the polar coordinate system is used:
find the stationary point of the functional

$$\Phi(\sigma) = \lambda \overline{\Phi}^E(\sigma) + (1-\lambda)\,\overline{\Phi}^T(\sigma), \qquad \lambda \in [0,1]\,, \tag{15}$$

where

$$\Phi^E(\sigma) = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\varepsilon_i^{app}(\sigma) - \varepsilon_i^{\exp}}{e_i}\right)^2, \tag{16}$$

$$\Phi^T(\sigma) = \frac{1}{\Omega}\int\limits_{\Omega} \kappa^2(\sigma) d\Omega, \tag{17}$$

satisfying equality constraints:

$$\frac{\partial \sigma_r^r}{\partial r} + \frac{\sigma_r^r - \sigma_t^r}{r} = 0, \qquad \text{(equilibrium equation)}, \tag{18}$$

$$\sigma_{r|a}^r = 0, \qquad \sigma_{r|b}^r = 0, \qquad \text{(boundary conditions)}, \tag{19}$$

$$\sigma_z^r = \nu(\sigma_r^r + \sigma_t^r), \qquad \text{(incompressibility equation)} \tag{20}$$

and inequality constraints:

$$|\varepsilon_i^{\exp} - \varepsilon_i^{app}(\sigma)| \leq e_i, \qquad \text{(admissible local errors)}, \tag{21}$$

$$\sqrt{\Phi^E} \leq e_E, \qquad \text{(admissible global error)}. \tag{22}$$

The mean solution curvature is calculated using the following definition, given in the Cartesian coordinates:

$$\kappa^2(f) = \frac{1}{4}(f_{xx} + f_{yy})^2 + \frac{1}{8}(f_{xx} - f_{yy})^2 + \frac{1}{2}f_{xy}^2 \tag{23}$$

and transformed to the polar coordinate system.

5. Numerical results

At first a choice of the most efficient combination of the standard EA operators was sought. Searching the best combination of operators and adjusting their parameters, acceleration up to several times may be reached. Using the best combination found, namely rank selection, heuristic crossover, an non-uniform mutation, particular already mentioned techniques were investigated yielding efficient acceleration of the optimization process. Some results of our efficiency analysis were described in [4, 15]. Brief overview is presented below.

Numerous numerical tests carried out clearly show a possibility of increasing solution efficiency using all proposed acceleration techniques. Acceleration of computations was measured using speed-up factors defined in [15]. Application of our smoothing technique based on the MWLS allowed to obtain up to 4 times efficiency increase. In those tests balancing procedure based on the linear correction function was used. A wide discussion of a'posteriori error analysis and related techniques for improving efficiency was given in [15]. Using these techniques the speedup about 2-4 was reached. However, when appropriately combined with additional smoothing procedure, the speed-up raised up to about 7.5 times [15]. The numerical analysis was done using mostly 1D and 2D bar bending benchmark problems. However, recent research using further benchmarks, like pressurized cylinder (1D and 2D), has also confirmed earlier observations. The greatest acceleration till now was obtained for solution approach using a step-by-step mesh refinement combined with the other techniques. When a series of denser and denser meshes was appropriately used, the speed-up factor of about 120 was gained [4].

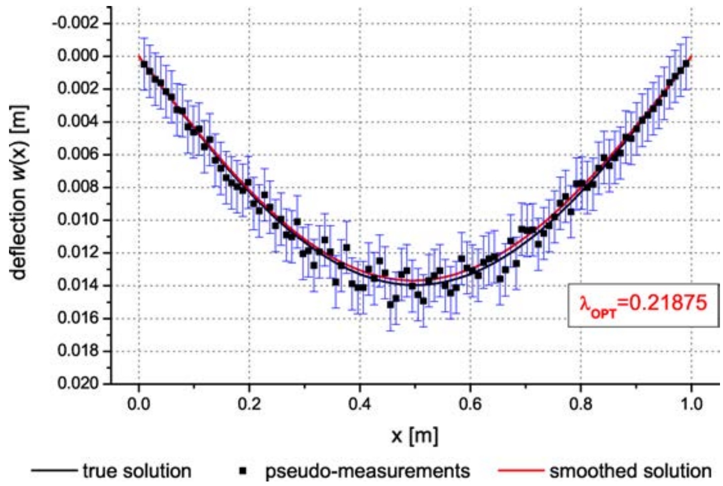
Summarizing, preliminary results of the executed tests clearly show a significant improvement of the optimization process in comparison with the standard EA. It is also worth noticing, that the improved EA allowed obtaining solutions in cases when the standard EA failed, e.g. for too large number of decision variables.

In this paper, we are presenting results of application of the improved EA to the sample benchmark problems of the PBA, formulated in Sec. 4. The main objective of executed tests was to find, whether the applied algorithms were efficient enough to solve such large problems. The final objective of our research is such improvement of the EA so that they can efficiently deal with optimization problems using up to several thousands of decision variables.

5.1. Smoothing of simulated beam deflections

Numerical data used in this experiment were randomly generated using the true solution of loaded free-supported beam as a base curve. The random data generator used Gaussian distribution. Such a simulation of the experiment allowed for controlling the admissible data errors. Generated pseudo-measurements were smoothed next using the PBA approach. In Fig. 1 you may see the original and smoothed solutions obtained when using data with admissible errors up to 10% (Fig. 1a) and up to 20% (Fig. 1b).

a)



b)

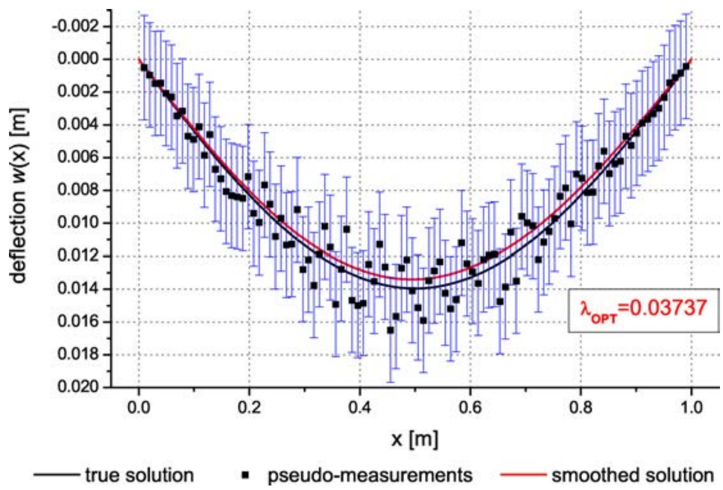


Fig. 1. Smoothed solutions obtained for data with admissible errors up to 10% (a) and up to 20% (b).

Using the PBA we may effectively smooth numerical and experimental data, reducing mean square and maximum errors. In Fig. 2 you may find absolute errors calculated on non-smoothed and smoothed data. Data sets used in that numerical experiment were generated by increasing the admissible errors from 2% up to 100%. The true errors where calculated using the following, standard norms:

$$e_{ms} = \left(\frac{1}{N} \sum_{i=1}^{N} (\, w_i - \overline{w}_i)^2 \right)^{1/2}, \qquad \text{(mean square)}, \tag{24}$$

$$e_{\max} = \max_{i=1,\,\dots,\,N} \{ |w_i - \overline{w}_i| \}, \qquad \text{(maximum)}, \tag{25}$$

where $\overline{w}_i$ is the true solution.

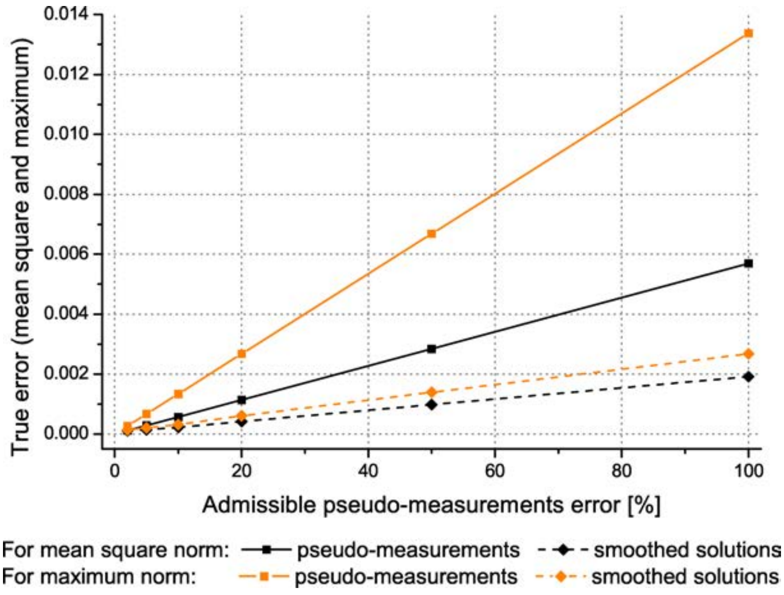


Fig. 2. Mean square and maximum errors calculated for non-smoothed and smoothed solutions.

5.2. Smoothing of real beam deflections

Real experimental deflections may be obtained, e.g., by vision measurement systems. Results of such optical measurements may be smoothed in very similar way and applied, e.g., for load identification. Such an experimental measurement technique was developed, e.g., in the Department of Robotics and Mechatronics at the AGH University of Science and Technology [7]. The results have been shared with us. In Fig. 3 one may see smoothed solutions using various boundary conditions. In the first case, the constraints were exactly the same, as in (12)–(14). In the second one, we assumed that the beam was fully clamped and added additional conditions for derivatives.

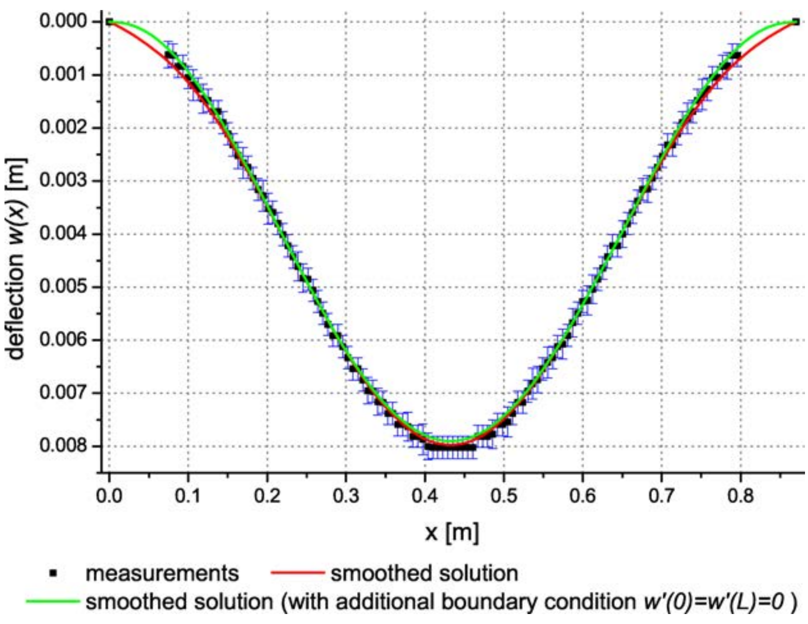


Fig. 3. Smoothed solutions obtained for real experimental data.

5.3. Residual stresses reconstruction in the thick walled cylinder

Randomly generated pseudo-measurements were also used in a set of tests concerning residual stresses reconstruction in the thick walled cyclically pressurized cylinder. For numerical data generation, a strain gauge technique was simulated. Assumed were delta type rosettes, giving three components of strains. All calculations were carried out in the 2D domain. However, for the clarity of presentation, only the data and results in 1D radial cross-section of the domain are shown. Methodology of executed tests was the same as in the case of beam deflections smoothing.

Figure 4 shows samples of generated pseudo-data with admissible errors up to 20%. Radial, hoop and axial residual stresses calculated in the PBA analysis of these data are shown in Fig. 5.

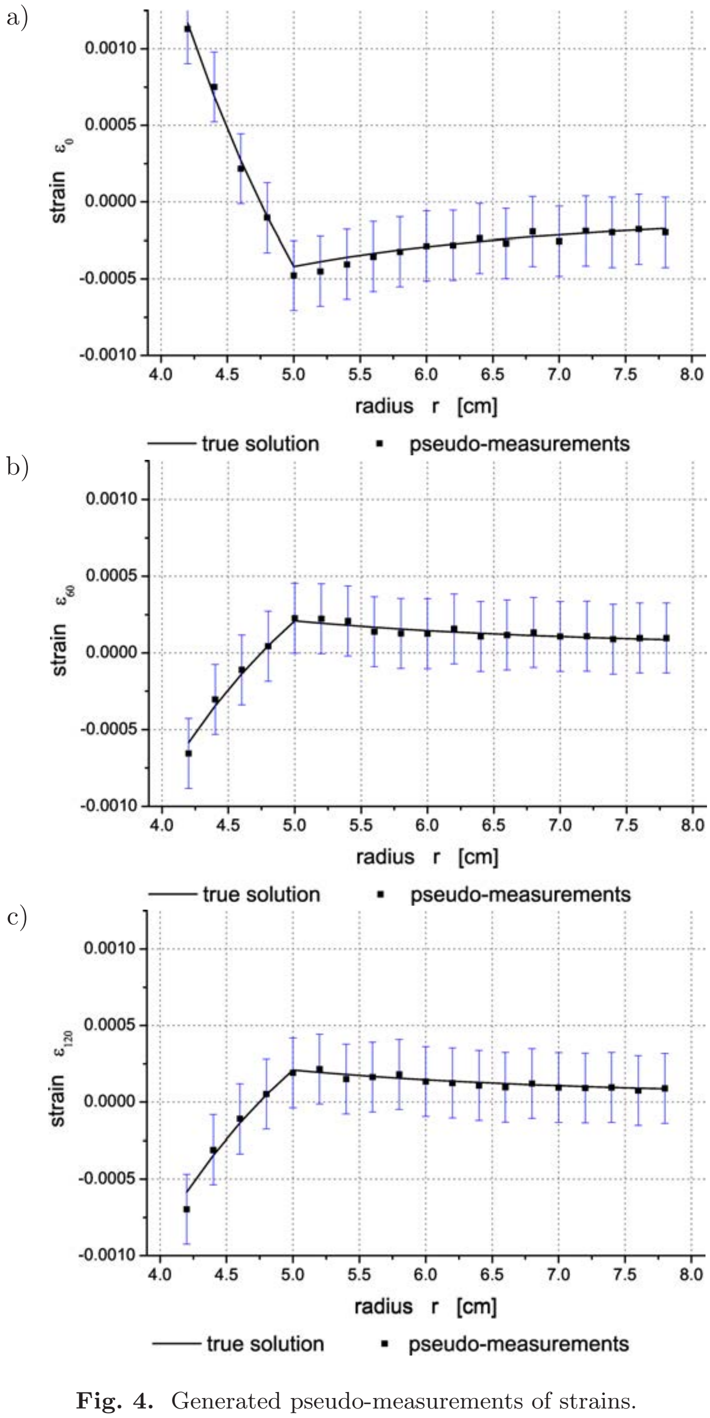


Fig. 4. Generated pseudo-measurements of strains.

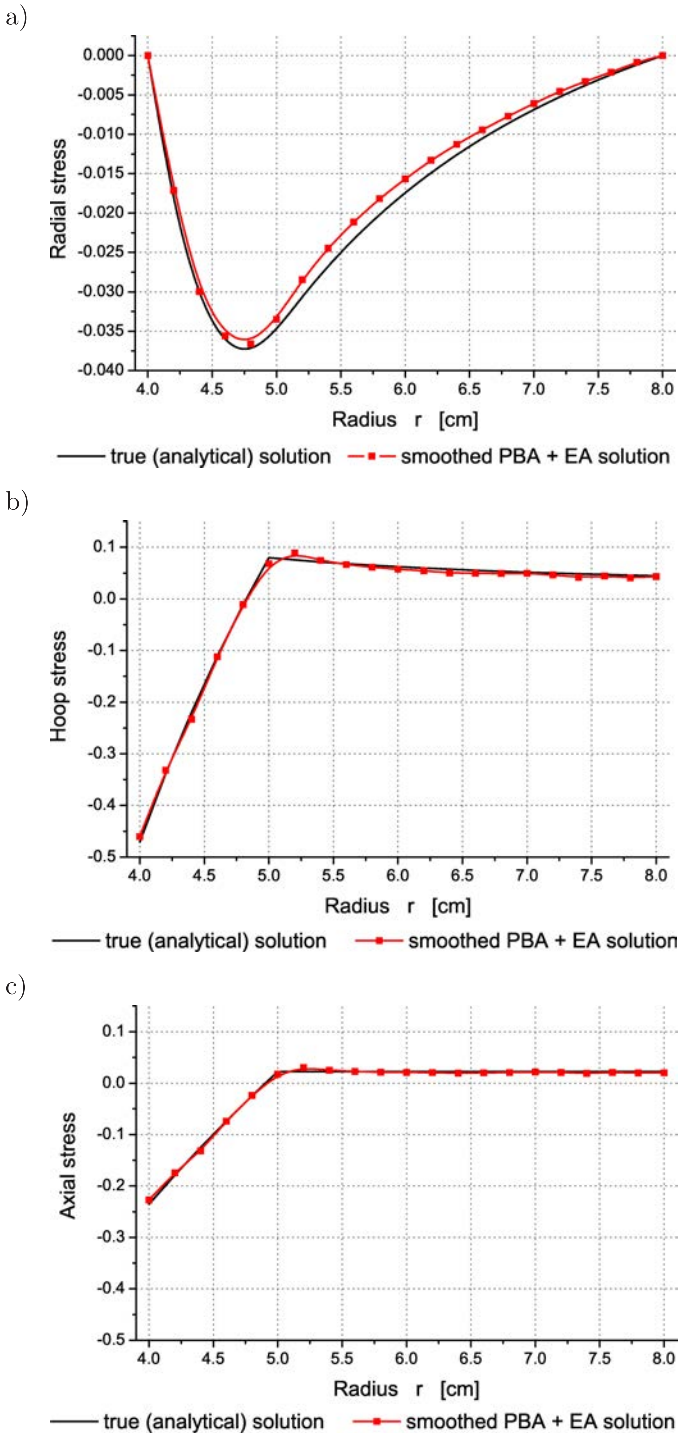


Fig. 5. Calculated radial (a), hoop (b) and axial (c) residual stresses.

In Fig. 6 one may see residual stresses obtained using pseudo-measurements of strains generated with various admissible errors. Only radial stresses are shown here.

Due to stochastic nature of the generated pseudo-measurements, and also stochastic nature of evolutionary computations applied, all tests should be repeated many times. Figure 7 shows results obtained using 10 independent data sets. Dispersion of the calculated random results and their averaged values are also shown. Such tests allow to draw a conclusion that the improved EA approach applied to the PBA problems gives repeatable results.

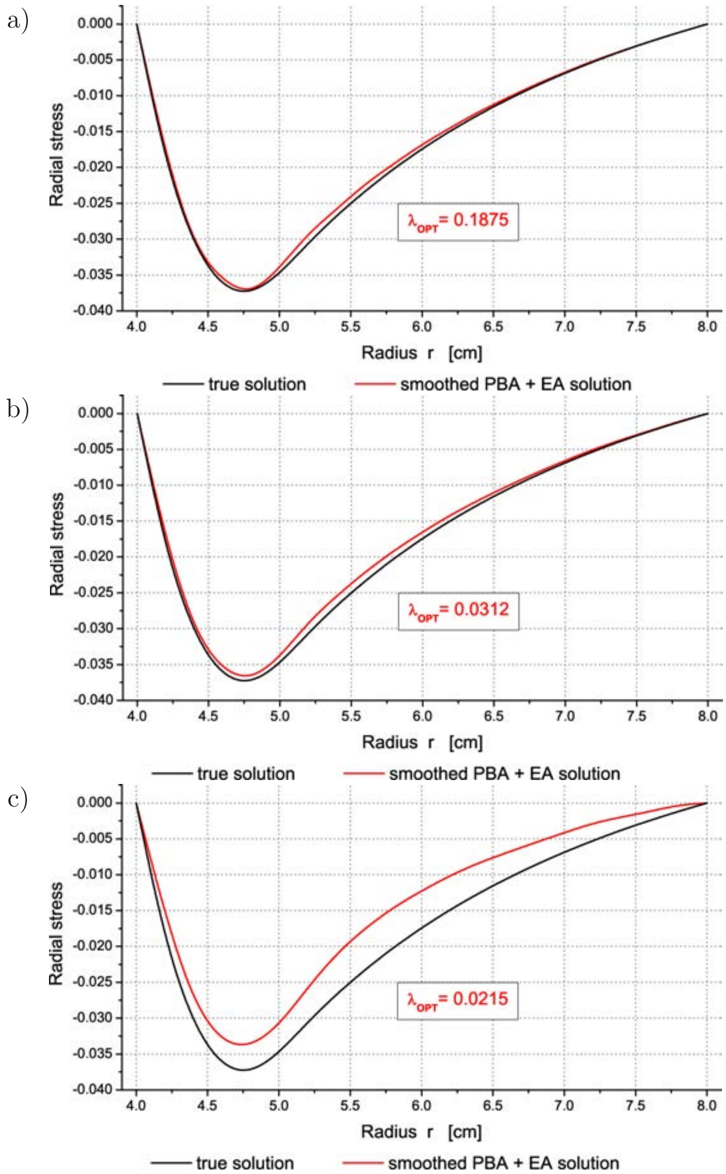


Fig. 6. Radial residual stresses obtained using randomly generated strains with admissible errors up to 5% (a), 10% (b), and 50% (c).

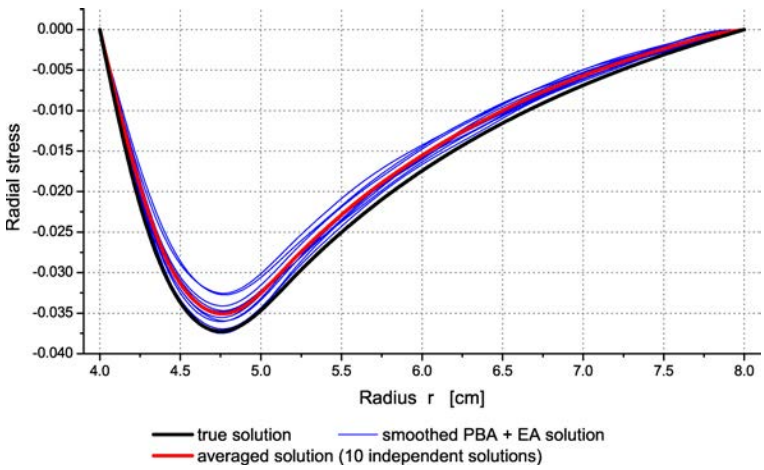


Fig. 7. Radial residual stresses calculated using 10 independent data sets.

6. Final remarks

Results obtained indicate a clear possibility of practical application of the improved EA to the PBA of experimental and/or numerical data for large optimization problems, the inverse ones including. The accelerated EA were successfully used for sample benchmark problems. Application of the accelerated EA to the PBA is still at the initial stage of research development; however, preliminary results are very encouraging. Continuation of this research is needed. Further research includes continuation of various efforts oriented towards acceleration of the EA-based solution process, and application of this approach to large, non-linear, constrained optimization problems (convex and non-convex) resulting from the PBA applied to experimentally measured data for real engineering problems, e.g., residual stress analysis in railroad rails and vehicle wheels.

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