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ON DEDICATED EVOLUTIONARY ALGORITHMS FOR LARGE NON-LINEAR CONSTRAINED OPTIMIZATION PROBLEMS IN APPLICATION TO RESIDUAL STRESSES ANALYSIS

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Abstract. This work considers development of dedicated Evolutionary Algorithms (EA) with several new specialized acceleration techniques introduced. Our long-term research is oriented towards development of efficient solution methods for a wide class of large, non-linear, constrained optimization problems. We are presenting here a preliminary application of the improved EA to sample benchmark problems of residual stresses analysis. The final objective of our research is such analysis done for railroad rails, and vehicle wheels. Knowledge of the tensile residual stresses is crucial for reliable prediction of rails and wheels service life resulting from their fatigue failure. Both the theoretical and experimental investigations of residual stresses may be expressed in terms of large, non-linear, constrained optimization problems. Due to the size and complexity of the optimization problems involved, our research is focused, first of all, on the EA efficiency increase.

1 INTRODUCTION

This work considers development of dedicated Evolutionary Algorithms (EA) with several new specialized acceleration techniques introduced. Many scientific and engineering tasks may be formulated as large optimization problems, and require efficient solution methods. Therefore, our long-term research [4] is oriented towards development of such methods for a wide class of large, non-linear, constrained optimization problems, where a discrete function is sought, e.g. expressed in terms of its nodal values. These values are defined on a mesh formed by arbitrarily distributed nodes. We are presenting here a preliminary application of the improved EA to sample benchmark problems of residual stresses analysis. The final objective of our research is such analysis done for railroad rails, and vehicle wheels [8,14,15]. Knowledge of the tensile residual stresses is crucial for reliable prediction of rails and wheels service life resulting from their fatigue failure [14]. Both the theoretical and experimental investigations of residual stresses may be expressed in terms of large, non-linear, constrained optimization problems [14,15]. Especially when for data smoothing the Physically Based Approximation (PBA) is used [9,14]. In contrast to most of the deterministic methods, the EA

may be successfully applied with equal efficiency to both the convex and non-convex problems, however, their general efficiency is rather low. Due to the size and complexity of the optimization problems involved, our research is focused, first of all, on the efficiency increase of the EA.

2 PROBLEM FORMULATION

We consider a wide class of large, non-linear, constrained optimization problems. Usually these problems are formulated as optimization of functionals, where a function $u(\mathbf{x})$, $\mathbf{x} \in R^N$ is sought, usually in the discrete form of the vector $\mathbf{u} = \{u_i\}$ consisting of nodal values u_i, $i = 1, 2, \ldots, n$. These nodal values are defined on a mesh formed by arbitrarily distributed nodes. Here N is the dimension of the physical space (1D, 2D or 3D), and n is a number of decision variables. In general, considered optimization problems may be posed as follows:

Find a function $u = u(\mathbf{x})$, that yields the stationary point of the functional $\Phi(u)$, satisfying the equality $\mathbf{A}(u) = 0$, and inequality constraints $\mathbf{B}(u) \le 0$.

The PBA approach is a specific example of the above general formulation. In the PBA all information about the considered problem may be used. The whole available experimental, theoretical, and heuristic knowledge is introduced in the functional and related constraints. The problem is posed in the following general way:

Find the stationary point of the functional

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

satisfying the equality constraints $\mathbf{A}(u) = 0$ (usually of theoretical nature), and inequality constraints $\mathbf{B}(u) \le e$ (usually of experimental nature). Here, $\Phi^E(u)$ and $\Phi^T(u)$ are the experimental and theoretical parts of the functional, scaled to be dimensionless quantities, u is the required solution, λ is a dimensionless scalar weighting factor, and e is an admissible tolerance.

Particular, detailed formulation of the PBA approach for residual stresses reconstruction in railroad rails, and vehicle wheels may be found in [9]. Theoretical model of residual stresses analysis in bodies under cyclic loadings is based on shakedown theory and may be also formulated as such general optimization problem [14,19].

Such optimization problems may involve large number of decision variables and require efficient solution methods.

3 APPLIED ALGORITHMS

3.1 Evolutionary Algorithms

The EA are precisely understood here as Genetic Algorithms with decimal (floating-point) chromosomes. The standard algorithm consists of three operators: selection, crossover and mutation [3,11]. Significant acceleration of the EA-based solution approach may be achieved in various ways, including appropriate hardware, software, and algorithm improvements. Hardware acceleration techniques include distribution and parallelization of calculations on various multiprocessor systems, e.g., GPUs, FPGA devices, SMP machines or standard computer clusters. Efficient software implementations dedicated for particular hardware

architectures are crucial as well. However, our research is mainly concentrated now on development of new algorithms and improvements of certain existing ones. Distributed and parallel computation are used as well, but mostly as a support for new acceleration techniques.

Algorithmic acceleration of an optimization process may be obtained by, e.g., development of hybrid algorithms [2,5] combining the EA with deterministic methods (such as feasible direction method), introduction of new, problem-oriented operators [6,7], choice of the most efficient combination of particular variants of operators, and evaluation of the best values of their parameters. Moreover, we have recently proposed, and preliminarily tested, several acceleration techniques based on simple concepts [4,16,17].

In order to achieve an acceleration of the optimization process, the modified EA use smoothing and balancing techniques, solution averaging, a'posteriori error analysis and related techniques, as well as adaptively refined series of meshes, and possible combinations of the above. Proposed techniques are well supported by non-standard use of parallel and distributed calculations. 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.

3.2 Smoothing and Balancing

When additional information about solution smoothness is available, the Moving Weighted Least Squares (MWLS) approximation technique [18,20] is applied in order to smooth raw solutions obtained from the standard EA. Additional smoothing may be applied periodically during the whole optimization process.

In problems of mechanics each smoothing may result in the global equilibrium loss of a considered body. The equilibrium is restored by the standard EA in a series of iterations. However, it may be also restored at once by means of an artificial balancing of body forces, performed directly after the smoothing [4]. In the considered tests, balancing procedure was used based on the linear correction function. Formulation of this procedure will be given in the description of the benchmark problems.

3.3 A'posteriori Error Analysis and Related Techniques

In the case of deterministic methods, the a'posteriori error analysis is well developed, and widely used now [1]. Some concepts of such error analysis may also be partially extended into the case of the EA solution approach. However, a new definition of a reference solution is needed. Therefore, we have proposed a concept based on the stochastic nature of evolutionary computation [16].

Due to such nature, the best chromosomes taken from various independent populations may differ from each other. Reference solutions required to estimate local errors are proposed to be obtained by a weighted averaging of the best solutions taken from the independent EA processes. The weighted averaged solution is expected to have a better chance to be closer to the exact one than majority of its particular components contributing to such average. After a'posteriori error estimation, and evaluation of relevant error maps, information about the magnitude and distribution of the local errors is used by appropriately improved crossover, and mutation operators in order to intensify calculations in large error zones [16].

Information about the global errors may also be introduced as an additional criterion in selection process [16].

Moreover, an additional acceleration may be achieved by collecting the best chromosomes, taken from all populations, and generating a new population of "representatives". Convergence in such population should be better than in the other populations.

In order to accelerate the optimization process a cloning strategy may be also used. Cloning may be applied to the weighted mean chromosome and/or to the best representatives [16]. For instance, 10% of the worst chromosomes in all populations may be replaced by the clones.

A'posteriori error analysis and related techniques may be well supported by the parallel and distributed calculations [16] in addition to other standard advantages provided by multiprocessor systems [10,13]. In such case all independent populations are calculated simultaneously in a parallel way. Of course, calculations carried out in each population may also be partitioned among processing units. Such approach essentially improves efficiency of the solution process.

More detailed information and wider numerical analysis of mentioned techniques using chosen benchmark problems may be found in [16].

3.4 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, e.g. on the mesh density in the domain. Therefore, when using an adaptive step-by-step mesh refinement, the analysis starts from a coarse mesh, allowing to obtain a solution much faster than in the fully dense grid case. When decreasing the number of nodes, the convergence rate is increased, and the time spent on each iteration is reduced. However, the solution obtained on a coarse mesh may usually be 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 done so far. The initial function values at these nodes are found by using an approximation built upon the coarse mesh nodal values. A general approach for most optimization problems may be obtained by using the Moving Weighted Least Squares (MWLS) approximation [18,20]. However, other approximation or interpolation methods may be considered. In some problems, the best results may be obtained for simple linear interpolation of the nodal function values. Efficiency of this approach may depend on the solution nature and approximation method applied.

Furthermore, the step-by-step mesh refinement may be also used in the a'posteriori error analysis. Solutions obtained after each mesh refinement (preliminary approximation followed by smoothing) are used as initial reference solutions for the error estimation. Such combined strategy, using all techniques mentioned above, may involve the following steps [4]:

- Evaluation of the solution on a coarse mesh.
- Smoothing of this rough solution.
- Mesh refinement and approximation of the initial values in the inserted nodes.
- Use of the obtained solution as an initial reference for the error estimation.
- Use of the weighted solution averaging for further reference solution generation, and the a'posteriori error analysis.
- Repetition of the above procedure until sufficiently dense mesh is reached.

4 BENCHMARK PROBLEMS

A variety of simple benchmark problems was chosen in order to evaluate correctness, and efficiency of the proposed acceleration techniques, as well as their ability to deal with large, and very large optimization problems. In particular, we have analyzed the residual stresses in an elastic-perfectly plastic bar subject to cyclic bending, and in a thick-walled cylinder made of the same material, and subject to cyclic loadings, like internal pressure, torsion and tension [4]. These problems may be analyzed as either 1D (taking into account existing symmetries) or as 2D ones as well. Another advantage of considered benchmark problems is possibility of testing almost any number of decision variables involved. The exact solutions needed for such comparisons are, of course, known.

We have also investigated several benchmark problems using the PBA approach for both experimental and numerical data, including smoothing of beam deflections, and reconstruction of residual stresses arising in bodies under cyclic loadings. However, these benchmark problems and obtained results are not discussed in this paper.

4.1 Benchmark problem 1

Considered is residual stresses analysis in an elastic-perfectly plastic bar of the rectangular cross-section subject to cyclic bending.

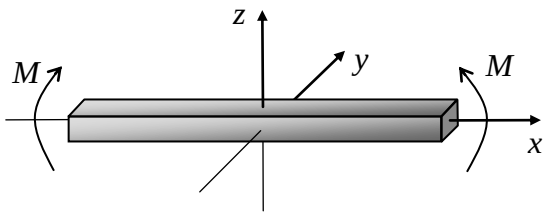

Figure 1: Model of bar subject to pure cyclic bending by the moment *M*

Formulation of the problem – 1D model

Find stresses $\sigma = \sigma(z)$ satisfying the minimum of the total complementary energy

$$\min_{\sigma} \int_0^H \sigma^2 dz \tag{2}$$

and constraints:

- global self-equilibrium equation

$$M = \int_0^H \sigma\, z\, dz = 0 \tag{3}$$

- yield condition for total stresses

$$\left|\sigma + \sigma^e\right| \le \sigma_Y \tag{4}$$

where σ_Y is the yield stress (plastic limit), and σ^e is the purely elastic solution of

the problem. After discretization, where the sought normal stress $\sigma = \sigma(z)$ is replaced by the piecewise linear function spanned over the nodal values σ_i, the following formulation is obtained:

Find stresses $\sigma_1, \sigma_2, ..., \sigma_n$ satisfying

$$\min_{\sigma_1,\sigma_2,...,\sigma_{n-1}} \left(\sum_{k=1}^{n-1} \sigma_k^2 + \frac{1}{2}\sigma_n^2 \right), \qquad \sigma_n = -\frac{2}{z_n} \sum_{k=1}^{n-1} \sigma_k z_k \tag{5}$$

and equality constraints

$$-\sigma_Y \le \sigma_k + \sigma_k^e \le \sigma_Y, \qquad k = 1,2,...,n \tag{6}$$

Numerical integration is used providing the exact results for linear functions.

Balancing procedure in 1D

The balancing procedure proposed for this benchmark problem is based on an assumption that the lost global equilibrium may be restored by adding an appropriate linear correction term $\sigma(z) = a\,z + b$. In the bar cross-section the resultant, unbalanced axial force *N* and the relevant static moment M_Y are evaluated using the EA solution based stress data:

$$N = \int \sigma \, dz \tag{7}$$

$$M_Y = \int z\,\sigma \, dz \tag{8}$$

Using the same formulas for the linear correction term, one may find unknown coefficients *a* and *b*. Finally, obtained are:

$$a = \frac{M_Y}{I_Y}, \quad \text{and} \quad b = \frac{N}{2H} \tag{9}$$

where I_Y is the moment of inertia of the bar cross-section.

Formulation of the problem – 2D model

In 2D model, the fitness function (total complementary energy) is defined as follows:

$$I = \int_{-b/2}^{b/2} \int_{-H}^{H} \sigma^2 \, dzdy \approx \frac{h^2}{9} \left(\sum_{k=1}^{n} \sigma_k^2 \, \alpha_k \right) \tag{10}$$

where α_j are Simpson integration coefficients. The sought solution has to satisfy the following constraints:

- global self-equilibrium equation

$$M = \int_{-b/2}^{b/2} \int_{-H}^{H} \sigma\, z \, dzdy \approx \frac{h^2}{9} \left(\sum_{k=1}^{n-1} \sigma_k z_k \alpha_k + \sigma_n z_n \alpha_n \right) \rightarrow \sigma_n = -\left(z_n \alpha_n\right)^{-1} \sum_{k=1}^{n-1} \sigma_k z_k \alpha_k = 0 \tag{11}$$

- yield condition for total stresses

$$-\sigma_Y \le \sigma_k + \sigma_k^e \le \sigma_Y, \qquad k = 1,2,\ldots,n \tag{12}$$

Balancing procedure in 2D

The balancing procedure may be developed in a way similar to the 1D case. In 2D case, the coefficients of the linear correction function $\sigma(y,z) = a\,y + b\,z + c$ are obtained as follows:

$$a = \frac{M_Z}{I_Z}, \quad b = \frac{M_Y}{I_Y}, \quad \text{and} \quad c = \frac{N}{\Omega} \tag{13}$$

where I_Z , I_Y are moments of inertia, and Ω is bar cross-section.

4.2 Benchmark problem 2

Considered is an elastic-perfectly plastic thick-walled cylinder under cyclic internal pressure. The following optimization problem given in the polar coordinates for residual stresses was analyzed:

Find the minimum of the total complementary energy:

$$\min_{\sigma_r^r,\sigma_t^r,\sigma_z^r} \tfrac{1}{2E} 2\pi L \int_a^b [(\sigma_r^r - \sigma_t^r)^2 + (\sigma_t^r - \sigma_z^r)^2 + (\sigma_z^r - \sigma_r^r)^2]\, r\, dr \tag{14}$$

subject to the equilibrium equation

$$\frac{\partial \sigma_r^r}{\partial r} + \frac{\sigma_r^r - \sigma_t^r}{r} = 0 \tag{15}$$

boundary conditions

$$\sigma_{r\,|\,a}^r = 0, \qquad \sigma_{r\,|\,b}^r = 0 \tag{16}$$

the incompressibility equation

$$\sigma_z^r = \nu(\sigma_r^r + \sigma_t^r) \tag{17}$$

and the yield condition

$$\phi(\sigma_r^r, \sigma_t^r, \sigma_z^r, \sigma^e) \le \sigma_Y \tag{18}$$

where $\sigma_r^r, \sigma_t^r, \sigma_z^r$ are respectively the radial, circumferential and longitudinal residual stresses, $\sigma^e = \{\sigma_r^e, \sigma_t^e, \sigma_z^e\}$ is the purely elastic solution of the problem, σ_Y is the yield stress, a, b are respectively the internal and external cylinder radii, L is its length, and E is the Young modulus.

5 NUMERICAL RESULTS

The objective of the tests presented here is also a comparison of various variants of the improved EA with the standard one. The standard algorithm is understood here as one

consisting only of three basic operators: selection, crossover, and mutation. Before testing additional acceleration techniques, we chose first the most efficient combination of the standard but decimal EA operators. Searching the best combination of operators, as well as adjusting their parameters, the acceleration factor up to several times may be reached. From numerous variants of operators [6,7] we preliminarily chose several popular ones: the ranking, and tournament selection, arithmetic, and heuristic crossover, uniform, non-uniform, and border mutation. We also tested various combinations of them. Using the best combination found, namely the rank selection, heuristic crossover, and the non-uniform mutation, particular acceleration techniques already mentioned before were analyzed. Some other results of our efficiency analysis were also described in [16], and very briefly in [4,17].

Acceleration of computation was measured using four speed-up factors defined in [16]. These factors take into account convergence of mean solution error as a function of time, or as a function of number of iterations, as well as convergence of fitness function. These four speed-up factors together provide the investigated acceleration characteristics. Moreover, the solution precision increase after certain periods of time or after a number of iterations was measured.

5.1 A'posteriori error estimation

A wide discussion of the weighted solution averaging, a'posteriori error analysis, and related techniques for improving efficiency of optimization processes was given in [16]. Using all these techniques together the speed-up about 2-4 was reached. However, when appropriately combined with additional smoothing and balancing procedure, the speed-up factor was raised up to about 7.5 times [16]. The numerical analysis was done using mostly simple benchmark problems, such as bar bending, and pressurized cylinder.

We are presenting here only sample results of a'posteriori error estimation. They were obtained for Benchmark 1 (2D model) after 3000 iterations of typical optimization process. The reference solution was calculated by weighted averaging of the best solutions (chromosomes) taken from 12 independent populations. Such reference solution was used later on for local errors estimation and an error map generation. You may see such estimated error map (Figure 2 (a)), and compare it to the exact one (Figure 2 (b)). In Figure 3 (c) you may see the difference between both maps. In this case, the error values in mean-square norm were as follows: 0.326 for estimated error map, and 0.338 for the exact one. The mean-square norm of the difference between both maps was equal 0.095.

For evaluation of the quality of error estimation in the case of benchmark problems we may use the effectivity index [16]:

$$i = 1 + \frac{\left| \|e\| - \|\bar{e}\| \right|}{\|e\|} \tag{19}$$

where e is the exact local error, and $\bar{e}$ is estimated local error. For perfect estimation the effectivity index would be equal to 1. For considered example the effectivity index i = 1.04 was reached.

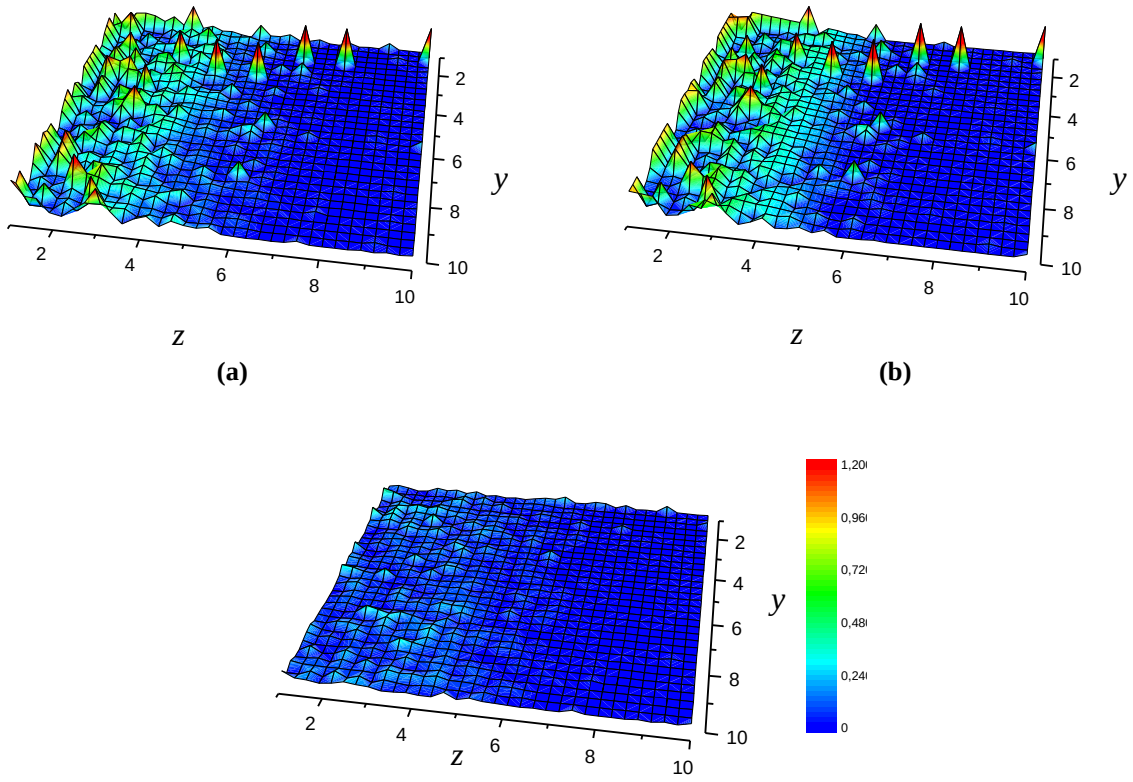

Figure 2: Example of a'posteriori error estimation: **(a)** Estimated error map **(b)** The true error map **(c)** Difference between the true and estimated error maps

5.2 Step by step mesh refinement

The typical results obtained by using algorithm described in Subsection 3.4 are shown in Figure 3. They were obtained from the residual stresses analysis in the bending bar benchmark problem (2D model).

In this case, the improved EA used a series of denser and denser meshes, as well as the a'posteriori error analysis. In Figure 3 one may see the true errors of the best solutions found after each step using the same mesh. The process started with 9 nodes (Figure 3 (a)), and was continued until the number of 1089 nodes was reached (Figure 3 (e)). Each nodal value corresponds to one decision variable (gene in a chromosome). When using the standard EA, even for much smaller number of nodes, the solution could not be obtained in a reasonable number of iterations. The whole considered process was continued for 3500 iterations. Precision of the final solution increased about 150 times when compared to one obtained by the standard EA. Furthermore, also in comparison to the standard EA, the acceleration factor of the optimization process up to about 200 times was reached.

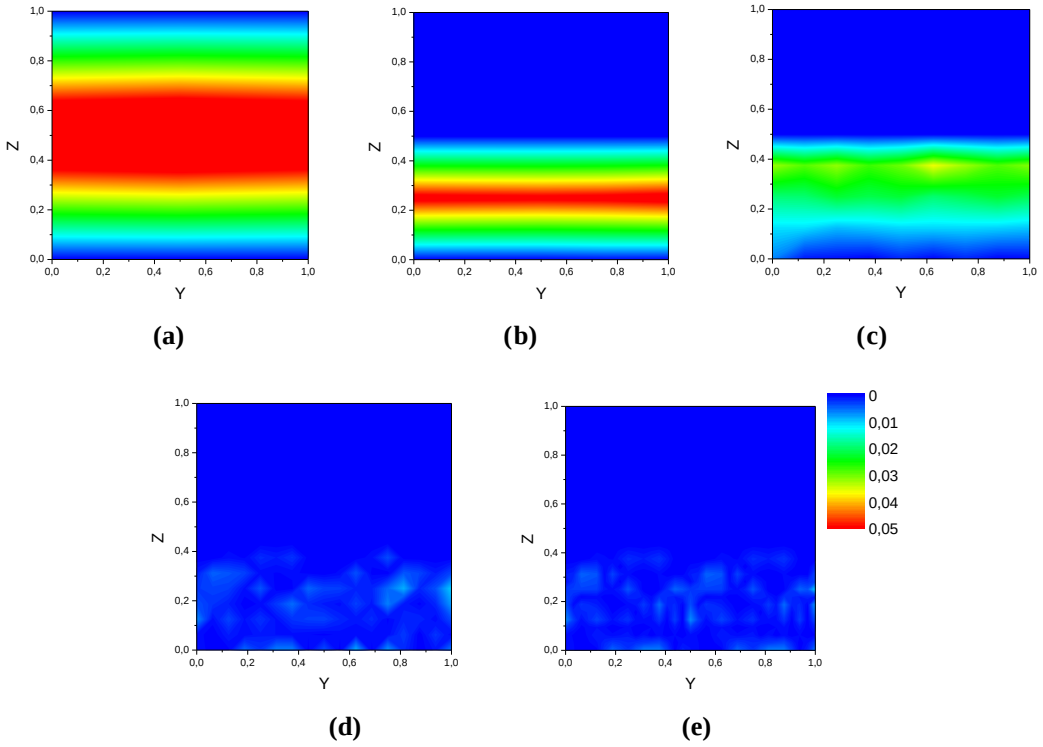

Figure 3: The true solution errors obtained in the residual stresses analysis in the bending bar (2D model). The algorithm used subsequent meshes with **(a)** 9 **(b)** 25 **(c)** 81 **(d)** 289 and final **(e)** 1089 nodes

Similar tests were executed for residual stress analysis in the cyclically pressurized cylinder (Benchmark 2). Brief information about those tests and results obtained may be found in [4]. The largest optimization problem for 2D model of such analysis involved over 2000 decision variables.

6 FINAL REMARKS

The general objective of this research is development of the EA method for efficient solution of large, non-linear, constrained optimization problems. Preliminary results of the executed tests clearly show a possibility of significant increasing solution efficiency using all proposed acceleration techniques. It is also worth noticing, that the improved EA allowed for obtaining solutions in cases when the standard EA failed, e.g. for large number of decision variables.

Future research includes continuation of various efforts oriented towards an improvement of the EA-based optimization approach, analysis of further benchmark problems, and application of such developed method to residual stresses analysis in railroad rails and vehicle wheels [8,14]. The EA based PBA approach for a wide class of smoothing of experimental data problems is also expected.

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