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ON ACCELERATING EVOLUTIONARY ALGORITHMS COMPUTATION APPLIED TO PHYSICALLY BASED APPROXIMATION

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Contents

Introduction

Research motivation

A variety of **engineering** and **scientific** tasks may be formulated as **large, non-linear, constraint optimization** problems, e.g.:

1. **Residual stress** analysis in railroad rails and vehicle wheels

   (**direct** theoretical problem).

2. **Physically based approximation of experimental data**, e.g.

   residual stress reconstruction using experimentally measured data e.g. strain gauge technique or Moire interferometry

   (**inverse** hybrid theoretical – experimental problem).

Efficient solution of such type optimization problems is crucial for various **practical engineering** applications.

Solution methods used (convex, and non-convex problems)

deterministic like

- **FDM** (Feasible Directions Method)
- Penalty Methods

and/or **stochastic** like

- **AI** (e.g. **Evolutionary Algorithms**)

Introduction

Research objective

General

Significant **acceleration** of the **EA** applied to **large, non-linear constraint optimization** problems, where a **function** (given e.g. by its **nodal values**) is searched.

The **speed-up** is based on:

- choice of the **most efficient combination** of the evolutionary operators: selection, crossing-over, mutation,
- use of several **new** simple **speed-up techniques proposed** here,
- further **development** of chosen **existing** acceleration methods.

Particular

Formulation and **testing applicability** of the accelerated **EA** to solution of engineering problems resulting from **Physically Based Approximation** of experimental and/or numerical data.

Physically based approximation (PBA)

Main features:

- simultaneous use of all available **information**

  experimental data (various measurements)

  theory (e.g. principles of mechanics, equilibrium equations, …)

  heuristic principles (e.g. smoothing)

- use rather **physics** than mathematics for smoothing

  principles, physical equations, boundary conditions

  true statistics of measurements, error bounds

  weighting factors dependent on information reliability

  probability type and distribution

- other interpretation of the PBA approach

  solution method of **inverse** problems

  hybrid method

  regularization method

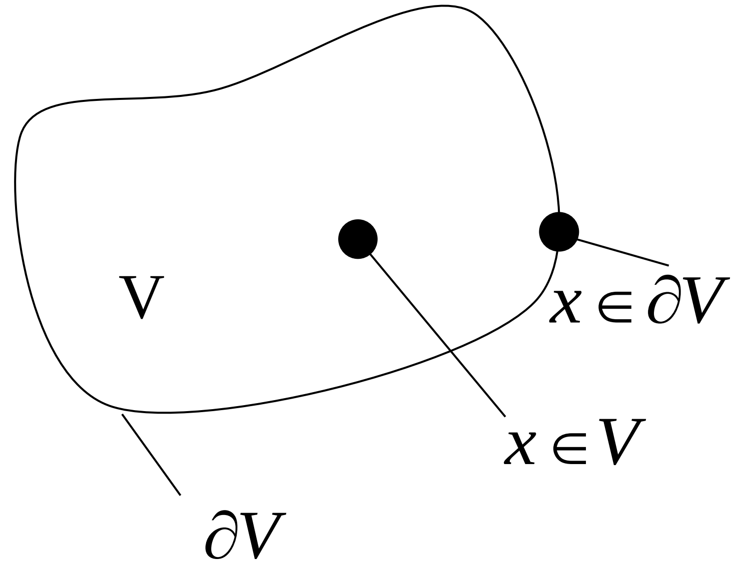
  smoothing method for a'posteriori error analysis

  mathematical formulation: **constrained optimization** method

Physically based approximation

Find $\boldsymbol{\sigma} = \boldsymbol{\sigma}(x)$ that yields the **stationary value** of the **functional**

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



and satisfy

equality constraints (theoretical)

$$A(\boldsymbol{\sigma}) = 0$$

inequality constraints (experimental)

$$B(\boldsymbol{\sigma}) \le e$$

where

$$\bar{\Phi}^T = \frac{\Phi^T}{\Phi^T_{REFERENCE}}$$ - dimensionless **theoretical** part of the weighted functional Φ^T

$$\bar{\Phi}^E = \frac{\Phi^E}{\Phi^E_{REFERENCE}}$$ - dimensionless **experimental** part of the weighted functional Φ^E

$\lambda \in [0,1]$ - weighting factor

e - admissible tolerance

Theoretical requirements

Determine

Functional Φ^T

Constraints $A(\boldsymbol{\sigma})$

Determine a functional

(i) Theory is **known** (in mechanics, e.g. the total complementary energy)

$$\Phi^T = \frac{1}{VG}\int \sigma^T C \, \sigma \, dV$$

$\boldsymbol{\sigma}$ - stress vector

C - compliance matrix

G - Kirchhoff modulus

for **local** formulation of the theoretical problem

$$\mathcal{L}\sigma = f \quad in \quad V$$

$$\mathcal{G}\sigma = g \quad on \quad \partial V$$

one has

$$\Phi^T = \int_V \left(\mathcal{L}\boldsymbol{\sigma} - f\right)^2 dV + \mu \int_{\partial V} \left(\mathcal{G}\boldsymbol{\sigma} - g\right)^2 dV$$

Theoretical requirements

(ii) theory is **not known** – heuristic principle – e.g. smoothness requirement

for scalar function f :

$$\kappa^2 = \frac{1}{2\pi}\int_0^{2\pi}\left[\frac{\partial^2 f}{\partial \nu^2}\right]^2 d\varphi$$, averaged curvature at point

$$\kappa^2 = \left(\frac{f_{xx}+f_{yy}}{2}\right)^2 + \left(\frac{f_{xx}-f_{yy}}{2^{3/2}}\right)^2 + \left(\frac{f_{xy}}{2^{1/2}}\right)^2$$

$$\Phi^T = V^{-1}\int_V \kappa^2 dV$$, mean curvature in domain

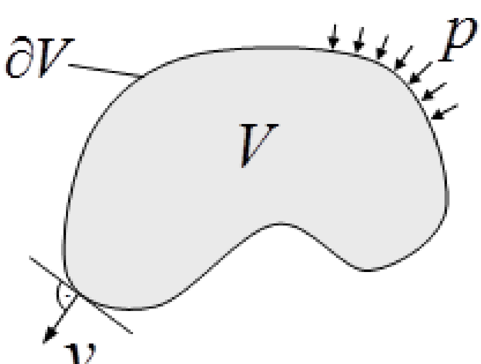
Determine constraints

Example of $A(\boldsymbol{\sigma}) = 0$ **constraints** for the total complementary energy functional equilibrium equations

$$\partial\boldsymbol{\sigma} = 0 \quad in \quad V$$

and static **boundary conditions**

$$\nu^T\boldsymbol{\sigma} = 0 \quad on \quad \partial V$$



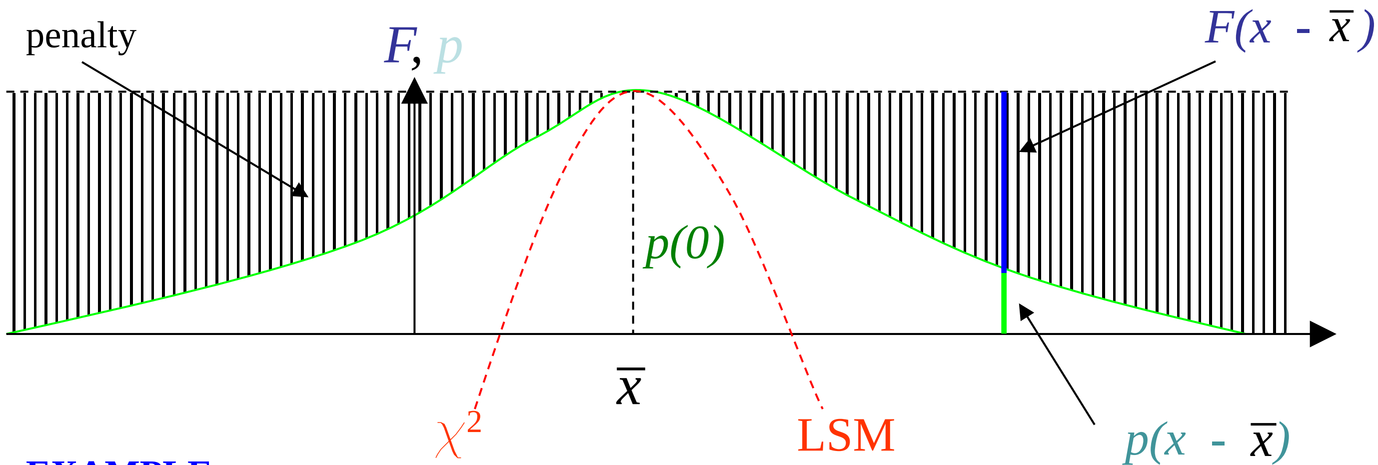
Experimental requirements

Introduce

Penalty function

$$\Phi^E = \frac{1}{N}\sum_{n=1}^{N} F\left(\frac{f_n(\sigma) - q_n}{e_n}\right)$$

q_n	- experimental data
e_n	- experimental error
$f_n(\sigma)$	- smoothed physical quantity
$n = 0, 1, \ldots, N$	- numbers of experimental data
$F(\ )$	- data scattering function



$F(\ ) = p(0) - p(\ )$

$p(\ )$ - probability density function

EXAMPLE

$$p_{gaussian} = \frac{1}{\pi^{1/2}} e^{-x^2} \quad \Rightarrow \quad F = \frac{1}{\pi^{1/2}}\left(1 - e^{-x^2}\right) = \frac{1}{\pi^{1/2}}\left(x^2 - \frac{1}{2}x^4 + \ldots\right)$$

Experimental requirements

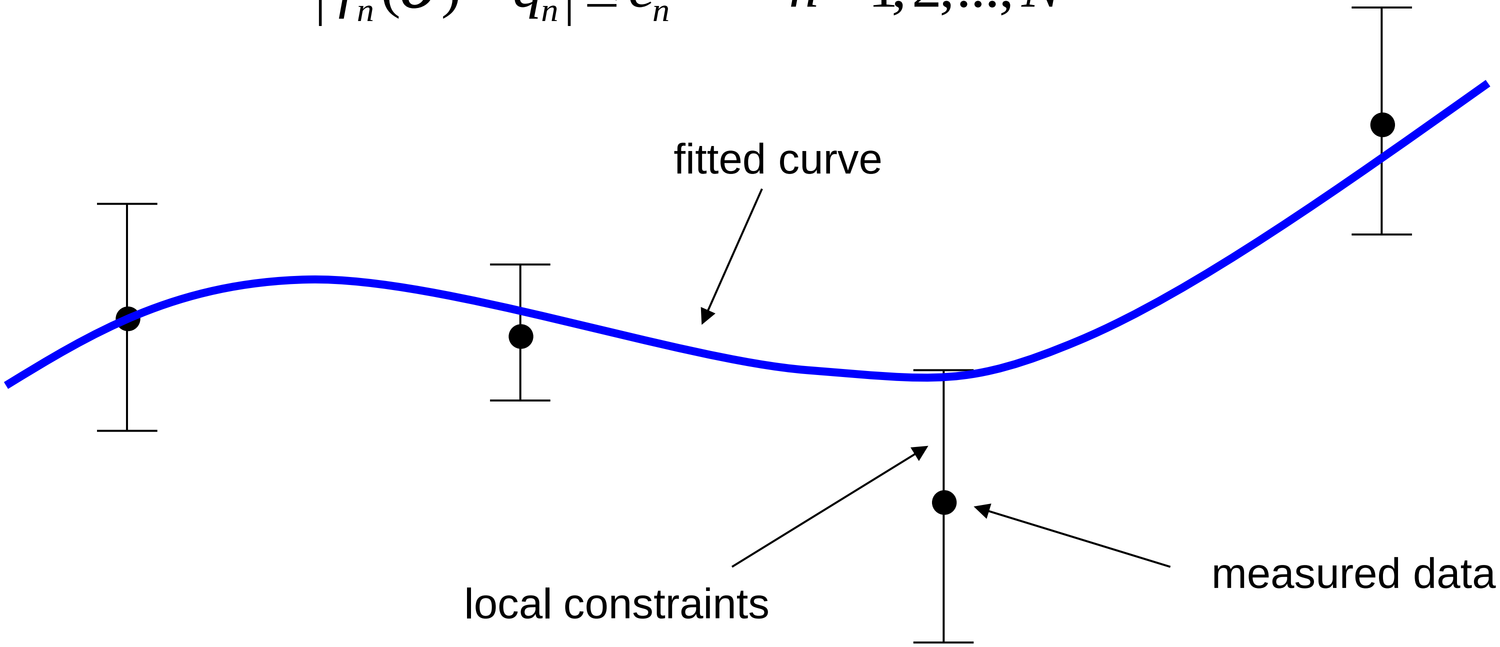
Constraints

Global

$$\sqrt{\Phi^E} \le \bar{e}$$

Local

$$\left| f_n(\boldsymbol{\sigma}) - q_n \right| \le e_n \qquad n = 1, 2, \ldots, N$$

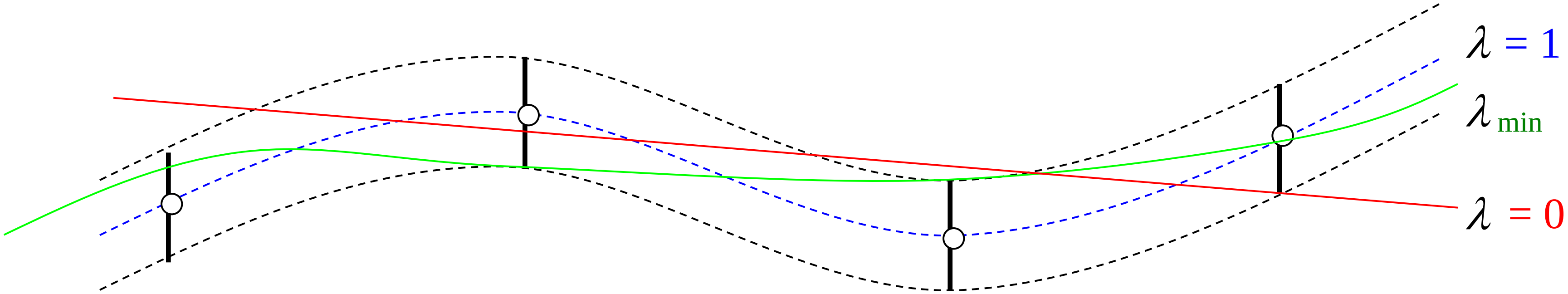


Formulation of the optimization problems

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

Difficulty: λ **= ?**

How to find the weighting factor, i.e. to determine a reasonable balance between **theory** and **experiment**



Chosen **formulation** **of optimization problems**

Two subsequent **optimization** problems are to be solved

(i) Find $\boldsymbol{\sigma}(\lambda)$ that yields the stationary value of the functional

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

and satisfy the theoretical constraints

$$A(\boldsymbol{\sigma}) = 0$$

(ii) Find such value of λ

$$\min_{\lambda} \lambda$$

that $\boldsymbol{\sigma}(\lambda)$ satisfies the experimental error bounds both

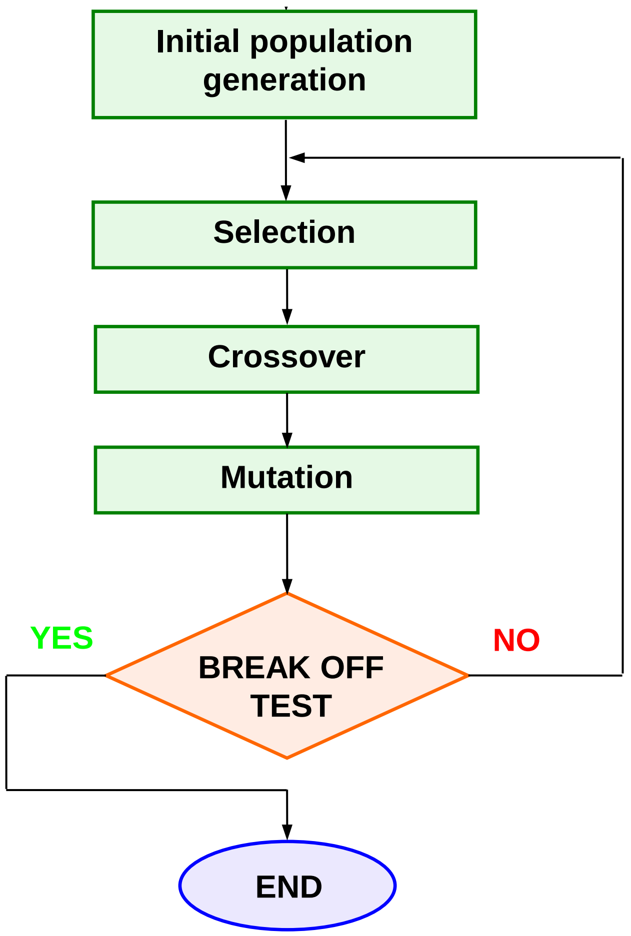
local $\left| f_n(\boldsymbol{\sigma}) - q_n \right| \le e_n \qquad for \quad n = 1, 2, ..., N$

and global $\sqrt{\Phi^E} \le \bar{e}$

Standard Evolutionary Algorithm used

Choice of the **most efficient combination** of evolutionary operators

- **Selection** operators:
  - **rank**
  - tournament
- **Crossing-over** operators:
  - simple
  - arithmetic
  - **heuristic**
- **Mutation** operators:
  - uniform
  - **non-uniform**
  - boundary



Acceleration techniques considered

Newly proposed simple acceleration techniques:

- **smoothing** of the direct EA solution,
- **balancing** of smoothed EA solution,
- use of **a' posteriori error analysis** and non-standard **parallel** and **distributed** calculations,
- adaptive step by step **mesh refinement**,

Development of chosen **existing** techniques:

- **new** evolutionary **operators** (e. g. gradient mutation, cloning),
- **hybrid** algorithms (EA + deterministic method).
- **distributed** and **parallel** algorithms.

A' posteriori solution error analysis

Solution of optimization problem

u^* **true**

$\tilde{u} = \tilde{u}_{h,p}$ **rough** solution

$\bar{u}$ improved **reference** solution - **hierarchic** approach

new solutions and postprocessing required

Local a' posteriori **error**

$e_T = \tilde{u} - u^*$ **true** error $e_E = \tilde{u} - \bar{u}$ **estimated** error

Global a' posteriori solution error

$e = \| e_T \|$ **true** error $\eta = \| e_E \|$ **estimated** error

Error norms: **mean square, maximum**

Estimation quality – **effectivity index**

$$i = 1 + \frac{\left| \|e\| - \|\eta\| \right|}{\|e\|}$$

Fitness function value f_{best} control

$$\xi = \left| \frac{f_{best}^{(m)} - f_{best}^{(m-1)}}{f_{best}^{(m)}} \right| \leq \xi_{admissible}$$

Generation of reference solutions

1. In the **deterministic methods** – well known, e.g. **hierarchic** approach

   h - type, **p** - type, **h**/**p** - type, and **residual**, **smoothing** approaches, also error indicators

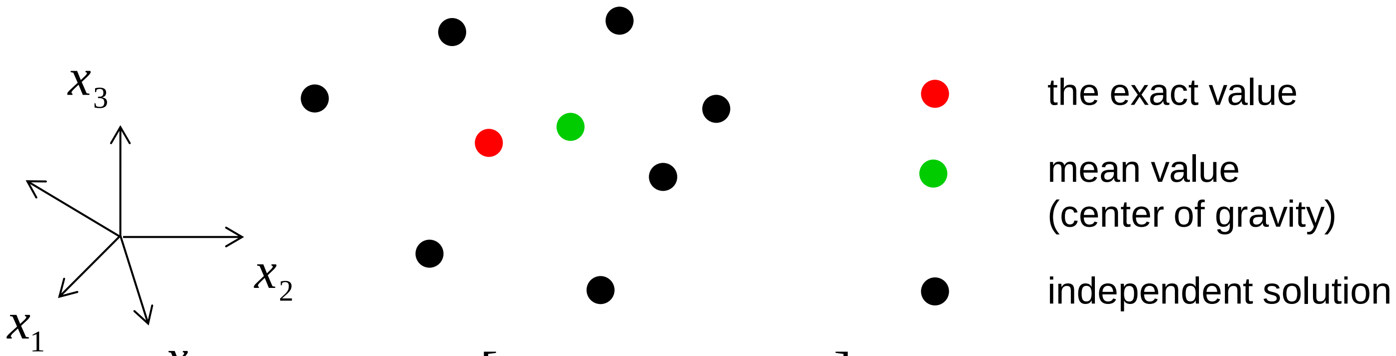
2. In the **Evolutionary Algorithms**

Approach

- generation of population of *m* **independent** solutions (chromosomes),
- **weighted averaging** of these results over the whole population,
- **postprocessing** (HO smoothing) of the above averaged discrete solution by means of the MWLS (or PBA) approximation,

Notice

h - type and/or **p** - type estimation approach would be also possible.



$$\mathbf{x} = [x_1, x_2, x_3, \dots, x_n]$$

Use of a' posteriori error analysis for the EA solution process **acceleration**

Approach **concept**

- Find or estimate EA solution **error** in the **whole** domain.

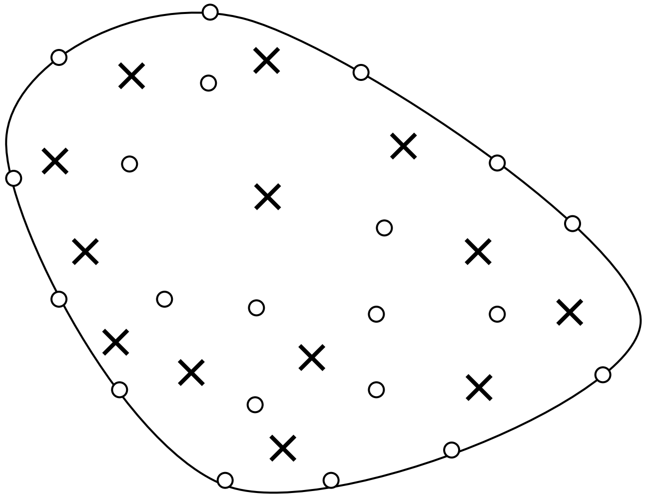
- **Intensify calculations** in zones where solution **error** is **larger** than a prescribed value e.g. the mean error.

  Do this by means of **modification** of the basic EA operators:

  selection, **mutation** , and **crossing-over**.

Step by step mesh refinement

Adaptive approach



○ - nodes of the **old** cloud (with known solution)

× - **new** candidates for the cloud

Generation **criterion** of new nodes

error $\bar{e}_x > \tau \cdot \bar{e}_{\max} \quad , \quad 0 < \tau < 1$

mesh density gradient $\dfrac{\left| d_i - d_j \right|}{\rho_{ij}} > \theta_{adm}$

Break off criterion

$$\forall \bar{e}_x < e_{adm}$$

Initial function values in inserted nodes may be calculated using **interpolation** spanned over coarse mesh

Use of **a'posteriori error analysis** for estimating the quality of nodes distribution and adaptation approach

Use of mesh refinement with a'posteriori error estimation

Strategy

(i) calculation of solution on a coarse mesh

(ii) smoothing of rough solution (e.g. using MWLS method)

(iii) mesh refinement and the best approximation (or interpolation) of initial function values at inserted nodes

(iv) use of obtained solution as the initial reference solution for a'posteriori error estimation

(v) use of weighted solution averaging for further reference solutions generation and a'posteriori error analysis

(vi) repetition of the procedure given above until a sufficiently dense mesh is reached

Benchmark problem (1): Smoothing of beam deflections

Problem **formulation**:

Simulated pseudo experimental $w_j^{\exp}, \;\; j = 0,1,\ldots,N$ are given

Find

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

$$\Phi^E(w) = \frac{1}{N}\sum_{j=0}^{N}\left(\frac{w_j - w_j^{\exp}}{e_j}\right)^2$$

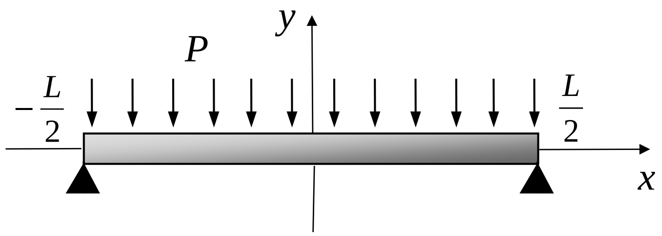
$$\Phi^T(w) = \frac{1}{L}\int_0^L \kappa^2 dx$$

satisfying:

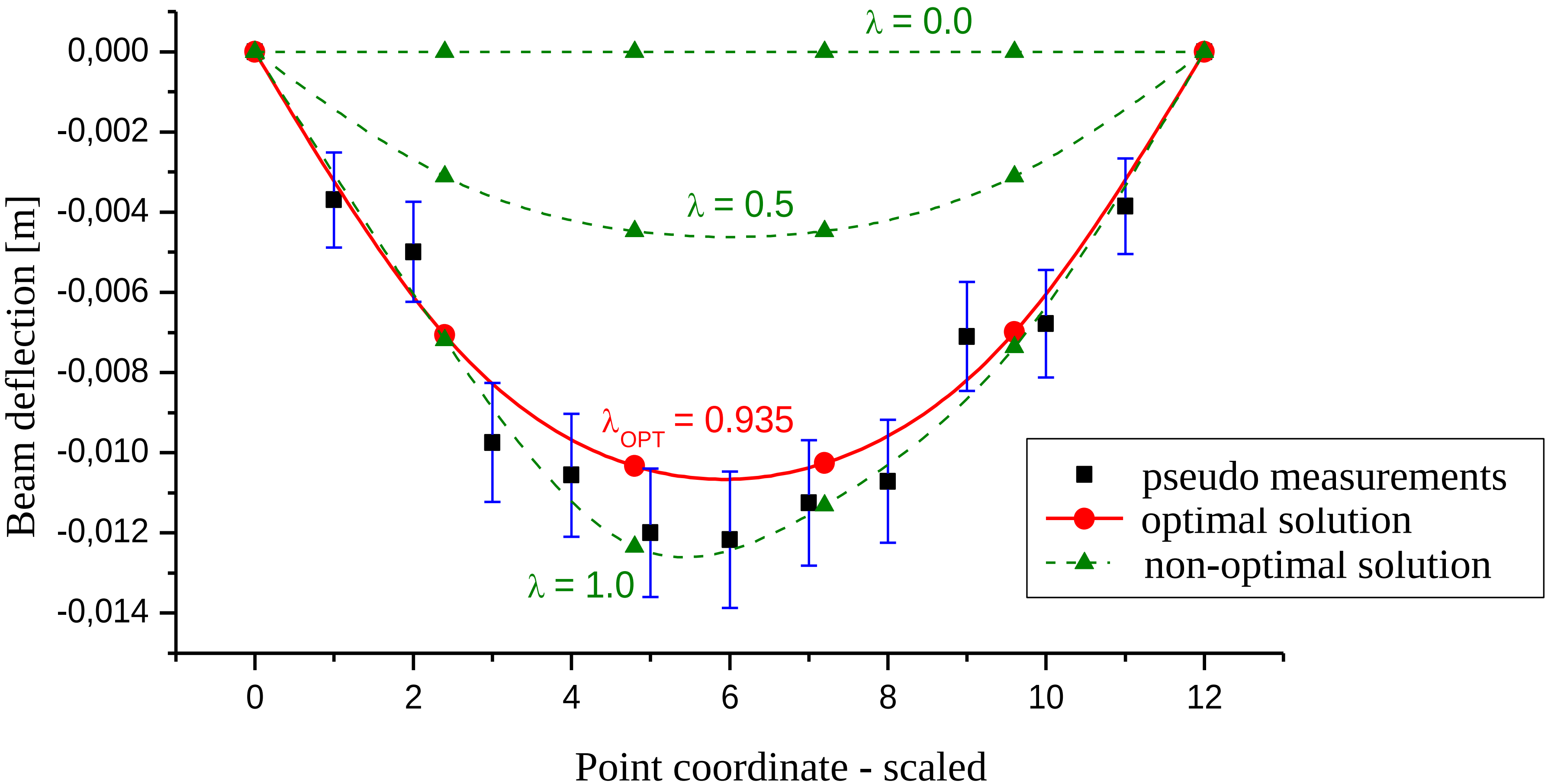
$$w_0 = w_N = 0$$

$$\left|w_j - w_j^{\exp}\right| \le e_j$$

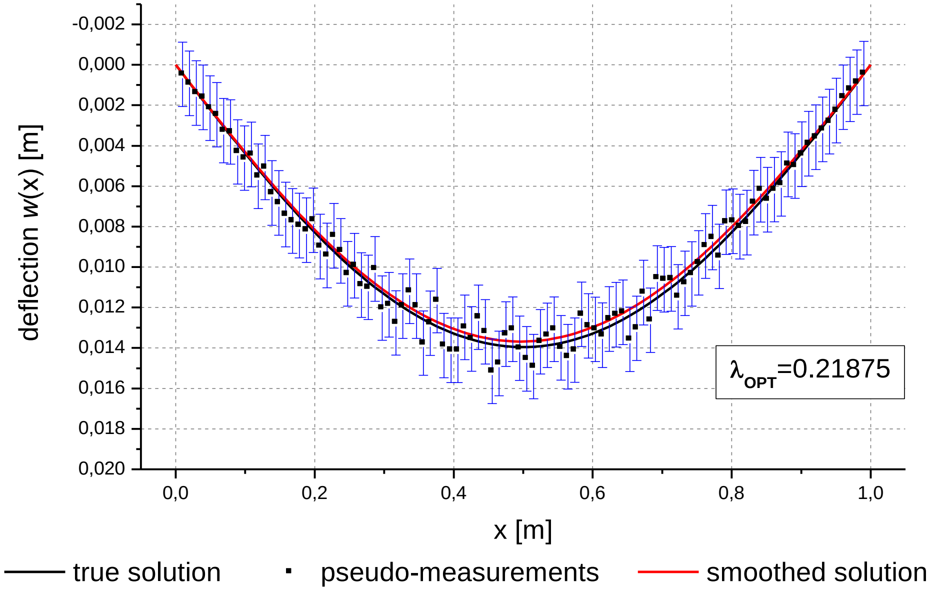
$$\sqrt{\Phi^E(w)} \le e_E$$

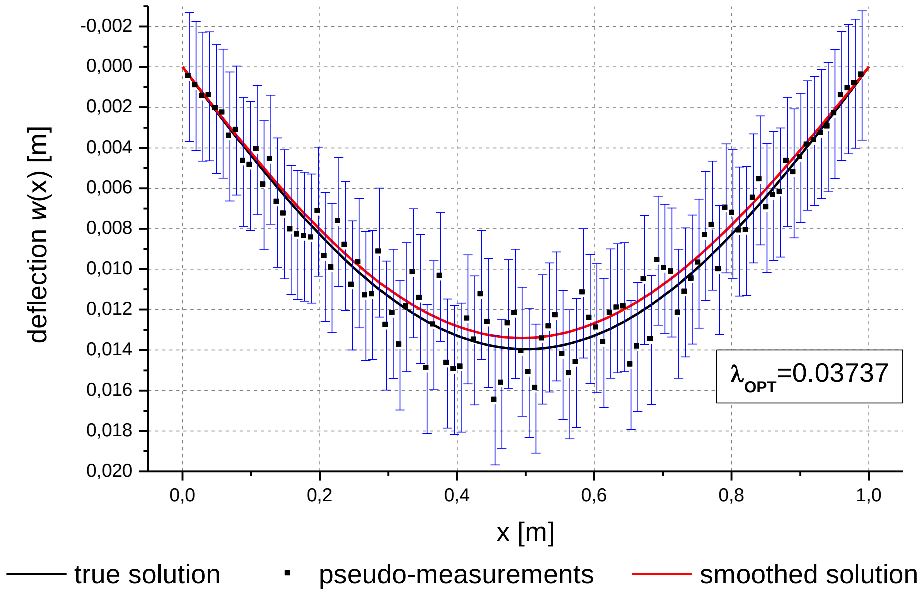


Smoothing of beam deflections

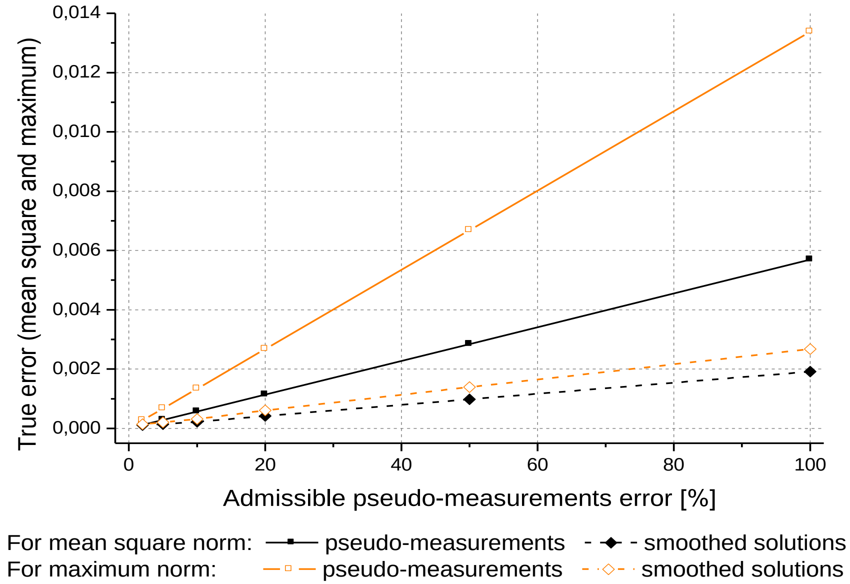


Smoothing of beam deflections





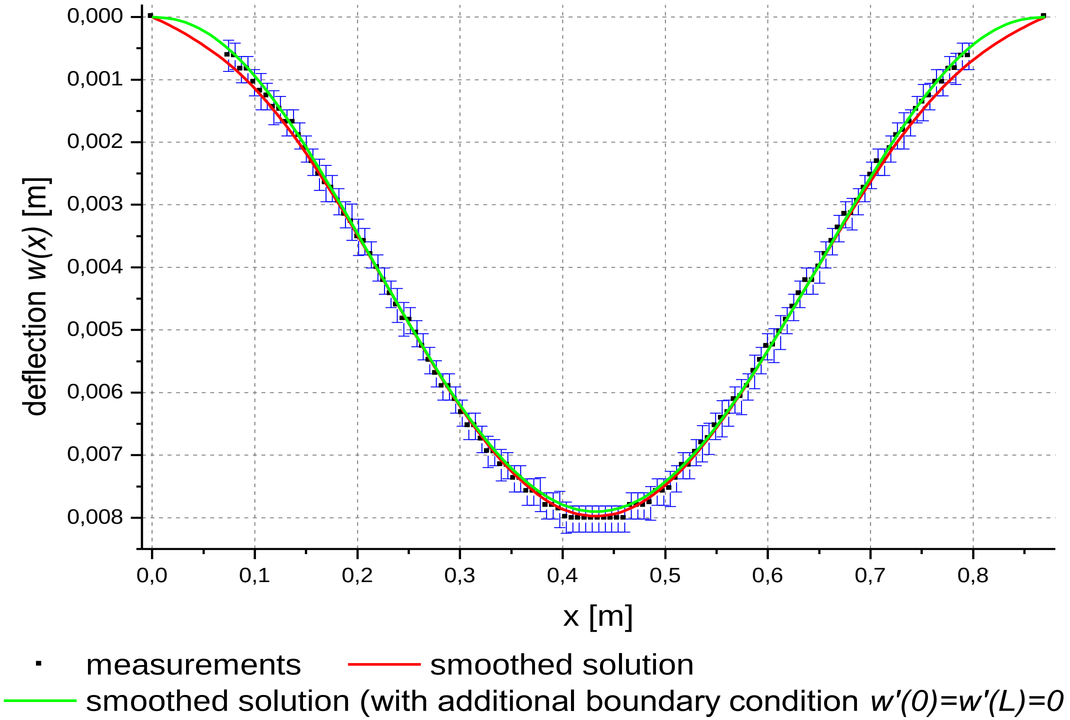
error up to: **(a) 10 %** **(b) 20 %**



Smoothing of beam deflections

Lab stand for **true** **experimental measurements**

Courtesy of Chair of Robotics and Mechatronics AGH Kraków



Benchmark problem (2): Residual stress reconstruction in thick-walled cylinder under cyclic pressure (2D model)

Stage I

Find the stationary point of the functional

$$\Phi = (1-\lambda)\overline{\Phi}^{T} + \lambda\,\overline{\Phi}^{E}$$

satisfying the equality constraints

$$\frac{\partial \sigma_r^r}{\partial r} + \frac{\sigma_r^r - \sigma_t^r}{r} = 0$$ equilibrium eq.

$$\sigma^r_{r|a} = 0, \quad \sigma^r_{r|b} = 0$$ boundary cond.

$$\sigma_z^r = \nu(\sigma_r^r + \sigma_t^r)$$ incompressibility eq.

Stage II

Find $\min\limits_{\lambda} \lambda$, $\lambda \in [0,1]$

satisfying the inequality constraints

$$\left|\varepsilon_i^{\exp} - \varepsilon_i^{app}(\sigma)\right| \le e_i$$ admissible local err.

$$\sqrt{\Phi^E} \le \bar{e}$$ admissible global err.

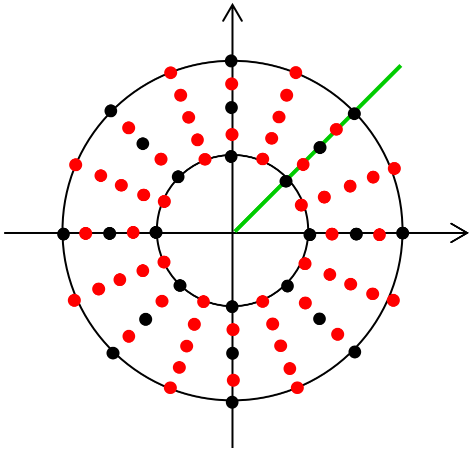
where

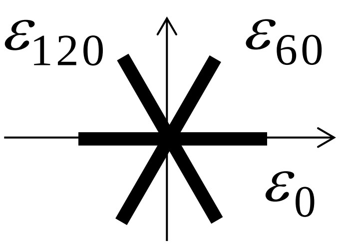
$$\Phi^E(\sigma) = \left(\frac{1}{N}\sum_{n=1}^{N}(\varepsilon_i^{\exp} - \varepsilon_i^{app}(\sigma))^2\right)^{\frac{1}{2}}$$

$$\Phi^T(\sigma) = \frac{1}{\Omega}\int_{\Omega}\kappa^2(\sigma)\,d\Omega$$

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

Simulation of strain gauge technique



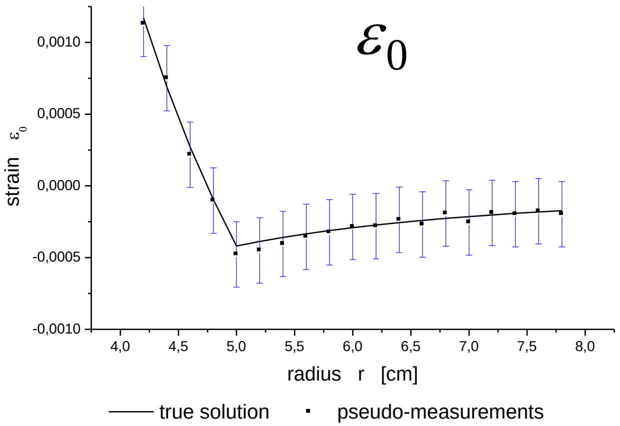


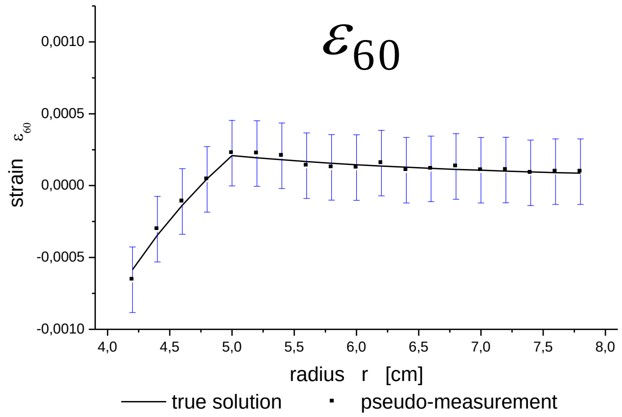
delta type **rosette**

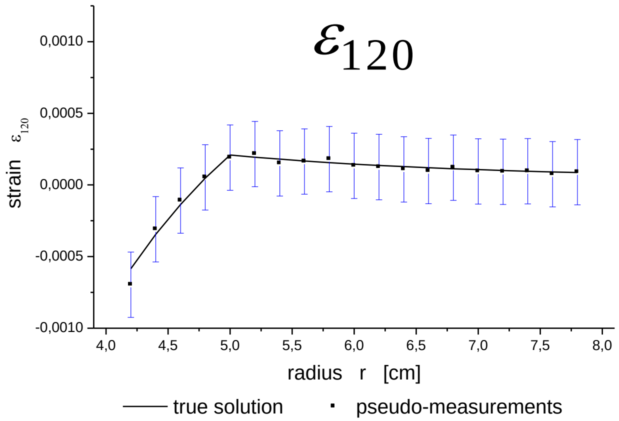
Final mesh: 21 x 16 (336 nodes)

Residual stress reconstruction - numerical results

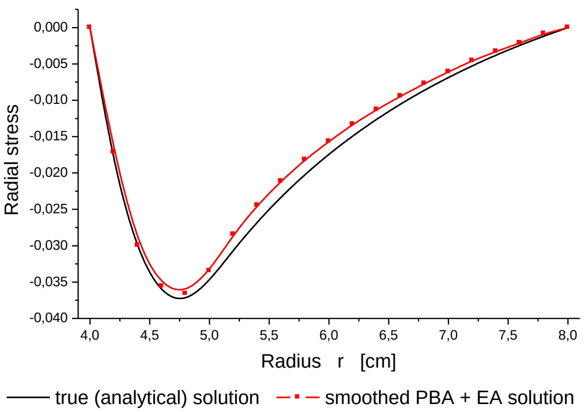
Random pseudo-measurements (strains) – error up to 20%

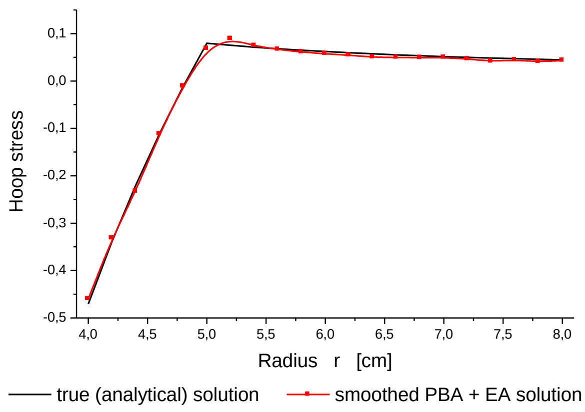


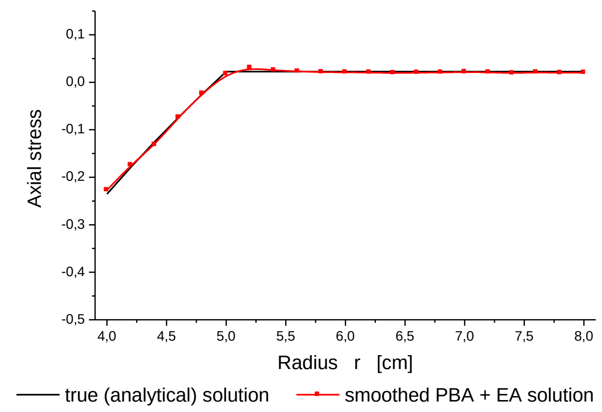




Solutions (stresses)

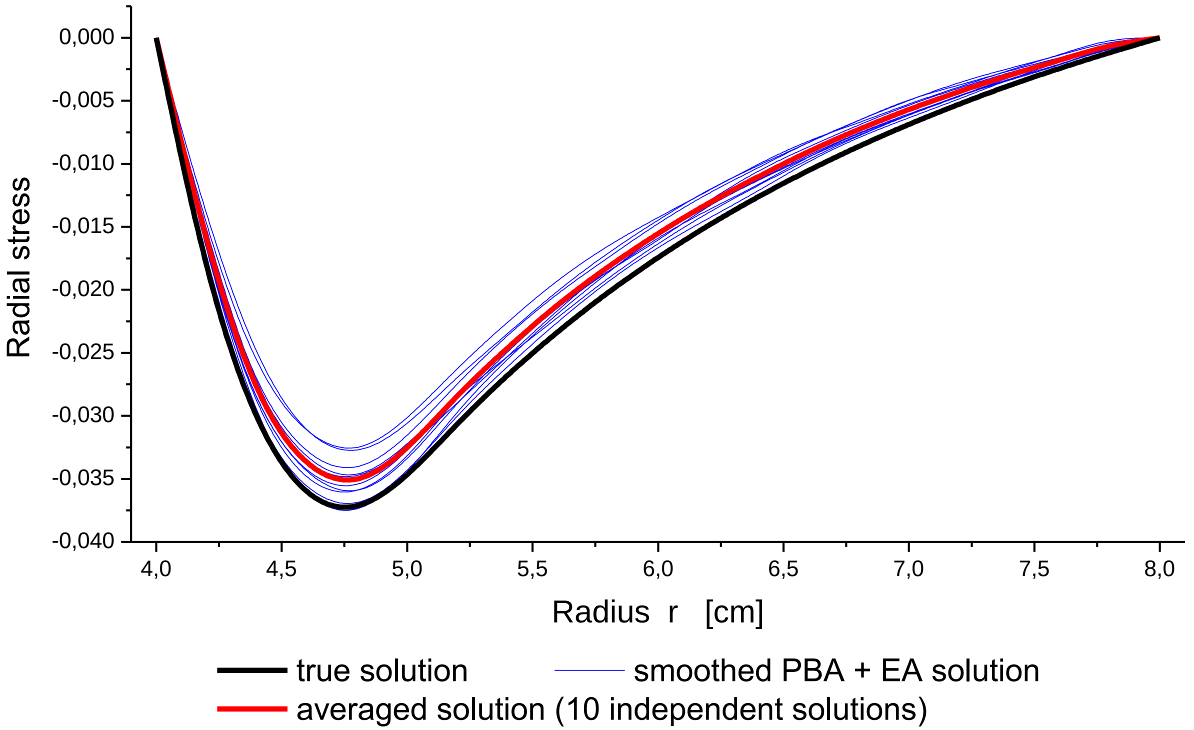






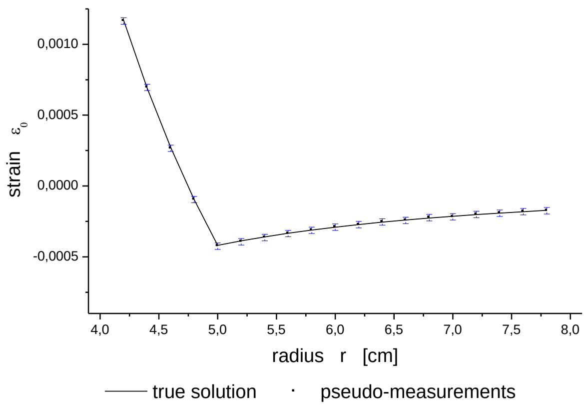
Residual stress reconstruction - numerical results

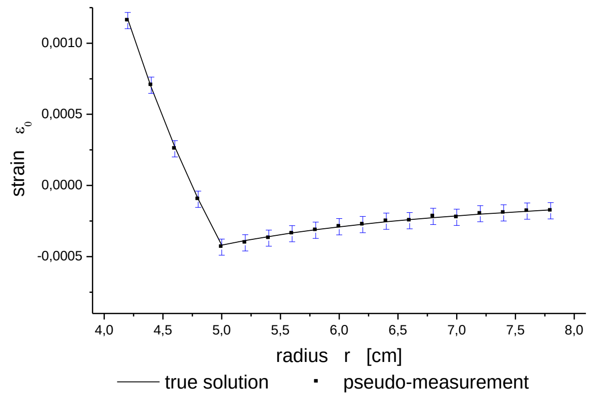
Solutions obtained for a series of random independent data sets

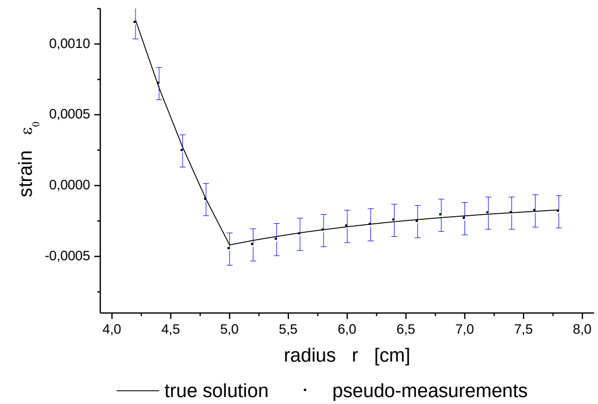


Residual stress reconstruction - numerical results

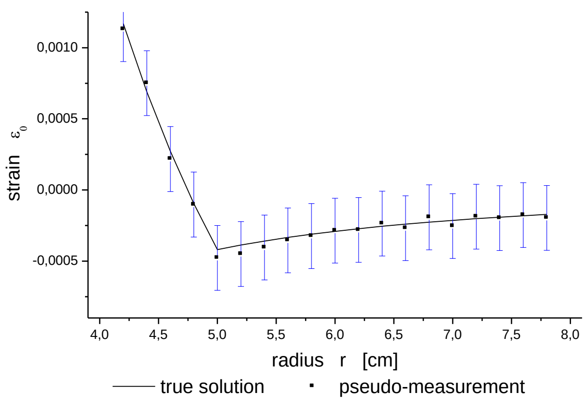
Pseudo-measurements (strains)

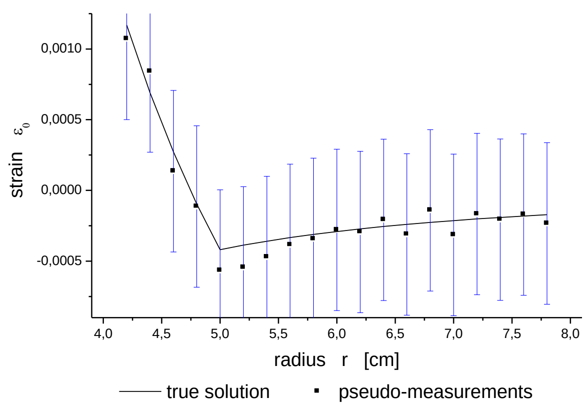


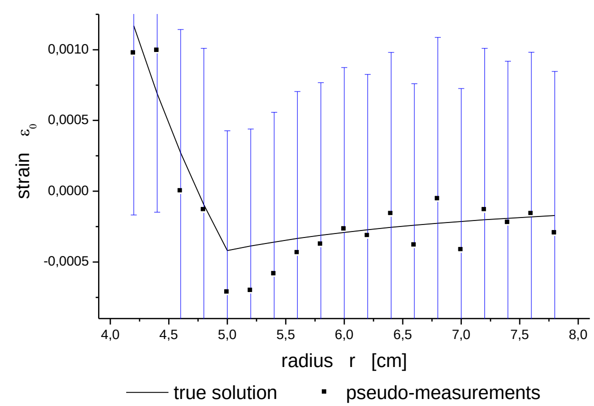




error up to: (a) 2 % (b) 5 % (c) 10 %



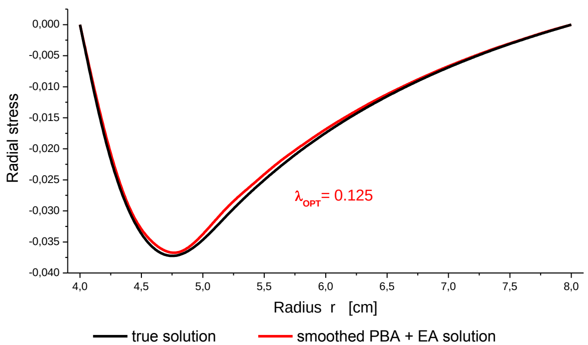




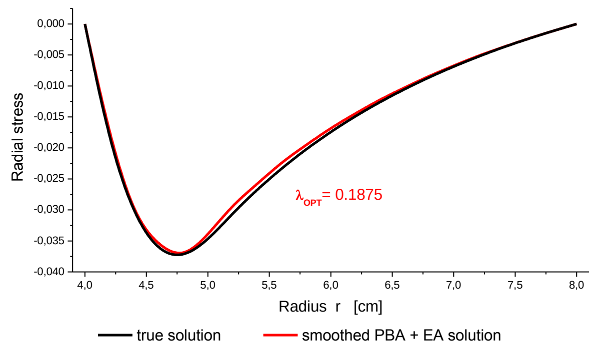
error up to: (d) 20 % (e) 50 % (f) 100 %

Residual stress reconstruction - numerical results

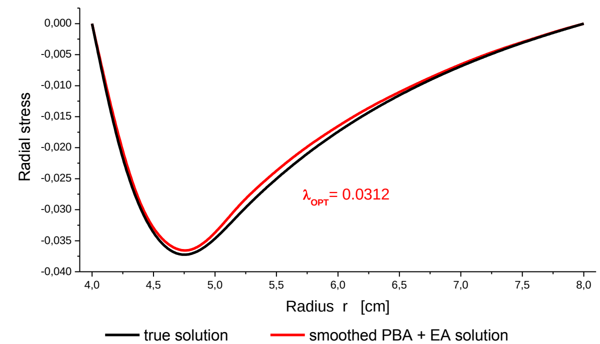
Solutions (stresses) - final mesh: 21 x 16 (336 nodes)



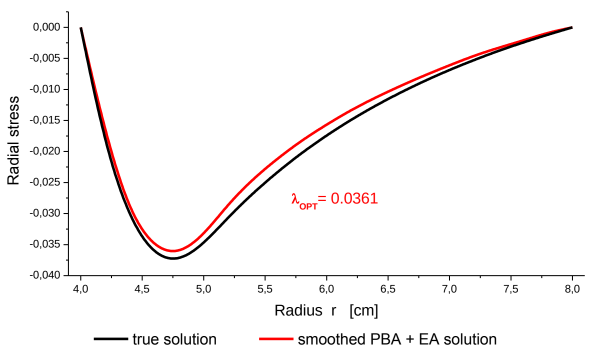
(a)



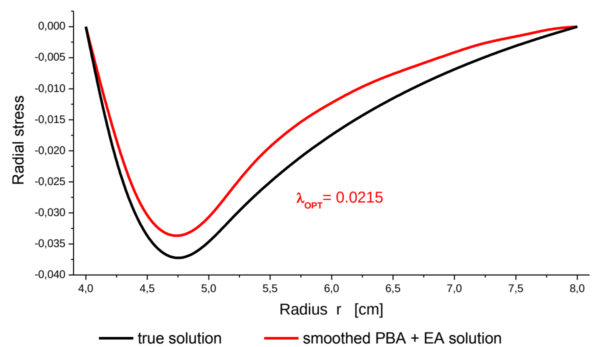
(b)



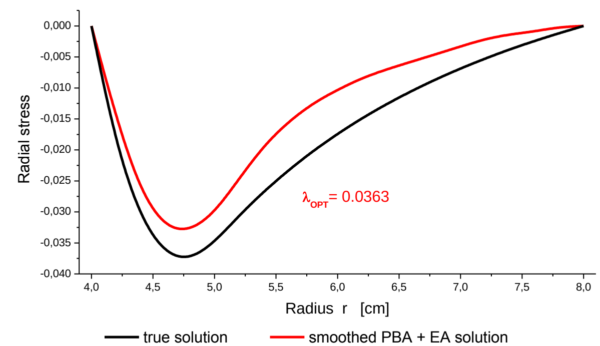
(c)



(d)



(e)



(f)

Final remarks

Summary

- Many **scientific** and **technical** tasks may be expressed in terms of **non-linear**, **constraint optimization problems**. In a wide class of such problems the objective is to find an **unknown function**, mostly in a discrete form.

- **Optimization** problems may be solved by means of either the **deterministic** or **probabilistic** methods. The first ones are very effective when dealing with the **convex** problems as opposed to usually slowly convergent **stochastic** methods, e.g. most AI ones, especially for **large** optimization problems. However, **efficiency** of the AI methods does **not change** much for **non-convex** problems, as opposed to the deterministic ones.

- The **objective** of this whole research, therefore, is to develop means of **essential acceleration** of the **Evolutionary Algorithms**, being one of the AI methods. Particular attention is paid here to use of **smoothing**, step by step **mesh refinement,** and our knowledge about estimated **solution error**, to essential **EA** acceleration. Several introduced speed-up concepts are tested on various, carefully selected **benchmark** problems.

Summary

- Preliminary **results** of executed tests are encouraging. For use of step by step **mesh refinement** together with **smoothing**, and a'posteriori **error analysis**, the overall speed-up factor about **150** times was reached so far.

- When well designed, the **accelerated EA** may provide solution much **faster** than the **standard EA** algorithm. Moreover, as opposed to the standard approach such solution may also be efficiently obtained for **large** optimization problems.

- Application of the **accelerated EA** was preliminarily examined for benchmark problems like smoothing of **beam deflections**, and **reconstruction** of residual stresses based on experimental data smoothing by means of the **PBA**.

Further research planned

- Continuation of various efforts oriented towards **increasing** the **EA efficiency**, including testing new concepts, and combination of all types of acceleration considered for their simultaneous use.

- Analysis of further **benchmarks**.

- Application to real engineering problems like **residual stress** analysis in **railroad rails** and **vehicle wheels**, as well as to a wide class of experimental and/or numerical data smoothing problems formulated as the **PBA** ones.

Thank you very much for attention