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Postprocessing and reliability evaluation of one-dimensional numerical simulation results in mechanical problems

Jan Wojtas
Institute of Computer Science
Faculty of Physics, Mathematics and Computer Science
Cracow University of Technology
Warszawska 24, 31-155 Kraków, Poland
e-mail: jwojtas@pk.edu.pl

This work addresses extended formulation of a new approach proposed to control numerical data error [3, 5]. It includes developing postprocessing techniques for the approximation of data given in a discrete form and estimation (evaluation) of this data *a posteriori* error and the reliability index. Theoretical consideration and numerical analysis are based on the adaptive meshless finite difference (MFDM) approach.

Keywords: meshless FDM, experimental data approximation and smoothing, *a posteriori* error estimation of experimental data, adaptive methods.

1. Introduction

Almost all numerical procedures of computational mechanics are based on the discretization process in which the continuous model of the analyzed body is transformed into a discrete one.

The discretization process is made as well within the experimental study and constitutes the key point of a computer simulation. It has a strong influence on the exactness, efficiency, generality and usefulness of the obtained results. A correct discretization strategy and a discretization process control very often decide whether the solution for the analyzed problem is obtained or not [1, 3].

The key element of numerical simulation is the reliability assessment of the obtained results. In particular, this assessment concerns the accuracy of the adopted models and the determination (estimation) of the error made during the calculation with an indication of its minimization (or elimination) effective method [2, 4].

In this work, the implementation of a new method of numerical data a posteriori error estimation (MES or MRS results) in one-dimensional mechanics problems is undertaken. In particular, this study introduces the possibility of assessing the reliability of the results that have been obtained on the basis of the built-in global-local grid density index with an evenly distributed error.

The author has applied here the approach which uses a discrete function to describe the problem and the method of weighted moving least squares (WMLS) with constraints defined by differential-algebraic equations (e.g., beam deflection equation, boundary conditions). The presented approach concerns the so-called problem-oriented *a posteriori* error estimators. Particular attention was paid to the error function having additional conditions, so that it was possible to estimate the error of selected values (e.g., the component of strain, the energy or its increase [8]), and the final results reliability.

2. Global-local measures of this approach quality

The following designations for global norms were introduced:

$$\|U\|^2 = \frac{1}{h^2}\int\limits_{\Omega} fu\, d\Omega + \int\limits_{\Omega} f\nabla u\, d\Omega, \tag{1}$$

$$\|e\|^2 = \frac{1}{h^2}\int\limits_{\Omega} eu\, d\Omega + \int\limits_{\Omega} e\nabla u\, d\Omega, \tag{2}$$

where

$$\begin{aligned} fu &= (\mathbf{u}^h)^T\mathbf{u}, & eu &= (\mathbf{u}^* - \mathbf{u}^h)^T(\mathbf{u}^* - \mathbf{u}^h),\\ f\nabla u &= (\nabla\mathbf{u})^T\nabla\mathbf{u}, & e\nabla u &= (\nabla\mathbf{u}^* - \nabla\mathbf{u}^h)^T(\nabla\mathbf{u}^* - \nabla\mathbf{u}^h), \end{aligned} \tag{3}$$

where $\mathbf{u}^h$ is a vector of numerical data (at the so-called experimental points), $\mathbf{u}^*$ is a vector of fictitious (recovered) data, and h is a dimension of the local area assigned to a node.

2.1. Density parameters of a net in the problems of numerical data estimation

The global error must be smaller than some predetermined part (percentage) of the total norm, i.e.,

$$\|e\| \le \eta\,\|U\|\,, \tag{4}$$

where η is the relative value of the allowable global solution error. Equation (4) allows to define the so-called global error parameter as

$$\xi_g = \frac{\|e\|}{\eta\,\|U\|}. \tag{5}$$

When a parameter ξ_g value satisfies the condition $\xi_g \le 1$, it means that the global criterion is met, while the $\xi_g > 1$ condition indicates that it is necessary to further improve the grid.

However, this is insufficient. Therefore, the second, local criterion was considered. The distribution of nodes within the improved grid meets the optimization criterion. This local condition can be formulated as follows:

$$\|e\|_i = \|e\|_{r_i}\,, \tag{6}$$

where $\|e\|_i$ is the current error norm and $\|e\|_{r_i}$ is the desired value of the error norm in this point. Equation (6) can be used to define the local error parameter $\overline{\xi}_i$ at the point i as

$$\overline{\xi}_i = \frac{\|e\|_i}{\|e\|_{r_i}}. \tag{7}$$

It can be noted that value $\overline{\xi} = 1$ defines the optimal mesh density, while $\overline{\xi} > 1$ and $\overline{\xi} < 1$ indicate that the mesh density needs to be reduced or increased accordingly. For the process of mesh optimization, a definition of the norm $\|e\|_{r_i}$ is crucial.

The most popular criterion for mesh optimization is the criterion based on an even distribution of errors in all nodes. The grid (according to this criterion) is optimal if the (global) error has an even distribution in all nodes. Based on this definition, we can define an acceptable error in each node as the ratio between the global error and the number of nodes in the grid. Due to the additivity of the squares of standards, an acceptable error can be saved as

$$\|e\|_{r_i} = \frac{\|e\|}{\sqrt{n}}. \tag{8}$$

From Eqs (8) and (7) the local density parameter can be defined as

$$\overline{\xi}_i = \frac{\|e\|_i}{\|e\| \, n^{-1/2}}. \tag{9}$$

The alternative optimality criterion based on equal distribution of the error density function in a node says that the mesh is optimal if the square of the error per unit area (volume) of the polygon assigned to this node (e.g., Voronoi polygon) is the same within the whole grid

$$\frac{\|e\|_i}{(\Omega_i)^{1/2}} = \frac{\|e\|}{(\Omega)^{1/2}}. \tag{10}$$

In Eq. (10), Ω_i and Ω mean respectively the area (volume) assigned to the node and the whole domain.

We can therefore write an expression for the desired error norm for each point as

$$\|e\|_{r_i} = \|e\| \left(\frac{\Omega_i}{\Omega}\right)^{1/2}. \tag{11}$$

Now the error parameter $\overline{\xi}_i$ based on Eqs (11) and (7) can be shown as

$$\overline{\xi}_i = \frac{\|e\|_i}{(\Omega_i)^{1/2}} \left[\frac{\|e\|}{\Omega^{1/2}}\right]^{-1} = \frac{\|e\|_i}{\|e\|} \left(\frac{\Omega}{\Omega_i}\right)^{1/2}. \tag{12}$$

Now, theoretical or point-based density parameters can be derived from the above-mentioned optimality conditions as

$$\overline{\xi}_i^{\,\text{theor}} = \frac{\|e\|_i}{\eta \, \|U\| \, (n)^{-1/2}}, \qquad \overline{\xi}_i^{\,\text{theor}} = \frac{\|e\|_i}{\eta \, \|U\|} \left(\frac{\Omega}{\Omega_i}\right)^{1/2} \tag{13}$$

for the equal distribution of error, as well as for the equal, weighted (field size assigned to the node) distribution of the error at each experimental point respectively.

3. Global-local indicator of improving mesh density as a measure of the reliability of the obtained results

The methods of converting errors into such a mesh density are presented below. They provide an even distribution of errors for the proposed density distribution of nodes. This is a basic requirement (and an advantage) of adaptation methods. As it turns out, to define the correct density of nodes we need to enter both the local and global density index.

The local indicator for improving the mesh density at point i can be defined as

$$\overline{\xi}_{\sigma Li} = \frac{\left|\sigma_i^{\text{exact}} - \sigma_i^{\text{approx}}\right|}{\|e\|}. \tag{14}$$

The average error in the area with the number of points equal to n can be specified as

$$\|e\|_\sigma = \frac{1}{\sqrt{n}} \sqrt{\sum_{i=1}^{n} \left(\sigma_i^{\text{exact}} - \sigma_i^{\text{approx}}\right)^2}. \tag{15}$$

The total weighted norm is defined as

$$\|U\|_\sigma = \frac{1}{\sqrt{n}} \sqrt{\left(\sum_{i=1}^{n} \sigma_i^{\text{exact}}\right)^2} \tag{16}$$

and then the global node density indicator can be defined as

$$\xi_\sigma = \frac{\|e\|_\sigma}{\eta \cdot \|U\|_\sigma}, \tag{17}$$

where η is the imposed error level.

Using the previously defined norms, the global-local grid density index is defined as the following (ver. 1):

$$\xi_{\sigma Li} = \xi_\sigma^2 \cdot \overline{\xi}_{\sigma Li} = \left(\frac{\|e\|_\sigma}{\eta \cdot \|U\|_\sigma}\right)^2 \cdot \frac{\left|\sigma_i^{\text{exact}} - \sigma_i^{\text{approx}}\right|}{\|e\|_\sigma} = \frac{\|e\|_\sigma}{\eta^2 \cdot \|U\|_\sigma^2}\left|\sigma_i^{\text{exact}} - \sigma_i^{\text{approx}}\right|. \tag{18}$$

As it can be seen from the above formula, the global-local density index has a multiplicative form, with the global index included in the square formula. The global-local grid density index can also be defined as the following (ver. 2):

$$\xi_{\sigma Li} = \xi_\sigma \cdot \overline{\xi}_{\sigma Li} = \left(\frac{\|e\|_\sigma}{\eta \cdot \|U\|_\sigma}\right) \cdot \frac{\left|\sigma_i^{\text{exact}} - \sigma_i^{\text{approx}}\right|}{\|e\|_\sigma} = \frac{1}{\eta \cdot \|U\|_\sigma}\left|\sigma_i^{\text{exact}} - \sigma_i^{\text{approx}}\right|. \tag{19}$$

Due to the correlation between the global-local grid density index and the error norm, this index is used to assess the reliability of the obtained results.

4. Definition of an error functional for experimental and numerical data approximation

We assume the existence of data defined on a discrete set of points. These data can come from the measurements as well as from the calculations, and the data will be processed using an approach with simultaneous fulfillment of additional conditions. In mechanics, these conditions could be, for example, equilibrium or geometry equations. In the most general approach, in the computational process, two grids are assumed: one is the output one, on which the data is defined, and the second is the computational one. This is a more general approach than it was proposed in [6, 7], where measurement and calculation points were assumed to be the same points.

Let us assume the following:

Data: the vector $\widetilde{\mathbf{u}} = \{\widetilde{u}_1, ..., \widetilde{u}_n\}$ of measured quantities;

Unknown: vector $\mathbf{u} = \{u_1, ..., u_m\}$ of unknown values, generally located at some other points (in terms of their number and position) than the measured values $\mathbf{u} = \{u_1, ..., u_m\}$.

The values of the unknown $\overline{u}$ can calculated at points corresponding to experimental measurements through the relation

$$\overline{\mathbf{u}} = \mathbf{A}\mathbf{u}, \tag{20}$$

where $\overline{\mathbf{u}} = \{\overline{u}_1, ..., \overline{u}_n\}$ and the matrix $\mathbf{A}$ [m × n] infers from the relation $\overline{\mathbf{u}}$ and $\mathbf{u}$, obtained by an approximation (e.g., moving weighted least squares – MWLS). Now the main task is to:

Find: $\min_u (\mathbf{A}\mathbf{u} - \widetilde{\mathbf{u}})^2$ meeting the additional equations:

$$\mathbf{H}\mathbf{u} = \widetilde{\mathbf{F}}, \tag{21}$$

where the matrix $\mathbf{H}$ [n × k] and the right side vector $\widetilde{\mathbf{F}} = \{\widetilde{F}_1, ..., \widetilde{F}_k\}$ are constructed as the result of describing some additional conditions by means of finite differences.

With such assumptions, the error function can be presented using the following form:

$$R(\mathbf{u}, \boldsymbol{\lambda}) = \frac{1}{2}(\mathbf{A}\mathbf{u} - \widetilde{\mathbf{u}})^2 + (\mathbf{H}\mathbf{u} - \widetilde{\mathbf{F}})^T \boldsymbol{\lambda}, \tag{22}$$

where λ is a vector of Lagrange multipliers.

Minimizing the assumed error function against unknown $\mathbf{u}$ and λ, we obtain the following system of equations:

$$\frac{\partial R}{\partial \mathbf{u}} = \mathbf{A}^T\mathbf{A}\mathbf{u} - \mathbf{A}^T\widetilde{\mathbf{u}} + \mathbf{H}^T\boldsymbol{\lambda} = 0, \qquad \frac{\partial R}{\partial \boldsymbol{\lambda}} = \mathbf{H}\mathbf{u} - \widetilde{\mathbf{F}} = 0. \tag{23}$$

The above set of equations can be reduced to two systems of linear equations, from which we can calculate unknowns:

$$\boldsymbol{\lambda} = \left(\mathbf{H}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{H}^T\right)^{-1}\mathbf{H}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\widetilde{\mathbf{u}} - \left(\mathbf{H}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{H}^T\right)^{-1}\widetilde{\mathbf{F}}, \tag{24}$$

$$\mathbf{u} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\widetilde{\mathbf{u}} - (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{H}^T \cdot \left\{\left(\mathbf{H}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{H}^T\right)^{-1}\mathbf{H}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\widetilde{\mathbf{u}} - \mathbf{H}^T\left(\mathbf{H}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{H}^T\right)^{-1}\widetilde{\mathbf{F}}\right\}. \tag{25}$$

In the matrix form, the above system of equations can be written as

$$\begin{bmatrix} \mathbf{A}^T\mathbf{A} & \mathbf{H}^T \\ \mathbf{H} & \mathbf{0} \end{bmatrix} \times \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{A}\widetilde{\mathbf{u}} \\ \widetilde{\mathbf{F}} \end{bmatrix}. \tag{26}$$

The solution of the system of equations (23) is the vector u of the function values, for which the error function (22) has the minimum value and the equations of constraints (21) specified in finite differences are met. The method presented here has been applied to improve the results of calculations/measurements in a number of mechanics tasks, among others in the bending beam problem, which is described below.

5. Numerical example of a bending beam

The steel beam ($E = 205 \times 10^6$ kPa) with cross-sectional dimensions 1.0×1.0 cm and length $L = 1.00$ m was taken into consideration. The beam was loaded by uniform loading $q = 1.00$ kN/m.

The calculations were carried out for an irregular mesh of nodes, using the beam deflection equation as the conditions for restrictions for internal, in the form:

$$w''(x) = -\frac{M(x)}{EJ}, \tag{27}$$

where $w(x)$ – a deflection of the beam at its point x, $M(x)$ – a value of the bending moment in point x, E – a Young modulus, J – a moment of inertia.

The distribution of nodes and the measured values of deflections were generated as random values. Figure 1 shows the values of deflections: measured, corrected and the exact ones. The use of optimization with constraints impels the change of values so that they will improve the fulfillment of the constraints equation within the considered area. This means choosing from the family of acceptable curves, defined by the constraints equation of the single curve, for which the error function obtains the minimum value. As it is shown in Fig. 1, the character of the curve with the corrected values corresponds to the constraints equation.

To evaluate the quality of the solution, the relative and absolute errors were determined at individual nodes, referring the obtained values to the known exact ones. Graphs with errors are shown in Fig. 2. The relative and absolute errors do not give a full picture of the quality of the obtained solution, as they show only the local change of the measurement/function value at the given point. For comparison with the above norms, the global-local error was determined from Eq. (19). Application of the global-local norm eliminates these inconveniences and allows to assess the credibility of the entire solution.

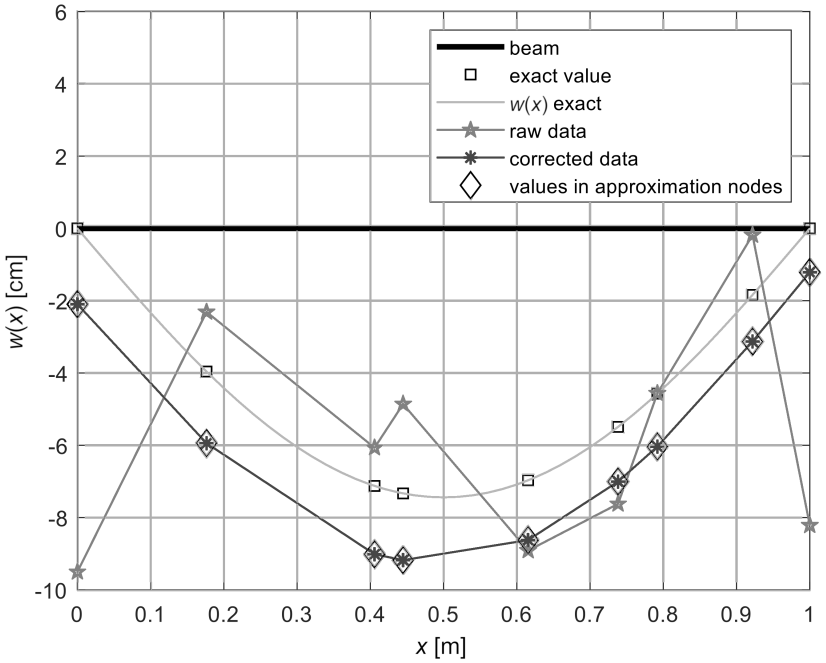

Fig. 1. Beam deflections values: measured, corrected and the exact ones for constrains within the concerned area.

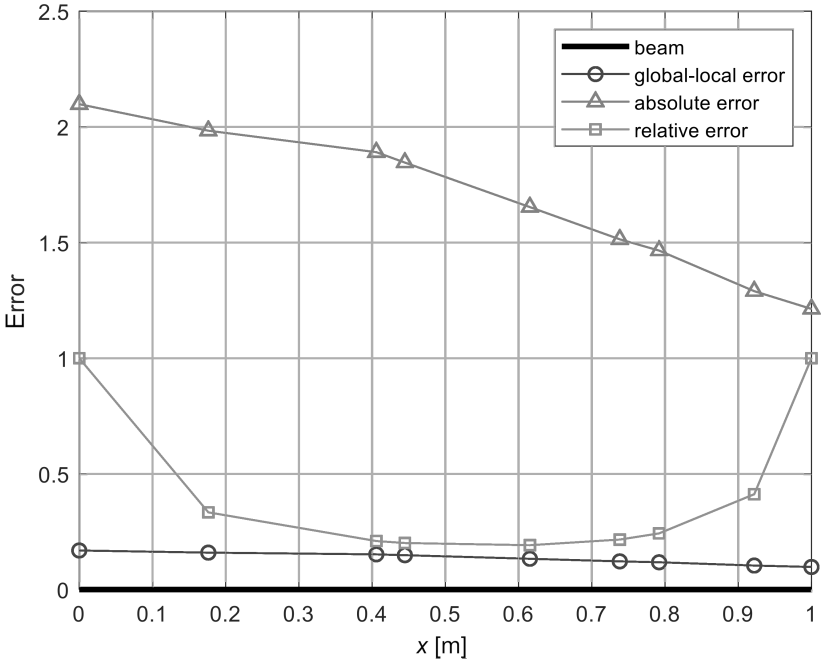

Fig. 2. Values of relative, absolute and global-local errors for intra-area constraints.

The global-local error allows to determine the size and global nature of the error (permanent or variable error) of the solution and it locally shows the quality of the solution at individual nodes. The graph of the global-local norm depicted in Fig. 2 presents almost a constant distribution of the errors within the entire domain (the local error value, for example, at the point $x = 0$, is slightly greater than the error at the point $x = 1$).

For comparison with the previous task, the same numerical data was verified using the beam deflection equation as the constraints equation for internal nodes and assuming additional restrictions in the form of static boundary conditions at the beam support points: $w(0) = w(1) = 0$.

For such a formulation of this task, the strict solution will always be obtained for the corrected values, regardless of the introduced measured values (see Fig. 3).

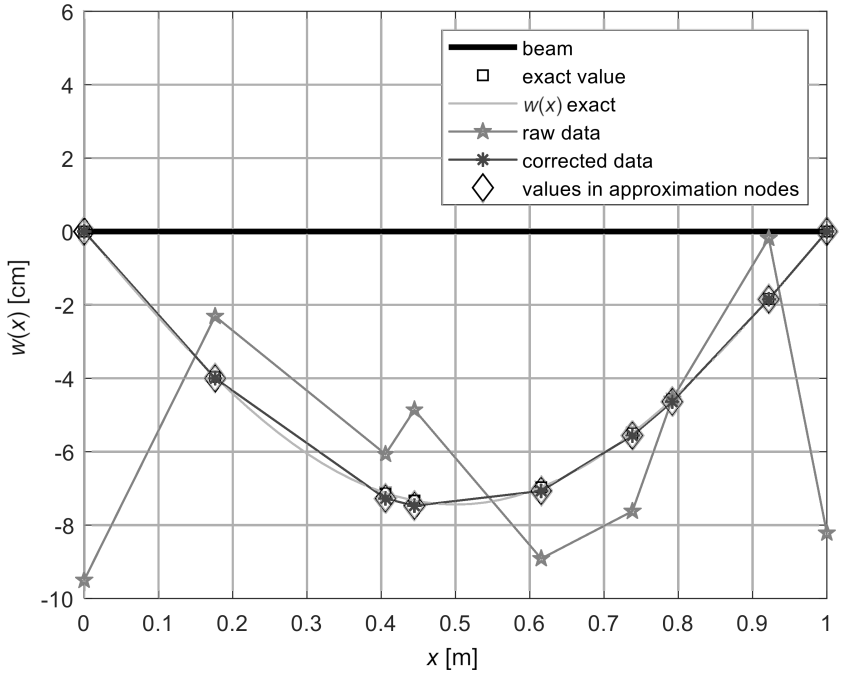

Fig. 3. Beam deflections values: measured, corrected and exact for restrictions inside the area and at the edge.

Figure 4 shows graphs of errors. The relative and absolute errors do not inform about the credibility of the obtained solution. The global-local norm within the whole area is close to zero, which means that the quality of the obtained solution is very high.

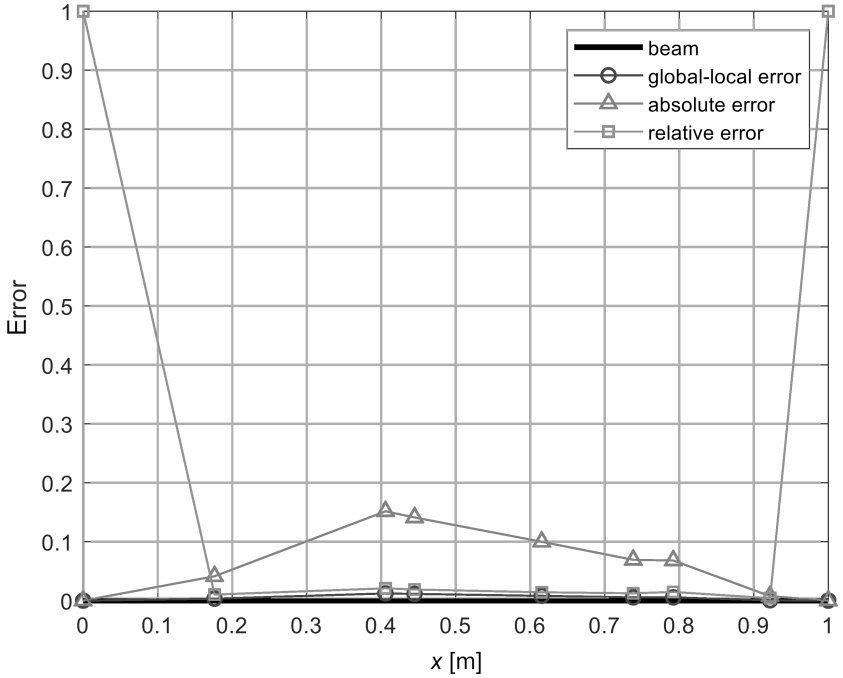

Fig. 4. Values of relative, absolute and global-local error for restrictions inside the area and at the edge.

The solutions presented above were obtained assuming that the input data grid and the calculation grid overlap. For comparison, the following is the solution for the task in which a computational grid consists of five points and does not coincide with the data grid, which has nine points. Values corrected at points corresponding to the ones within the data grid were determined using Eq. (20).

The matrix A $[9 \times 5]$ can be derived from the relation existing between $\overline{u}$ and u, obtained by the Lagrange interpolation, where $\overline{u}$ are the values of the sought function, calculated at points

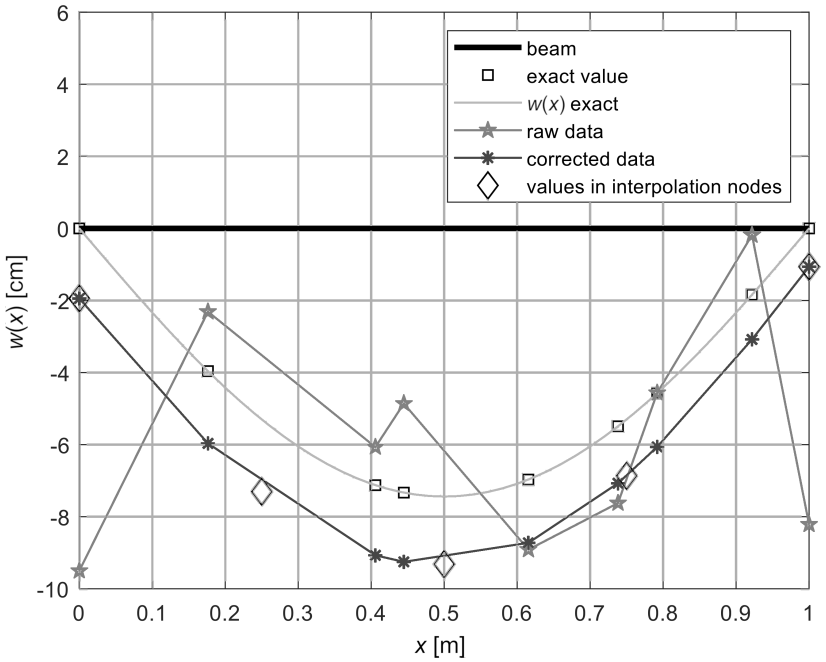

Fig. 5. Beam deflections' values: measured, corrected and the exact ones for constraints within this area – data grid and calculation grid do not coincide.

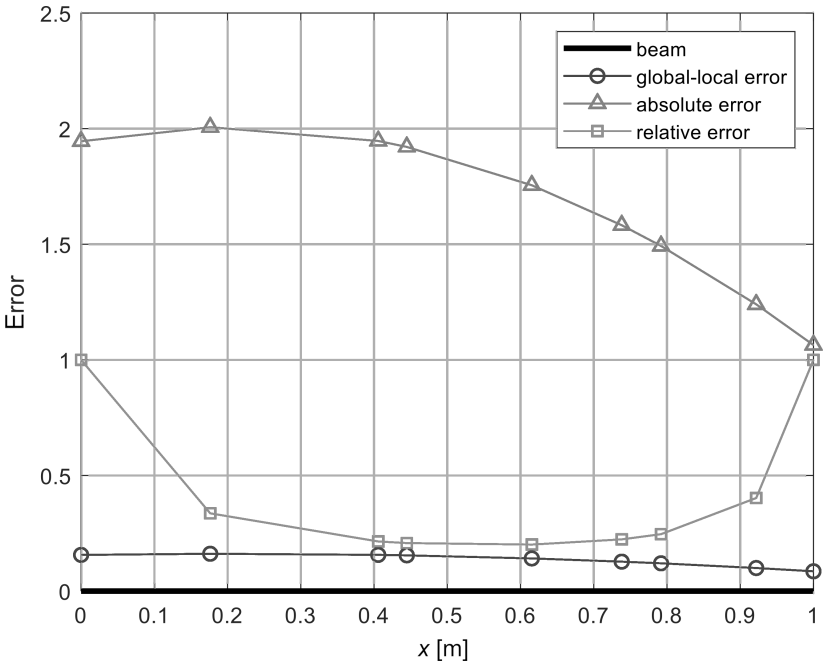

Fig. 6. Values of relative, absolute and global-local errors for intra-area constraints – data grid and calculation grid do not coincide.

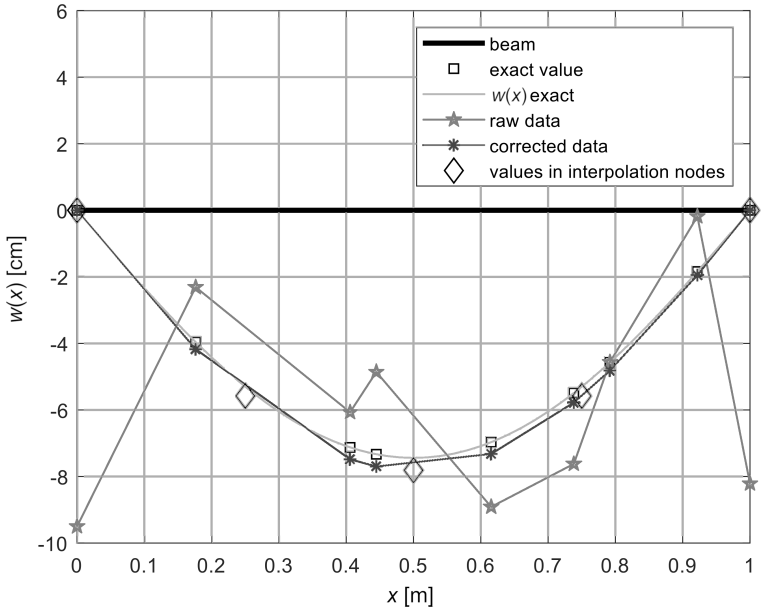

Fig. 7. Beam deflections' values: measured, corrected and exact for restrictions inside the area and at the edge – data grid and calculation grid do not coincide.

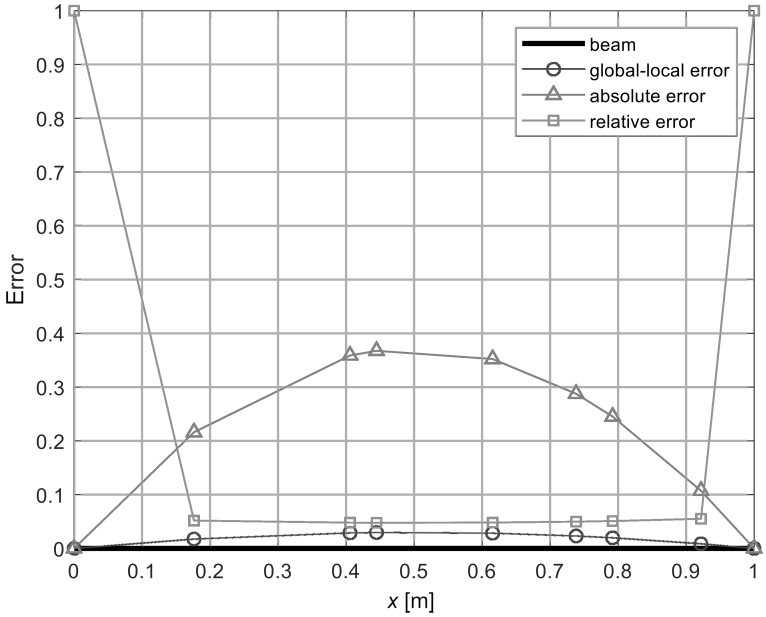

Fig. 8. Values of relative, absolute and global-local error for restrictions inside the area and at the edge – data grid and calculation grid do not coincide.

corresponding to the input data, and u are the values of the sought function, computed in the calculation grid points.

6. Summary

This study used the approximation method proposed in [3, 5] for a given discrete set of values using the mesh-sess MRS formulation with additional restrictions.

This concept was used to estimate *a posteriori* errors of numerical data in a one-dimensional problem. It contained a technique of discrete data post-processing with additional conditions, a way

of estimating the *a posteriori* error of these data and the assessment of the reliability of the obtained results using the so-called global-local grid node density index with an evenly distributed error.

The proposed global-local grid density index correctly determines the reliability of the obtained results. It points the places where the measuring grid should be denser so it may be implemented for the adaptation process.

The introduced criteria for assessing the results reliability are well suited to discrete BMRS and MES methods. Also, they can be implemented for computer simulations and verifications of the results of experimental measurements.

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