Computing and Informatics, Vol. 30, 2011, 639–653

IMPROVEMENTS IN THE GLOBAL A-POSTERIORI ERROR ESTIMATION OF THE FEM AND MFDM SOLUTIONS

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Communicated by Jacek Kitowski

Abstract. The present paper deals with the estimation of the solution error of the boundary value problems of mechanics science. The well-known ideas of error estimators are presented, as well as new original ones, which use the concept of the improved HO reference solution, obtained using the Meshless Finite Difference Method analysis. Such HO estimators may be applied not only in the MFDM, but also in the Finite Element Method error analysis. This issue is presented here for the first time ever. The approach is tested on chosen 2D benchmark problems. The results are very encouraging.

Keywords: A-posteriori error analysis, higher order approximation, Finite Element Method, correction terms, Meshless Finite Difference Method

1 INTRODUCTION

This paper is devoted to the estimation of a-posteriori solution error of the boundary value problems of mechanics. Nowadays, precise solution error estimation is one of the fundamental tasks in each numerical analysis [1, 23, 25, 29]. In most cases, it is a complex and very time consuming process when a high quality reference solution is required. In each analysis, it replaces the true analytical solution that is known for the benchmark problems only. The broad range of solution error estimators [1, 29] was introduced, defined and tested for the Finite Element Method (FEM, [28]).

However, there may be still a need for development of new ones. Following this idea a-posteriori error approach based on the concept of the Meshless Finite Difference Method is developed (MFDM, [13, 14]). It is based here on a new Higher Order (HO) reference solution of especially high quality.

Therefore in the present work the outlines, exemplary applications and recent developments of the Meshless Finite Difference Method are presented first. This is a meshless solution approach fully competitive to the FEM. As opposite to the FEM analysis, only nodes, without any pre-imposed structure, are required in the MFDM. Consequently, local approximation of the unknown function is prescribed in terms of nodes only.

A simple and effective concept of the so called Higher Order (HO) MFD solution mentioned above is briefly presented as well. This type of an improved MFD solution requires only double solution of simultaneous algebraic equations, with the same left hand side. Only the right hand side of those equations is modified, by means of the appropriate HO correction, resulting from the Taylor series expansion of the standard MFD operator.

Among many applications, the HO MFD solution may be successfully applied in solution as well as in residual error estimations. For results of the MFDM analysis, such solution provides the best quality estimation, when compared with the other estimators. It is also expected to be more precise than the other commonly used estimators for the FEM analysis.

The proposed approach is tested on several 2D benchmark examples. Solution estimations obtained using HO estimators are compared with those obtained using standard estimators, for the MFDM and FEM analysis separately. The results are very encouraging.

2 DESCRIPTION OF A PROBLEM SOLUTION

The boundary problems of mechanics may be posed in various formulations, including the local one, when the set of differential equations involving the unknown function u is given at arbitrary point P of the domain Ω by point together with the proper boundary conditions

$$\left\{ \begin{array}{l} Lu = f \\ Gu = g \end{array} \right. \qquad u = u(P) \qquad \left\{ \begin{array}{l} P \in \Omega \\ P \in \partial\Omega \end{array} \right. \tag{1}$$

where L, G denote differential operators inside the domain Ω and on its boundary $\partial\Omega$, respectively. Other type of b.v.p. formulation is the global one, in which the energy functional

$$\mathrm{I}(u)=\frac{1}{2}b(u,u) - l(u) \tag{2}$$

should be minimised or the variational principle

$$b(u,v) = l(v) \quad \text{for} \quad v \in \mathrm{V}_{adm} \tag{3}$$

satisfied, both prescribed to the whole domain Ω at once. Here $b(u,v)$ and $l(v)$ are bilinear and linear functionals, respectively. Test function v comes from the admissible space V_{adm}.

Mixed types of the b.v.p. formulations are also possible, for instance in the local-global formulations variational principle is satisfied only locally, on the local subdomains, prescribed to selected points (e.g. to nodes). Here, discusion about possible b.v.p. formulations is limited to several most commonly applied ones. However, more details about this matter may be found in [2, 3, 14].

In most cases, the above problems have to be solved using appropriate discretization tools, like the FEM or the MFDM. In such methods, both domain and function have to be discretized, providing the mesh size h and approximation order p. As the result, one obtains the numerical solution u, which differs from the exact analytical one $u^{(T)}$. The solution error may be measured as follows:

$$e = \left\| u^{(T)} - u \right\| . \tag{4}$$

Here $\|\cdot\|$ denotes the appropriate norm, involving integration, either over the whole domain or over a chosen local subdomain only. This type of error evaluation is called the global one. Two types of such global norms, namely the energetic and mean ones, are commonly applied in calculations.

$$\eta_E = \sqrt{b(e,e)} \quad , \quad \eta_{L_2} = \sqrt{\frac{1}{\Omega}\int\limits_{\Omega} (e)^2 \, d\Omega} \tag{5}$$

The global error evaluation is more frequently used in the FEM, where the domain discretization is based on the elements. Appropriate error estimation [1, 9, 14, 25] requires high quality reference solution $\bar{u} \approx u^{(T)}$ replacing in (4) the exact analytical solution $u^{(T)}$. Therefore, one obtains the global estimate

$$\eta = \|\bar{u} - u\| . \tag{6}$$

Its quality depends on the accuracy of the $\bar{u}$. In the present paper, we deal with several types of such global error estimates, namely hierarchic, smoothing and residual ones. They are common for the FEM analysis [1, 28, 29]. However, all of them may also be applied in the MFDM.

In the standard hierarchic estimators, new mesh has to be generated (h-type) or approximation order needs to be raised (p-type). Therefore, solution of completely new discrete problem is required. In the case of smoothing estimators, the solution error is estimated using the difference between a rough u' and smoothed $\bar{u}'$ solution derivatives.

$$\eta = \|\bar{u} - u\| \sim \|\bar{u}' - u'\| \tag{7}$$

The most common smoothing estimator used in the FEM is the Zienkiewicz-Zhue one [29].

The last type of estimators considered here is based on the distribution of the exact residual error which is defined as

$$r = L\hat{u} - f \tag{8}$$

where $\hat{u}$ is a continued nodal solution. In the residual estimator of explicit type one has

$$\eta = \sqrt{h^2 \left\| r \right\|_{L_2}^2 + \frac{1}{2} h \left\| J \right\|_{L_2}^2} \tag{9}$$

where J denotes jump term of the solution $u^{(T)}$ on the (sub)domain boundary. The implicit type requires solution of the b.v.p. with the residuum (8) used as the right hand side

$$b(e, v) = l(v) \quad \text{for} \quad v \in \mathrm{V}_{adm}. \tag{10}$$

Eventually, the solution error is obtained after solving a discrete form of the Equation (10).

Our goal is to prove that the HO MFD reference solution may be applied in both the FEM and MFDM error solution analysis, producing the best estimation, when compared to the estimators outlined above. Moreover, as it will be shown, it uses the same discretized problem as for the estimated solution, but it does not need so much computational effort.

3 APPLIED ALGORITHMS AND METHODS

In this section, outlines of the Mehsless Finite Difference Method are presented. The MFDM [13, 14] is one of the basic discrete solution approaches to analysis of the boundary value problems of mechanics. It belongs to the wide group of methods called nowadays the Meshless Methods (MM, [3, 13, 14, 27]. The MM are contemporary tools for analysis of boundary value problems. In the meshless methods, approximation of a sought function is described in terms of nodes, rather than by means of any imposed structure like elements, regular meshes etc. Therefore, the MFDM, using arbitrarily irregular clouds of nodes, and the Moving Weighted Least Squares (MWLS, [11, 14]) approximation falls into the category of the MM, being in fact the oldest [14], and possibly the most developed one of them.

The basic MFDM solution approach consists of the following steps:

- generation of the cloud of nodes,
- cloud of nodes topology determination,
- MFD star determination,
- function discretization (selection of degrees of freedom) and Moving Weighted Least Squares approximation,
- generation of the MFD operators,
- numerical integration (for the global formulations only),

- generation of the MFD equations,
- discretization of the boundary conditions,
- solution of the S(L)AE, obtained from the above,
- appropriate postprocessing.

The bases and the recent state of the art in the research on the MFDM, as well as several possible directions of its development are briefly presented in [14, 25]. Here only some general remarks are given concerning especially cloud of nodes generation, local function approximation, numerical integration and boundary conditions discretization. They are of essential importance to the HO MWLS approximation and improved a-posteriori error analysis. Although the MFDM is the oldest, and therefore the most developed meshless method, its solution approach is still being currently developed. The latest MFDM extensions include the higher order approximation based on correction terms, multipoint approach, a-posteriori error estimation as well as an adaptation approach, and are presented in [15, 16, 17, 19, 20, 21, 22, 23, 24, 25, 25].

The MFDM may deal with boundary value problems posed in every formulation [14, 25], where the differential operator value at each required point may be replaced by a relevant difference operator involving a combination of searched unknowns of the method. Thus any formulation mentioned in the previous section may be used here. However, independently of the bvp formulation type applied, one always starts from the generation of a cloud of nodes, that may be irregularly scattered, but usually are without any imposed structure on them, like finite element or regular mesh, and have no mapping restrictions to the regularized stencil. In such a cloud of nodes, some additional ones may be easily added, removed or shifted, if necessary, causing only small changes in nodes structure.

Basically any nodes generator might be applied. However, it is very convenient to use a nodes generator specially designed for the MFDM, e.g. the Liszka type [12, 13, 18], that is based on the nodes density control. Nodes are 'sieved out' from the regular very dense background mesh, according to a prescribed density. Although such a generator provides arbitrarily irregular cloud of nodes, it is useful to determine its topology afterwards. This includes generation of the subdomains prescribed to nodes – i.e. Voronoi polygons (in 2D or polyhedrons in 3D), and (in 2D) the Delaunay triangles – placed between nodes. The topology information may be applied for star generation and/or for integration purposes.

Once the nodes for MFD stars are selected (e.g. using topology oriented criteria like Voronoi neighbours), the local approximation of the unknown function is performed at every point of interest (node, Gauss point). It is done using the Taylor series expansion, and the MWLS approximation [11, 14]. It is crucial to the method that the MFD star may consist of more nodes (m) than the minimum required to provide the approximation order (p). Evaluation of the MWLS approximation requires the minimisation of the weighted error functional

$$J = (\boldsymbol{q} - \boldsymbol{P}\boldsymbol{D}u)^t \boldsymbol{W}^2 (\boldsymbol{q} - \boldsymbol{P}\boldsymbol{D}u) \tag{11}$$

where $\boldsymbol{P}$ – interpolants matrix, $\boldsymbol{D}u$ – derivatives vector (up to the p^{th} order), $\boldsymbol{q}$ – MFD star nodal values vector, and $\boldsymbol{W}$ – diagonal weights matrix. Weighting functions are singular for the central node of the MFD equations. In this way, interpolation is enforced there. As a consequence, the essential boundary conditions are satisfied without any additional techniques.

After minimisation of (11), one obtains the complete set of derivatives, up to the p^{th} order

$$\boldsymbol{D}u = \boldsymbol{K}\,q \quad , \quad \boldsymbol{K} = (\boldsymbol{P}^t\,\boldsymbol{W}^2\boldsymbol{P})^{-1}\boldsymbol{P}^t\,\boldsymbol{W}^2 \tag{12}$$

which are, in fact, the coefficients of the local approximation. Moreover, the approximation error may be easily estimated, by considering several additional terms of the Taylor series expansion. It is worth stressing that other meshless methods often use equivalent polynomials for the function approximation [3], instead of the truncated Taylor series. However, although the results of the approximation are the same, the polynomial approach does not provide at once so much valuable information (e.g. about local errors and derivatives).

Some extensions of the MWLS approximation, like use of the generalised degrees of freedom or local constrains are presented in [14].

In the case of global formulations integration is required. The following techniques may be used:

- integration around nodes over the Voronoi polygons, which is the best solution for the even order differential operators,
- integration between the nodes over the Delaunay triangles (2D), which produces the most accurate results for the odd order differential operators,
- integration on a background mesh, independent of the nodes distribution,
- integration over the zones of influence of the weighting functions of the MWLS approximation,
- integration over the local subdomains (MLPG, [2]).

Generation of the MFD operators which appears in formulations (1)÷(3) is done using the MWLS approximation, and appropriate formulae composition. Generation of the MFD equations depends on the formulation type. In the case of local formulation (1) one may use the collocation technique, whereas in the case of global formulations (2) and (3) one has to minimise the energy functional or to use the relevant variational principle.

The essential boundary conditions are automatically satisfied by using singular weights in the MWLS approximation. However, discretization of the natural or mixed boundary conditions usually requires additional MFD approximation on the boundary. Such approximation may use only internal nodes from the domain, but it is of poor quality then. Introducing additional, external, fictitious nodes or generalised degrees of freedom may raise the approximation quality on the boundary.

The MFDM solution approach requires analysis of the S(L)AE. It is most convenient to use a solver which takes advantages of the method's nature, like the multigrid approach [5, 16]. Finally, the postprocessing of the numerical results is performed using the MWLS approximation once again.

There are many extensions of the basic MFDM solution approach. Among them one may mention:

- cloud of nodes adaptation [18, 23, 24, 25],
- various MWLS extensions [14],
- higher order approximation [15, 16, 17, 19, 20, 21, 22, 23, 24, 25],
- a-posteriori error analysis [1, 9, 23, 24, 25],
- multigrid solution approach [5, 18],
- MFDM in various bvp formulations, including the MFDM/MLPG combinations [2, 26],
- MFDM on the differential manifold,
- MFDM/FEM combinations [10],
- experimental and numerical data smoothing [8].

Here, higher order approximation will be discussed in a more detailed manner.

The solution quality may be improved by increasing the number of nodes or by raising the order of local approximation. This may be done using HO MFD operators [4, 7], generalised degrees of freedom [14], multipoint approach [8, 15, 16, 17] or Higher Order Approximation (HOA, [19, 20, 21, 22, 23, 24, 25]), based on correction terms. The last approach will be discussed here.

Instead of introducing new nodes or degrees of freedom into the simple MFD operator, some additional terms are considered. They result from the Taylor series expansions of the simple MFD operator coefficients. Beside the HO derivatives $\boldsymbol{D}u^{(H)}$, they may also contain the singularity $\boldsymbol{c}^t\boldsymbol{S}$ or discontinuity terms $\boldsymbol{e}^t\boldsymbol{J}$. HO derivatives may be calculated by means of using appropriate formulae composition and use of the basic MFD solution, corresponding to the simple (not improved) MFD operator.

The HOA concept is based on splitting the MWLS approximation terms into two parts, namely the low (L) and higher order (H) ones

$$\boldsymbol{P}^t\boldsymbol{D}u^{(L)} \quad + \quad \left(\boldsymbol{P}^{(H)}\right)^t \boldsymbol{D}u^{(H)} - \boldsymbol{c}^t\boldsymbol{S} - \boldsymbol{e}^t\boldsymbol{J} \quad = \quad \boldsymbol{q}. \tag{13}$$

These additional HO terms are treated as known values. In such a way, the final results (derivatives up to the p^{th} order) depend on the nodal values, and on the correction terms Δ mentioned above:

$$\boldsymbol{D}u^{(L)} = \boldsymbol{K}\boldsymbol{q} - \Delta, \quad \Delta = \boldsymbol{K}\left[\left(\boldsymbol{P}^{(H)}\right)^t \boldsymbol{D}u^{(H)} - \boldsymbol{c}^t\boldsymbol{S} - \boldsymbol{e}^t\boldsymbol{J}\right]. \tag{14}$$

It is assumed here that the approximation order is raised to $2p^{\text{th}}$. The HO derivatives are calculated in the most accurate manner then.

The HO MFD solution is obtained in two steps. In the first step, only the low order part of (13) is taken into account and the basic, low order solution $\boldsymbol{u}^{(L)}$ is obtained then. Afterwards, the implicit postprocessing values of the correction terms (14) are calculated, using formulae composition of the low order solution. They modify the right hand sides of the MFD equations, leaving the coefficient matrix unchanged. The new improved HO solution $\boldsymbol{u}^{(H)}$ is exact within the approximation order assumed ($2p^{\text{th}}$) and, in general, does not depend on the quality of the MFD operator.

HO solution may be applied in many aspects of the MFDM approach, especially for improving

- solution quality inside the domain [19],
- solution quality on the boundary [20],
- the a-posteriori error analysis [21, 22, 23, 24, 25],
- the adaptation process [23, 24, 15],
- and for modification of the multigrid solution approach [5, 18, 23, 24, 25].

Let us return to the development of the HO global error estimates. HO solution is applied here as the superior quality reference solution for several types of outlined estimators, namely hierarchic, smoothing and residual ones. HO reference solution provides error estimation of the $2p^{\text{th}}$ order (as opposed to the classic $p+1$ order of the improved, reference solution), where p denotes the basic approximation order considered, and as the opposite to the well-known standard estimators, it does not need so much computational effort.

The concept of the hierarchic estimators deals with an additional solution of the MFD equations, producing high quality HO solution. In that case, only the right hand side of those equations is modified whereas the numbers of nodes in both the cloud and MFD operator remain unchanged. In the case of smoothing estimators, one may use correction terms explicitly for improved estimation of the rough derivatives, since smoothing is built into the MWLS approximation and HO derivatives composition. Therefore, any additional smoothing technique is not needed. Moreover, improved estimation of the residual error may be applied in estimators of the residual type, in both the explicit (simpler but less accurate) and implicit forms.

In the present paper, we also propose to apply such technique in the analysis carried out by FEM. The correction terms may be found using the standard FEM solution, and Taylor series expansion of the simplest MFD operator required to solve a given b.v. problem. They are applied in order to obtain a FEM/MFDM reference solution, which may be used for a-posteriori error estimation. It is worth stressing that this approach does not need any additional topology information. It uses only the one which was generated a priori for the FEM analysis.

Series of 1D and 2D tests done clearly showed that the HO reference MFDM solutions may provide much better error estimation than the ones obtained from the classic estimators commonly applied in the FEM.

4 NUMERICAL RESULTS

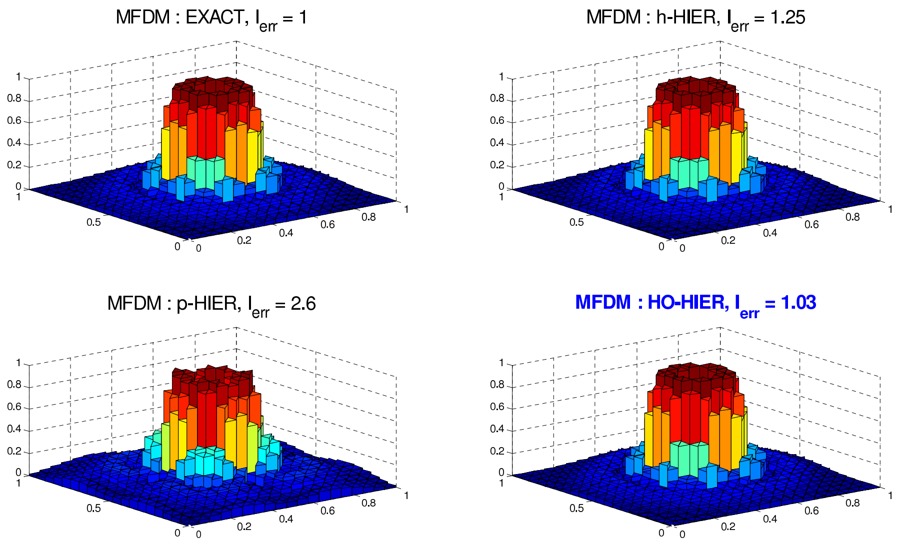

Fig. 1. Hierarchic estimators (h-type, p-type, HO-type) for the MFDM solution error

In this section exemplary numerical results for the typical 2D Poisson benchmark problem are presented with analytical solution exhibiting large amounts of gradient. Calculations were made for the mesh with 400 nodes subjected to the domain of the quadratic shape. Results of

- the exact solution error,
- h – hierarchic estimation,
- p – hierarchic estimation,
- HO – hierarchic estimation,
- ZZ – smoothing estimation,
- HO – smoothing estimation,
- residual estimation of explicit type,
- residual estimation of implicit type.

are presented for both the MFDM (Figures 1 and 2) and the FEM (Figures 3 and 4) analysis.

Both shape and effectiveness index

$$i = 1 + \frac{|e - \eta|}{|e|} \tag{15}$$

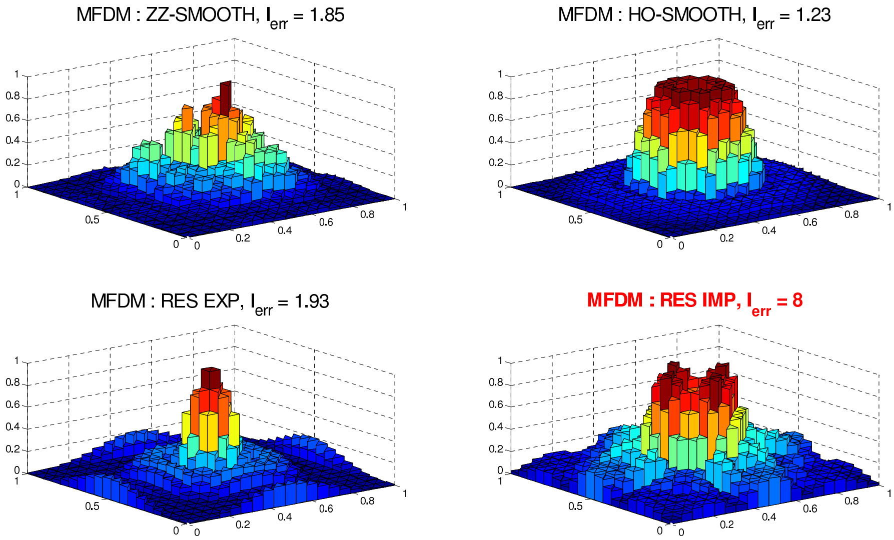

Fig. 2. Smoothing (ZZ-type, HO-type) and residual (explicit, implicit) estimators for the MFDM solution error

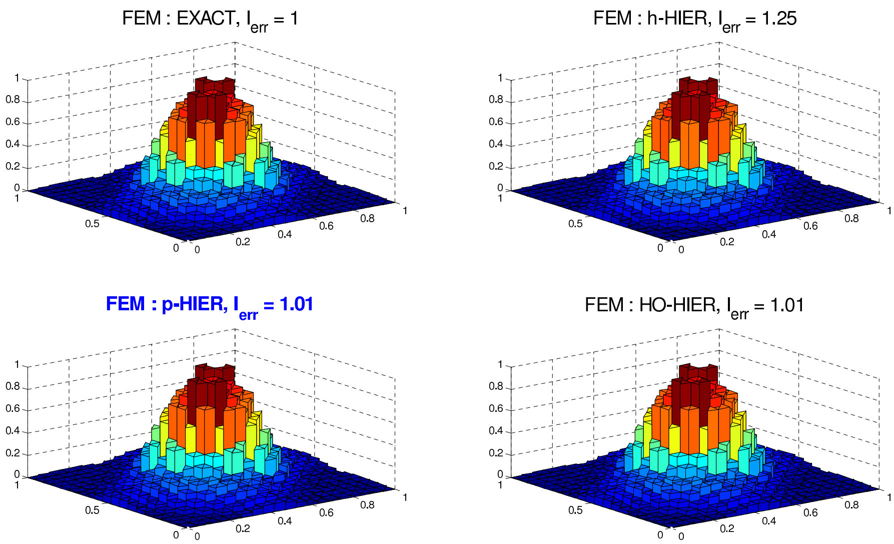

Fig. 3. Hierarchic estimators (h-type, p-type, HO-type) for the FEM solution error

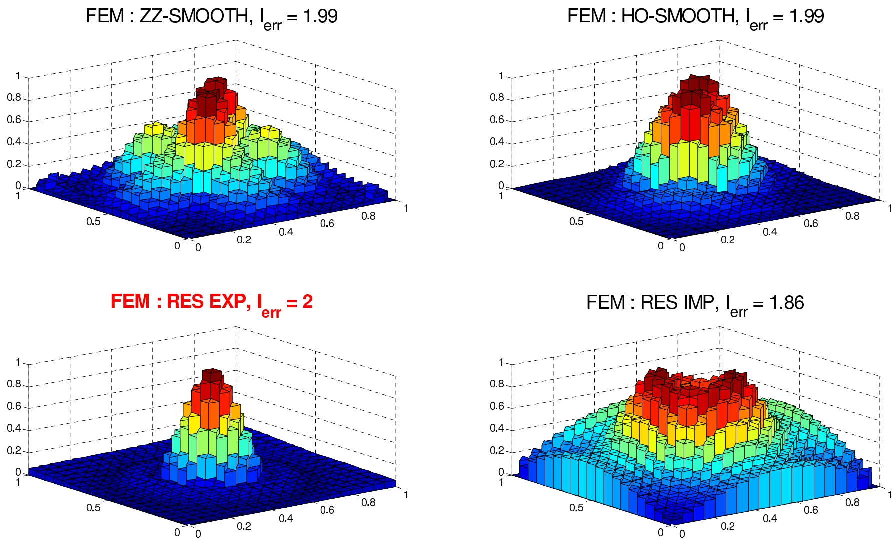

Fig. 4. Smoothing (ZZ-type, HO-type) and residual (explicit, implicit) estimators for the FEM solution error

values are taken into account and may be compared here. For the MFDM solution error estimation, the best results were obtained when using the HO-hierarchic estimator ($i = 1.03$) and HO-smoothing estimator ($i = 1.23$). For the FEM solution error estimation, the same precision ($i = 1.01$) was reached when using hierarchic estimators, of HO- and p-type. However, the HO-estimator does not require providing any new unknowns into the algebraic system whereas the p-estimator needs re-building the mesh with HO finite elements with additional internal nodes.

The analysis done required designing and building the appropriate computer program. It was written in C++ Visual Studio. In addition, Matlab graphical environment was used. Calculations for dense meshes and clouds of nodes were performed using ACK Cyfronet software (*Saturn*).

5 CONCLUSIONS

Simple and effective way of solution error estimation was proposed and tested here. It uses a concept of the Higher Order reference solution which may be applied in both the Meshless Finite Difference Method and, for the first time, in the Finite Element Method. It is based on additional correction terms which come from the Taylor series expansion of the unknown function in the MFDM analysis. Those terms consist of HO derivatives as well as singularity or discontinuity terms. They modify the right hand side of the MFD equations, providing high quality MFD solution without the necessity of providing new nodes into the simple MFD operator or new unknowns into the algebraic equation system.

HO estimates were compared to those which are commonly applied in other discrete methods, especially in the FEM. This includes hierarchical, smoothing and residual estimators. All of them need high quality reference solution as the equivalent of the unknown analytical solution. HO MFD solution may be applied here, giving the estimation of $2p$ order quality, where p is a basic approximation order. It provided better results for less computational effort, when compared to the high costs of other hierarchic estimators.

Series of preliminary 1D, and 2D benchmark problems solved demonstrated the potential quality and power of these error estimation concepts. However, many more tests are needed, especially non-linear ones and 3D problems. Several chosen true engineering applications are planned as well.

Acknowledgement

The authors would like to thank for the possibility of using the high performance super computers of the Polish academic centre CYFRONET in Cracow.

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