

# Multipoint meshless FD schemes applied to nonlinear and multiscale analysis

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**Abstract.** The paper presents computational schemes of the multipoint meshless method – the numerical modeling tool that allows accurate and effective solving of boundary value problems. The main advantage of the multipoint general version is its generality – the basic relations of derivatives from the unknown function depend on the domain discretization only and are independent of the type of problem being solved. This feature allows to divide the multipoint computational strategy into two stages and is advantageous from the calculation efficiency point of view. The multipoint method algorithms applied to such engineering problems as numerical homogenization of heterogeneous materials and nonlinear analysis are developed and briefly presented. The paper is illustrated by several examples of the multipoint numerical analysis.

**Keywords:** Meshless FDM, Higher order approximation, Multipoint method, Homogenization, Nonlinear analysis, Elastic-plastic problem

## 1 Introduction

Besides the most commonly applied method of computational analysis – the Finite Element Method, the alternative methods, such as various meshless methods are more and more developed [1] contemporary tools for analysis of engineering problems. The paper introduces computational schemes of the application of the recently developed higher order multipoint meshless finite difference method [2, 3] to the boundary value problems. The new multipoint approach (higher order extension of the meshless FDM (MFDM) [4]) is based on the arbitrary irregular meshes, the moving weighted least squares (MWLS) approximation, and the local or various global formulations of boundary value problems. The multipoint technique leads to greater flexibility when compared with the FEM, provides  $p$ -type solution quality improvement, and may be used to solve various types of engineering problems. Due to its characteristic features, the method application especially for the nonlinear and multiscale analyses needs specific solutions, which are presented in the paper.

The paper is organized as follows. Section 2 describes the idea of the multipoint meshless FDM and its two versions. The general version is especially useful to solve various engineering problems including nonlinear ones. The basic steps of the multipoint MFDM analysis are presented in this part. The algorithm of the method

application to the two-scale analysis of heterogeneous materials, based on the multipoint MFD characteristic features, is discussed in detail in section 3. The general multipoint strategy in the nonlinear analysis is outlined in section 4. Finally, a short summary and some concluding remarks are given.

## 2 The fundamentals of the new Multipoint meshless FDM

The idea of the multipoint method as the higher order FDM (translated as the “Hermitian method” in the English version of Collatz’s book) was proposed by L. Collatz [5] more than sixty years ago, and forgotten since then due to complex calculations, too difficult to apply without the modern computational techniques. The original multipoint concept has been modified and extended recently [3] to the new multipoint meshless FDM, which is based on an arbitrary irregular cloud of nodes, the MWLS approximation [4] instead of the polynomial interpolation, and the local or various global formulations of the boundary value problems. This allows to obtain a fully automatic high quality solution as well as an error estimation tool. Generalized and unified description of the multipoint method is presented in the articles [2, 3]. The concept of the multipoint approach is based on raising the approximation order of the unknown function by using a combination of its values together with a combination of additional degrees of freedom at all nodes of a stencil.

The idea of the approach is illustrated by derived multipoint difference operators of the various approximation orders of the following type

$$\sum_{j(i)} c_j u_j = \sum_{j(i)} \alpha_j f_j \quad (1)$$

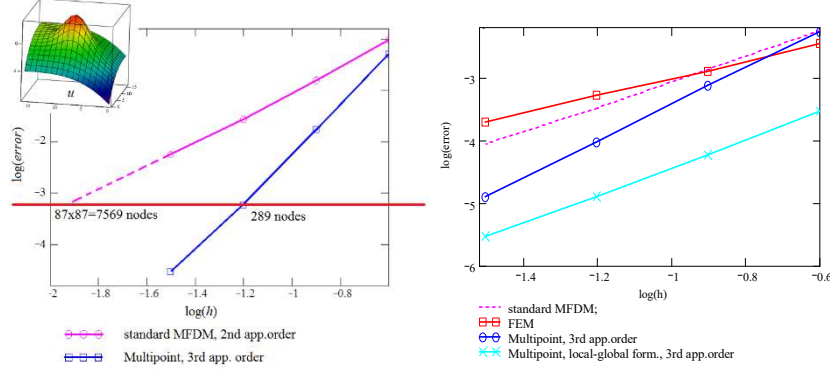
Here,  $i$  – is the central node number of the stencil consisting of nodes  $P_j$ ,  $j = 1...m$ ,  $f$  – the additional degrees of freedom (d.o.f),  $c_j$  and  $\alpha_j$  – coefficients. In this formula, a combination of the additional d.o.f. values *at each node* of the stencil (MFD star) is used instead of the function value  $f$  at the *central node only*, as it is in the classic (M)FDM solution approach.

The analysis of the method effectivity was done. As is depicted in Fig.1, to obtain the required level of solution error, the multipoint method needs a decreased number of nodes when compared with the standard MFD. Additionally, the convergence rate of derivatives obtained by the multipoint method has the same order as it is for the solution itself (phenomena of “superconvergence”). It is very important for engineering problems due to problem formulation posed in terms of the derivatives and unknowns (stresses, strains, etc).

### 2.1 The general approach of the multipoint method – versions

There are two basic versions of the multipoint method – the *specific* one, where the values  $f$  of the considered differential equation right-hand side are assumed as the additional d.o.f. (1), and the *general* approach – the unknown values of selected function derivatives are used as the additional d.o.f.

$$\sum_{j(i)} c_j u_j = \sum_{j(i)} \alpha_j u_j^{(k)} \quad (2)$$



**Fig. 1.** Solution convergence for the multipoint method, the standard MFDM, and the FEM (Poisson's BVP with the different right-hand side)

Although the specific formulation is simpler and easier in implementation, its application is more restricted, mainly to the linear boundary value problem (BVP) posed in the strong formulation. The general formulation [2] is more complex but it can be used for all types of the BVP, including nonlinear ones, and all types of problem formulation – strong (local), weak (global), and mixed (global-local, MLPG). The global relation between the additional d.o.f. (unknown  $k$ -th order derivatives) and the basic ones

$$\mathbf{U}^{(k)} = \mathbf{A}\mathbf{U}, \quad (3)$$

which follows from the multipoint general FD operator (2), is the key feature of the general version. Here  $\mathbf{A}$  – is the coefficient matrix.

Having found such dependencies for any derivative emerging in the considered BVP, any differential equation can be approximated. In this way, the general multipoint approach can be considered as a tool for solving a wide class of engineering problems.

## 2.2 The basic steps of the multipoint MFDM analysis

The basic multipoint MFDM algorithm (described in detail in [2, 3]) is based on the meshless FDM scheme [4] and consists of the several steps (Fig. 2), which are listed below with some comments:

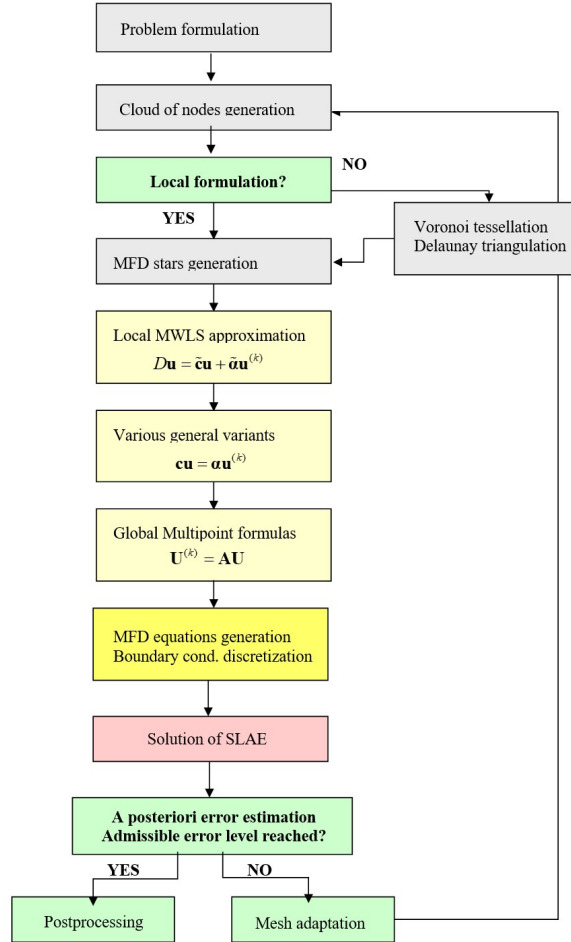
### Selection of the appropriate boundary value problem formulation:

local (strong), global (weak), or global-local (e.g. MLPG [6]). Global formulation may be posed in the problem domain  $\Omega$  as the following variational principle

$$b(v, u) = l(v), \quad \forall v \in V \quad (4)$$

as well as minimization of the energy functional given in the general form.

In the weak formulation (4), the trial  $u$  (searched problem solution) and test  $v$  function may be the same – it is the Bubnov-Galerkin approach, or different from each other – the Petrov-Galerkin one. In the last case, the multipoint method may be used also with various mixed global-local problem formulations. The MLPG5 (Meshless Local Petrov-Galerkin) global-local formulation [6], due to the use Heaviside-type test function may be computationally more efficient than the other formulations.



**Fig. 2.** The flow chart of the multipoint MFDM algorithm

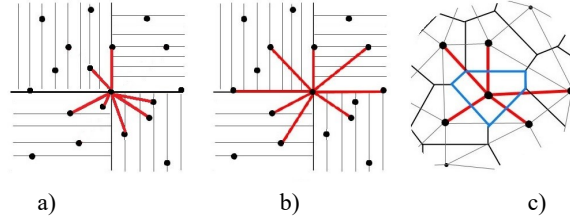
### Domain discretization

- nodes generation (e.g. by applying Netgen [8], or the Liszka's type generator [7]);
- domain partition by Voronoi tessellation and Delaunay triangulation;
- domain topology determination (neighborhoods).

Only a cloud of nodes is needed in the case of local problem formulation. For global or global-local formulation, the integration and, consequently, the integration cells, like Voronoi polygons (subdomains assigned to individual nodes) [9] or Delaunay triangles, are needed.

### Optimal MFD star (stencil) generation

The MFD star (stencil) is the basis of the MWLS approximation and can be generated by using various criteria (Fig. 3), like the nearest distance (the simplest one), the cross (the optimal one), or the Voronoi neighbors criterion (best, but more complex) [4, 9].



**Fig. 3.** Stencil criteria in 2D: a) nearest distance, b) cross criterion, c) the Voronoi neighbors

### Local approximation by moving weighted least squares (MWLS) method

The important part of the multipoint MFD algorithm is the computation of the FD operators using MWLS approximation. Construction of the local (based on the stencil) function approximation is performed by assuming appropriate d.o.f. at stencil nodes. The Taylor polynomial of degree  $p$  is considered in the MFD [3, 4] as the basis function. Minimization of the weighted error functional  $\partial J / \partial \{D\mathbf{u}\} = \mathbf{0}$  yields at each node the local multipoint MFD formulas for a set of derivatives  $D\mathbf{u} = D\mathbf{u}_i = \{u_i, u'_i, u''_i, \dots, u_i^{(p)}\}$  and finally for the local basic operators (2).

### Generation of the multipoint difference formulas

Simultaneous equations  $\mathbf{C}\mathbf{u} = \mathbf{a}\mathbf{u}^{(k)}$  are generated in the whole domain  $\Omega$  afterward. For the nonlinear problems or problems posed in global formulation, the approximation of unknown function  $u$  and its derivatives are provided by the *general* multipoint technique only. Several variants of the general multipoint approach may be used [2]. Finally, the solution provides the relation (3) formula for each  $k = 1, \dots, n$  derivative.

### Generation of the MFD simultaneous equations

Having found the FD formula (3) in the whole domain for all derivatives emerging in the considered BVP, these relations are applied to the given problem. After such discretization PDE depends on the primary unknowns  $u$  only.

### Solution of the system of linear algebraic equations (SLAE)

#### Error estimation

In general, the error  $e$  of the obtained solution  $u$  is evaluated by the exact (analytical) one  $u^E$  (benchmark tests only):  $e = u^E - u$ ; or in the case when it is unknown, by applying an improved solution  $u^H$  as the reference one  $e^H = u^H - u$ .

Due to the high quality of the multipoint result, it can be used to calculate the reference solution needed for a posteriori error estimation [12]. The  $p$ -type error analysis can be performed by comparison of the multipoint higher order solution with the one obtained by the second order MFD. The error analysis may be applied for two purposes: an examination of the solution quality and, if required, the mesh refinement. The mesh can be easily locally modified by moving existing or entering new nodes, which is simpler in the meshless methods than in the FEM.

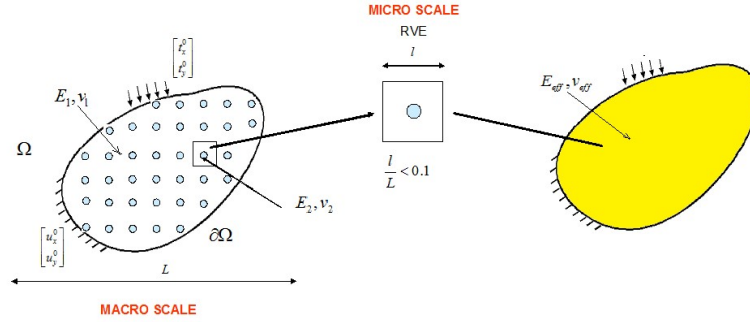
### Postprocessing of the results

At the postprocessing stage, after the nodal values of the displacement are obtained, the strains and stresses are evaluated. The advantage of the MFD-based methods is that difference formulas are generated at once for the full set of derivatives  $D\mathbf{u}$ , and the

characteristic feature of the multipoint general case is the relation between the unknown function and its derivative (3). All derivative operators depend on the domain discretization only. Therefore, the stress and strain fields can be easily calculated by using coefficient matrices (3).

### 3 Multipoint approach in the two-scale analysis of heterogeneous materials

The higher order multipoint approach may be applied at the macro as well as the micro levels in the procedure of homogenization [11, 13] (Fig. 4). At the macro level, the heterogeneous material with a periodic distribution of inclusions was considered. The values of the effective material constants were determined for a single representative volumetric element RVE with defined material parameters for the matrix and inclusions.



**Fig. 4.** Formulation of the homogenization problem

At the macro level, the problem for a heterogeneous or porous material may be posed in both weak and strong formulation, instead at the micro RVE level, the variational form (4) of the linear elasticity problem was assumed. In general, the homogenization solution approach based on two separate scales consists of the following steps [10]:

#### *Discretization of the domain*

- initial mesh generation for both – the macro and microstructures;
- selection of the points at the macroscale (typically the Gauss points), for which the effective parameters will be evaluated at the microscale;
- determination of type and size of the RVE.

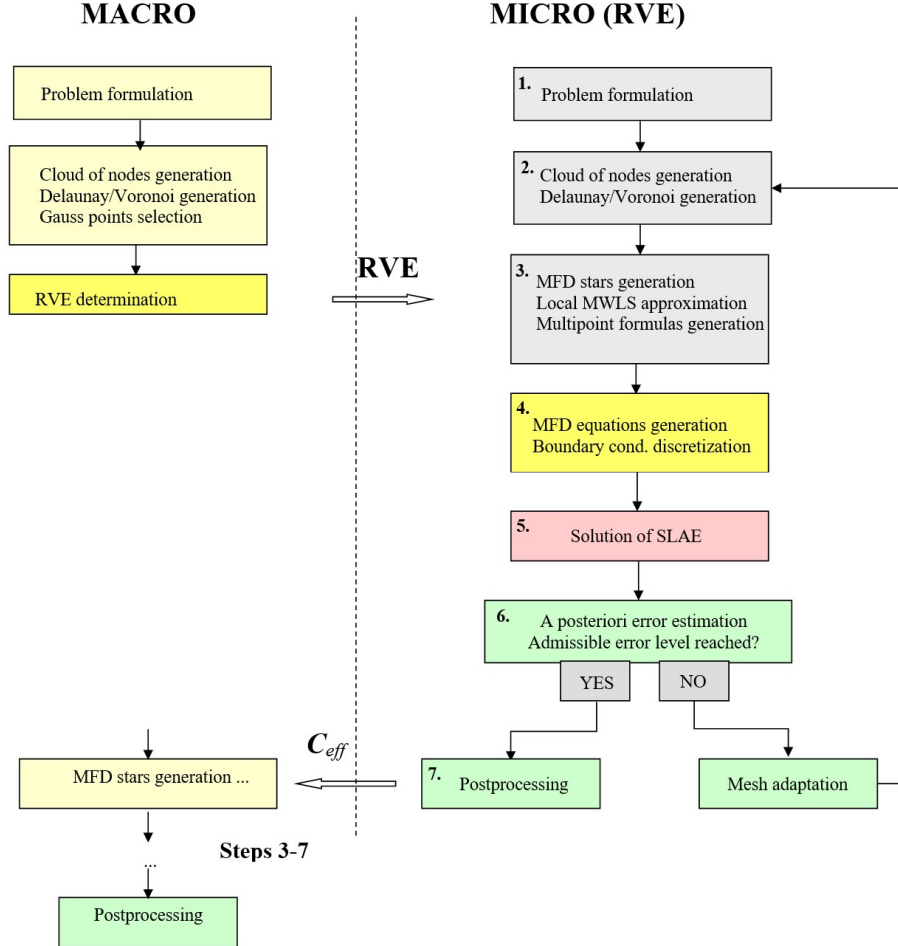
#### *Microscale analysis*

- solution of the BVP at the RVE;
- computation of the effective material tensor  $C_{\text{eff}}$ ;
- verification of the multiscale analysis;
- error estimation.

#### *Transfer of the homogenized effective parameters to Gauss points at the macrostructure*

#### *Macroscale problem solution*

#### *Postprocessing and error estimation.*



**Fig. 5.** The numerical homogenization algorithm

The multipoint approach to computational homogenization was developed and described in detail in the article [11] taking into account the characteristic features of the method. The homogenization algorithm is presented in Fig. 5 with some comments added below.

Steps 3-7 (Fig. 5) regard both the macro and micro levels but have different details:

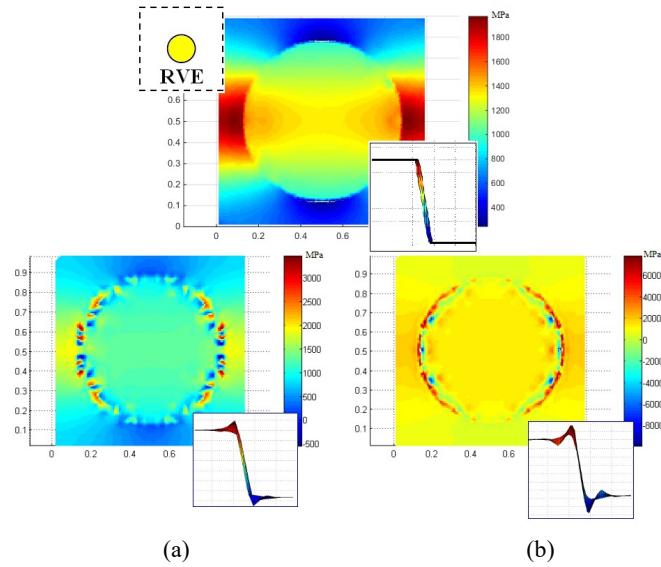
- At the macrostructure level, the selected *formulation* depends on the solved problem. At the micro level – the variational formulation (global or global-local) was assumed instead.
- On the *discretization* stage, the quality of the mesh (density, distribution of nodes) for the macrostructure is not so important and mostly depends on the geometry of the domain and solved problem. The RVE mesh may be generated either independently on the inclusion distribution or may be adjusted to them. In the latter case, a better

result is expected, but such influence is not very significant for sufficiently fine mesh [11].

- *Selection and generation of the stencils* (MFD stars) for the local approximation is very important in the RVE domain of the multiscale problem. The stencils should be adjusted to the inclusion distribution [11]. It is significant due to the oscillations phenomenon occurring near the inclusion boundary in another case (Fig. 6). Their amplitude was significantly influenced by the Gauss point number used for numerical integration. To generate the optimal stencils adjusted to the inclusion, the nearest criterion (the simplest one) or the Voronoi neighbors (more complex) stencil generation have to be applied. Although the asymmetrical stencils cause a slightly worse approximation quality, they allow obtaining good results at the inclusion boundary.

Inside the domain – at the main matrix of heterogeneous material or subdomains of inclusions, the best choice is to use the cross criterion due to its simplicity.

- In the case of local formulation (macrostructure) only trial function  $u$  has to be *approximated* by the MWLS method. In the weak formulation (the microscale), the Petrov-Galerkin approach (the trial  $u$  and test  $v$  function are different) was applied. The trial function  $u$  and its derivatives were approximated by the multipoint meshless FDM. The test function  $v$  and its derivatives at Gauss points can be calculated by the MWLS approximation based on the same stencils as  $u$ , or by simple interpolation on the integration subdomain, e.g. Delaunay triangle. In the preliminary tests, the type and order of approximation of test function  $v$  do not influence on results.



**Fig. 6.** Stress  $\sigma_{xx}$  : stencils adapted to the inclusion;  
stencils do not correspond to the inclusion with 1(a) and 3(b) Gauss point

- Various versions of the general multipoint case can be applied for *difference formulas generation* [2]. The best way due to the necessity of adjusting the stencil to the



inclusion at the RVE is version 4-”XY”, where  $u_{,x}$  as well as  $u_{,y}$  derivatives are used as the additional d.o.f. in the Multipoint FD operator.

- For the local problem formulation (in the macroscale only), the *system of difference equations is generated* by the collocation technique. The *numerical integration* is additionally required in the case of the global formulation. Simultaneous algebraic equations are generated directly from the variational principle (5) by aggregation from each integration cell (Delaunay triangle or Voronoi polygon, which could be different from the test or trial function subdomains) and taking into account the multipoint FD operators.
- At the *postprocessing* stage the strain and stress volume averages can be evaluated and the effective values of the material parameter tensor  $\mathbf{C}_{eff}$  are calculated.

The preliminary comparison of the effective material constants calculated by the MFDM algorithm, with the ones obtained by the FEM [17] as presented in Fig. 7, shows a more stable solution process in the case of the MFDM.

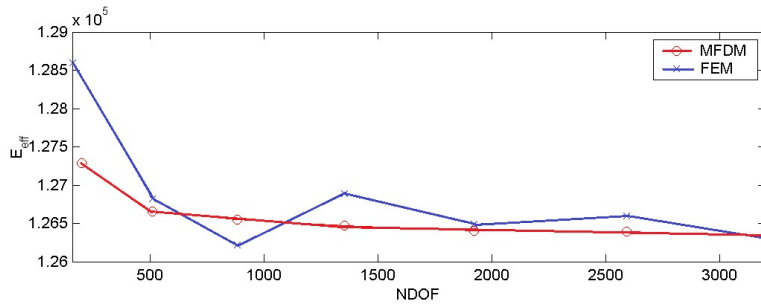


Fig. 7. Convergence of the effective Young's modulus obtained by the FEM and MFDM

#### 4 The nonlinear analysis by the Multipoint MFDM

The multipoint MFDM has also been developed for the analysis of geometrically and physically nonlinear problems [14]. The strategy of the multipoint method for nonlinear analysis consists of the same parts as in the case of the linear BVP described above and several additional steps related to nonlinearity. The whole algorithm may be divided into two stages.

The initial one concerns the calculation of the primary derivative relations of type (3) in the whole domain. The higher order and mixed derivative dependencies (3) can be obtained from the first order derivatives by the formulae composition approach as is shown in the following examples

$$\mathbf{u}_{,x} = \mathbf{A}\mathbf{u}, \quad \mathbf{u}_{,y} = \mathbf{B}\mathbf{u} \quad \Rightarrow \quad \mathbf{u}_{,xx} = \mathbf{A}^2\mathbf{u}, \quad \mathbf{u}_{,xy} = \mathbf{A}\mathbf{B}\mathbf{u}, \quad \mathbf{u}_{,yy} = \mathbf{B}^2\mathbf{u}, \quad \mathbf{u}_{,xyy} = \mathbf{A}^2\mathbf{B}\mathbf{u}$$

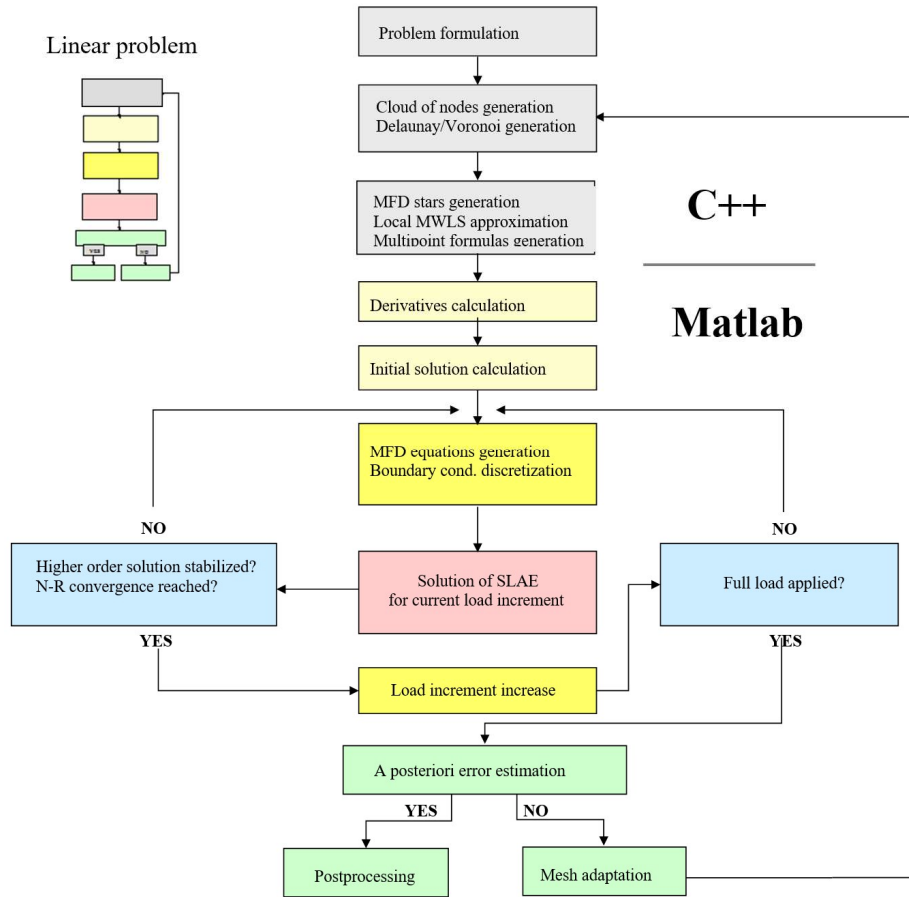
The process of the calculation of the primary derivatives in the general multipoint approach is quite complex and computationally demanding [2], but it does not depend on the analyzed problem. Moreover, the relations (3) have to be computed only once for

the assumed domain and discretization. This first part of the algorithm can be implemented in C++ or Fortran environment to obtain the coefficient matrices optimally.

Having found the global multipoint coefficient matrices for derivatives, the relations (3) can be applied to the given BVP in the second part of the algorithm. This part, strictly related to the analyzed nonlinear problem, may be easily computed in, e.g. Matlab environment. Due to its matrix-oriented programming language and extended graphic possibilities, Matlab is a perfect tool for this purpose. Besides the optimization of the computational time, this partitioning is especially useful for engineering tasks, where problem formulation may be changed but the discretization remains the same.

The nonlinear algorithm is based on the key features of the MFD and especially of the higher order multipoint method. First of all, it is the independence of the FD operators from the problem formulation. Using this feature, the nonlinear problem formulation PDE may be easily rewritten in terms of unknown function only.

The Multipoint meshless FDM solution algorithm is presented in the flowchart (Fig. 8).



**Fig. 8.** The flow chart of the nonlinear analysis algorithm

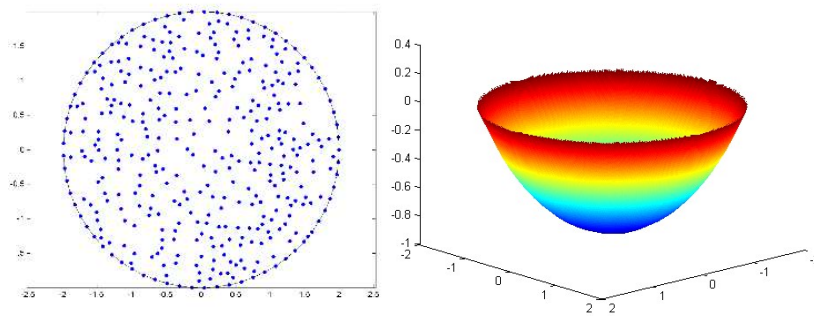
#### 4.1 Geometrically nonlinear problems

Obtained by the multipoint general approach simultaneous nonlinear algebraic equations can be solved by using an iterative technique. The most commonly applied procedure for this purpose is the Newton–Raphson method. The Jacobian tangent matrix on each iteration step has to be evaluated by the formula

$$\frac{\partial F_i}{\partial u_j} = \frac{\partial F_i}{\partial u_k} \frac{\partial u_k}{\partial u_j} + \frac{\partial F_i}{\partial u_k} \frac{(\partial u_x)_k}{(\partial u_x)_k} \frac{\partial F_i}{\partial u_j} + \frac{\partial F_i}{\partial u_k} \frac{(\partial u_y)_k}{(\partial u_y)_k} \frac{\partial F_i}{\partial u_j} + \dots$$

The first part of the Jacobian matrix ( $\partial F_i / \partial u_j^{(s)}$ ,  $s = 0, 1, \dots$ ) may be analytically calculated, e.g. by using the symbolic differentiation, while the second part (the derivatives  $\partial u_j^{(s)} / \partial u_i$ ) is evaluated numerically only once for the discretization. Appropriate multipoint difference operators (3) generated for the set of the partial derivatives can be used here. For example, if  $\mathbf{u}_x = \mathbf{A}\mathbf{u}$ ,  $\mathbf{u}_y = \mathbf{B}\mathbf{u}$ , then  $\frac{\partial \mathbf{u}}{\partial \mathbf{u}} = \mathbf{I}$ ,  $\frac{\partial \mathbf{u}_x}{\partial \mathbf{u}} = \mathbf{A}$ ,  $\frac{\partial \mathbf{u}_y}{\partial \mathbf{u}} = \mathbf{B}$ , where  $\mathbf{A}$  and  $\mathbf{B}$  – are the FD coefficient matrices,  $\mathbf{I}$  is the identity matrix. In this way, the calculation time can be significantly reduced.

Several simple benchmarks and nonlinear engineering problems, including the deflections of the ideal membrane and analysis of the large deflection of plates using the von Karman plate theory, were tested. Two iterative approaches were used – the simple one using the staggered scheme (4<sup>th</sup> order von Karman problem), and the Newton–Raphson (NR) iterative scheme. The ideal membrane deflections problem was solved by the incremental-iterative approach and the NR method. Despite a fully random irregular cloud of nodes assumed, a high quality almost axially symmetric solution was obtained (Fig. 9). The 14 pressure increments and only 73 iteration steps were needed to reach the required level of the error (assumed  $10^{-12}$ ) by the 3<sup>rd</sup> order general multipoint approach. It is a very encouraging result. The standard MFDM (using relaxation modification of NR algorithm [15]) requires twice more iteration steps to reach the appropriate level of error.



**Fig. 9.** Random irregular mesh and numerical solution for ideal membrane deflection

## 4.2 Physically nonlinear problems

In the case of physically nonlinear problems in elastic-plastic analysis, the iterative procedure may lead to increased errors in the neighborhood of the elastic-plastic interface, and the incremental-iterative approach is especially useful. The multipoint operators can be calculated only once at the initially assumed discretization, or the solution may be improved by using the adaptation process [16, 17] based on the error estimation near the elastic-plastic boundary.

The oscillation problem similar to the situation in the homogenization analysis was expected to occur in the physically nonlinear analysis along the elastic-plastic boundary. However, the preliminary numerical results do not demonstrate the oscillations. This can be due to the different types of problem formulation (the weak one in the numerical homogenization), might be related to the type of discontinuity or other discretization factors, and needs further investigation.

The additional part of the nonlinear strategy in the case of elastic-plastic analysis is presented in the scheme (Fig. 10)

The physically nonlinear de Saint-Venant's problem of a prismatic bar elastic-plastic torsion has been analyzed by the multipoint MFDM and outlined in the paper [14]. The boundary between elastic and plastic parts was determined by using the Nadai “roof” approach [18]. The problem was solved by the Newton-Raphson method. In Fig. 11 (b) the elastic-plastic boundaries for various increasing loads  $\theta$  of square-shape cross-section bar are presented. The Prandtl stress function of the torsional problem is depicted in Fig. 11(a).

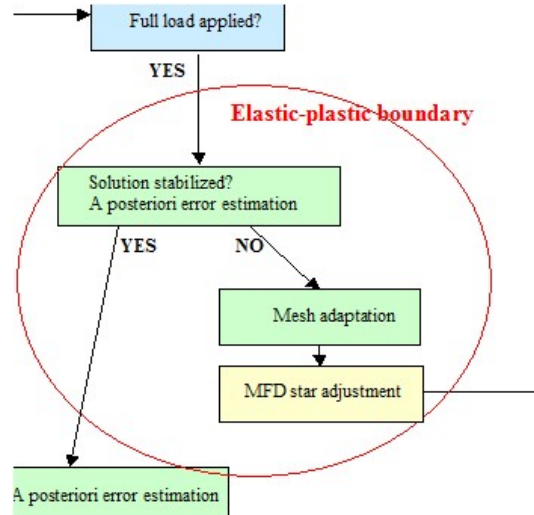
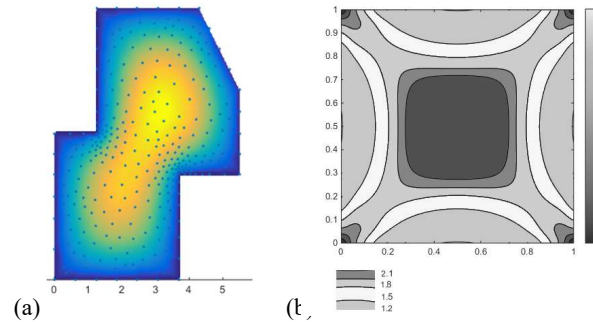


Fig. 10. An additional part of the multipoint nonlinear strategy for elastic-plastic analysis



**Fig. 11.** Prismatic bar torsion: (a) the Prandtl stress function for polygon cross-section; (b) elasto-plastic boundaries of the square cross-section for loads  $\theta = 1.2, 1.5, 1.8$  and  $2.1$

## 5 Final remarks

The paper introduces the application schemes of the new higher order multipoint meshless method for more demanding engineering problems such as numerical homogenization and nonlinear analysis. The appropriate algorithms were developed, characteristic features of the method application for particular types of engineering problems were examined, and necessary procedures were written and tested.

Like the other methods, the multipoint meshless approach has its advantages and disadvantages. They were examined, tested, and analyzed. The following characteristic features belong to the advantages of the multipoint method application to the analyzed problems:

- the possibility of using various formulations of BVP (weak, strong, mixed);
- modification and adaptation of whole mesh or only part of them without difficulties;
- higher order approximation and improved precision of the obtained solution on the arbitrarily irregular meshes, which allows for decreased number of nodes;
- the difference operators for the particular derivatives are generated besides the solution at once without additional computational cost;
- the multipoint FD operators depend on the domain discretization rather than on the analyzed specific problem;
- convergence rate of solution derivatives has the same order as it is for the solution itself (phenomena of “superconvergence”);
- the general approach of the multipoint MFDM allows for the analysis of various problems including nonlinear ones;
- in nonlinear analysis – computationally more efficient updating and evaluation of the tangent matrices needed in iteration approach;
- the multipoint solution may be used as the improved reference solution instead of the true analytical one for a posteriori error estimation.

In subsequent research, it is planned to combine both the nonlinear analysis and heterogeneous material homogenization and apply it for numerical modeling in e.g. concrete mechanics.

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