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ON APPLICATION OF THE MESHLESS FINITE DIFFERENCE METHOD TO NUMERICAL HOMOGENIZATION

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Abstract. *The most commonly used engineering tool for numerical analysis of variety of the heterogeneous materials is the Finite Element Method (FEM). However, this paper focuses on the alternative approach based upon the Meshless Finite Difference Method (MFDM). The purpose of the work is to present the some features, as well as the selected results of the numerical homogenization problem in terms of the Meshless FDM.*

The MFDM solution approach and its higher order extensions, e.g. the Multipont meshless method, may be used at both – the macro and the micro levels in the two-scale analysis of heterogeneous materials. The Multipoint MFDM concept is based on raising the order of approximation of the unknown function by introducing additional degrees of freedom in the stencil nodes, taking into account e.g. the right hand side of the considered differential equation. It improves the FD solution without increasing the number of nodes in the mesh and may also be used for a posteriori error estimation of the results.

At the macro level of two-scale modeling, the heterogeneous material with the inclusions spaced periodically was assumed. The values of effective material constants were determined by the homogeneous equivalents calculated at the micro level for a single representative volume element (RVE). The various types of the inclusion locations in the RVE were tested. The scope of numerical analysis also includes the examination of the influence of some factors on solution quality based on the MFDM and the higher order Multipoint MFDM approaches.

All results obtained so far are encouraging. However, it is only the early stage of the research. Further research is planned.

1 INTRODUCTION

Most of the innovative materials, such as composite and structural ones, as well as numerous natural materials have heterogeneous structure. Therefore, prediction of the mechanical properties of those materials is the important part of many fields of engineering, among them the mechanical and civil ones. Various homogenization approaches have been developed last years [2, 3, 4, 10, 13] to obtain the overall properties of heterogeneous materials and to simplify the analysis of engineering problems.

One of the popular multiscale technique provides overall behavior of the heterogeneous materials from known properties of their constituents e.g. fiber or inclusion and matrix through an analysis of a periodic single representative volume element (RVE) at the micro level. At the macro level, on the other hand, the heterogeneous structure of the composite material is replaced by a homogeneous equivalent obtained from RVE.

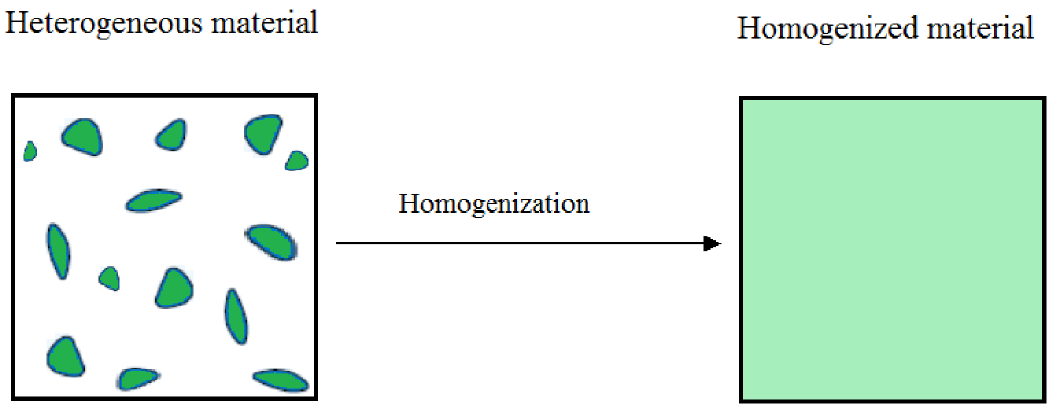


Figure 1: The homogenization approach

There are several methods used for the analysis of heterogeneous materials. The Finite Element Method (FEM) is the most commonly used engineering tool to analyze multiscale problem at both, the macro and the micro levels.

However, this paper focuses on the alternative approach based upon the Meshless Finite Difference Method (MFDM) [6, 12]. The purpose of the work is to present the formulation, as well as the some features and selected results of the numerical homogenization problem in terms of the Meshless FDM and its higher order modification – the Multipoint MFDM.

2 MESHLESS FDM AND MULTIPOINT MFDM APPROACHES

The meshless FDM solution approach [9, 12] and its higher order extensions [6, 11], e.g. the Multipont meshless method [5, 6], may be used at the macro and the micro levels in the two-scale analysis of heterogeneous materials [8, 11]. When compared with the finite element approach, the meshless methods may deal with the unstructured, totally irregular cloud of nodes rather than on elements. In the meshless FDM the local function approximation is built in terms of nodes only. In general, the location and density of nodes depend on the geometry and the physics of the given problem. Consequently, the MFDM allows to avoid the difficulties encountered in the traditional FE technique, such as time-consuming process of generation of the mesh of complex geometries, remeshing, and mesh distortions in large deformation problems.

The basic Meshless (Generalized) FDM scheme [12] consists of the several steps, which are listed below:

- selection of the appropriate boundary value problem formulation: local (strong), global (weak, e.g. variational) , or global-local (e.g. MLPG [1, 7]);
- domain discretization:
  - nodes generation (e.g. by applying the Liszka's type generator [9] based on the nodes density control),
  - domain partition by Voronoi tessellation and Delaunay triangulation,
  - domain topology determination (neighbourhoods);
- optimal stencil (MFD star) selection and generation;
- local approximation by moving weighted least squares (MWLS) method;
- generation of the difference formulas;
- discretization of the boundary conditions;
- generation and solution of the MFD simultaneous equations;
- postprocessing of the results.

The basic MFDM approach has been extended recently to the higher order Multipoint Meshless FDM [5, 6, 7].

The Multipoint MFDM concept is based on raising the order of approximation of the unknown function by introducing additional degrees of freedom in the stencil nodes, taking into account e.g. the right hand side of the considered differential equation (so-called the *specific* approach), or nodal derivatives (the *general* approach). In this way, in the multipoint MFD operators, the combination of values of searched function is equal to the combination of values of additional d.o.f. at all stencil nodes. It improves the FD solution quality without increasing the number of nodes in the mesh.

Let us consider the boundary value problem given in the domain Ω for the n-th order PDE in local (strong) formulation: $\mathcal{L}u = f$ with b.c. $\mathcal{G}u = g$, where $\mathcal{L}, \mathcal{G}$ are differential operators; or in equivalent global (weak) one formulated e.g. as a variational principle: $b(u, v) = l(v), \quad \forall\ v \in V$, where b – is a bilinear functional dependent on the test function v and solution u, V – is the space of test functions, l – is a linear form dependent on v.

In the MFDM solution approach, the standard difference operator based on MFD star may be presented in the following form

$$\mathcal{L}u_i \approx Lu_i \qquad \Rightarrow \quad Lu_i = f_i \qquad \sum_j c_{ij} u_j = f_i \,. \tag{1}$$

In the multipoint formulation, the MFDM difference operator Lu is obtained by using the Taylor series expansion of unknown function u including the higher order derivatives, and using additional degrees of freedom at nodes [6]. Instead of the function value at the *central node only*, one may apply e.g. a combination of the right-hand side values of the considered equation (specific case, eq.(2)), or nodal derivatives (general case [5], eq. (3)) *at any node* of MFD star.

$$\mathcal{L}u_i \approx Lu_i \qquad \Rightarrow \quad Lu_i = Mf_i \qquad \sum_j c_{ij} u_j = \sum_j \alpha_{ij} f_j \tag{2}$$

$$\sum_j c_{ij} u_j = \sum_j \alpha_{ij} u_j^{(k)} \tag{3}$$

The following denotations have been assumed here: j – number of a node in a selected stencil, Mf_i – a combination of additional d.o.f. In general, L may be either referred to the left side of differential eqs or to the integrand in the global formulation of b.v. problem, and to the boundary conditions.

The main feature of the multipoint MFDM general case is the relation between the additional d.o.f. (k-th derivative values) and the basic ones (searched function u values) in the whole domain Ω. The required number of such relations for N-dimensional problem can be reduced to N, calculated only the first derivative relations. The higher order derivatives may be developed next using the formulae composition approach. In this way, the general formulation may be used for all types of b.v. problems including the nonlinear one.

3 APPLICATION OF THE MFDM AND ITS EXTENSION TO HOMOGENIZATION

A heterogeneous elastic material with the inclusions spaced periodically was assumed. The length l of the micro scale is assumed to much smaller than the characteristic length L of the macro domain. The macro scale constitutive behaviour is determined by analysis of an RVE subjected to three types (in 2D) of boundary conditions [2, 13]. These numerical tests enable computation of all entries of the homogenized tensor of material properties.

3.1 Formulation at the macro scale

The macro scale problem of the plane stress analysis consists of finding the displacement field $\boldsymbol{u}_0$, as well as the stress $\boldsymbol{\sigma}_0$ and the strain $\boldsymbol{\varepsilon}_0$.

The b.v. problem at the macro level is defined as follows:

$$\begin{cases} \operatorname{div}\boldsymbol{\sigma}_0 = -\boldsymbol{f} & \text{in } \Omega \\ \boldsymbol{\sigma}_0 = \boldsymbol{C}\boldsymbol{\varepsilon}_0 & \text{in } \Omega \\ \boldsymbol{\varepsilon}_0 = \operatorname{sym}\left(\nabla \boldsymbol{u}_0\right) & \\ + \text{boundary conditions} & \end{cases}, \tag{4}$$

where $\boldsymbol{C}$ denotes the matrix of elastic effective material parameters, $\boldsymbol{f}$ **–** is the field of body forces.

3.2 Formulation at the micro scale

The plane stress analysis is carried out at the micro scale defined over RVE. The boundary value problem on the RVE level may be defined as follows.

The equilibrium state equation is assumed

$$\operatorname{div}\boldsymbol{\sigma} = 0 \qquad \text{in } \Omega\,. \tag{5}$$

The symmetric stress $\boldsymbol{\sigma}$ is related to the strain $\boldsymbol{\varepsilon}$ by the Hook's low

$$\boldsymbol{\sigma} = \boldsymbol{c}\boldsymbol{\varepsilon} \qquad \text{in } \Omega \tag{6}$$

where $\boldsymbol{c}(x,y)$ denotes the tensor of elastic material parameters and $\boldsymbol{\varepsilon} = \operatorname{sym}\left(\nabla \boldsymbol{u}\right)$ is the strain.

The Dirichlet boundary conditions

$$\boldsymbol{u} = \boldsymbol{u}^0 \qquad \text{on } \partial\Omega_u \tag{7}$$

were assumed for the displacement $\boldsymbol{u}$ to model tension in two directions as well as shearing of the RVE.

Effective material properties are determined by using volume average of the stress $<\boldsymbol{\sigma}>$ and the strain $<\boldsymbol{\varepsilon}>$

$$\langle \boldsymbol{\sigma} \rangle = \boldsymbol{C} \langle \boldsymbol{\varepsilon} \rangle , \tag{8}$$

which provide nine equations with nine unknowns.

3.3 Numerical homogenization based on the MFDM approach

The numerical analysis has been based on the discretization of macro and micro structures in terms of the meshless FDM. To define the overall properties of the heterogeneous materials a variational-based approach has been assumed. The MFDM discretization may be based on any irregular clouds of nodes without any imposed structure, like in the FEM, or regularity rule, like in the standard FDM. The cloud of approximation nodes for the RVE may be generated either independently on the inclusions distribution or may be adjusted to them.

The next principles in the application of the MFDM and its higher order extensions to the numerical homogenization are assumed [7]:

- In case of FEM, both the trial u and the test v functions are approximated by means of the same basis functions (Bubnov-Galerkin approach). In case of MFDM, two different bases (Petrov-Galerkin approach) may be applied;
- The approximation of unknown function u and its derivatives is provided by the appropriate meshless FD (1) or multipoint MFD (3) operators;
- In case of the weak formulation the numerical integration is additionally required in the MFDM approach. It is performed by the Gauss qudrature on subdomains such as the Delaunay triangles (integration between nodes) or Voronoi polygons (integration around nodes);
- The values of the test function v and its derivatives at Gauss point P_k are calculated by MWLS approximation based on the MFD star, or interpolation based on integration subdomain

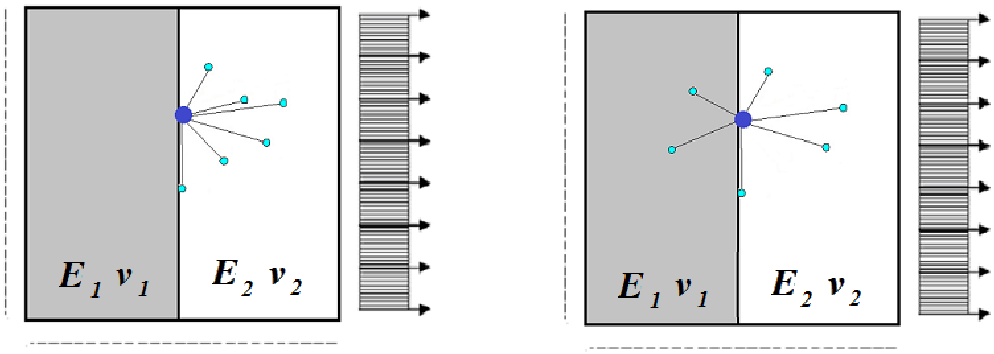
$$v(P_k) \approx \sum_j b_{j(k)} v_j \,, \qquad v_x\big|_{P_k} \approx \sum_j {}^{x}b_{j(k)} v_j \,, \qquad v_y\big|_{P_k} \approx \sum_j {}^{y}b_{j(k)} v_j \,. \tag{9}$$

The simultaneous equations are generated directly from the variational principle by aggregation (from each integration cell), and taking into account MFD or multipoint MFD operators [8]. After obtaining the nodal values of the displacement u_x and u_y, the effective values of the material parameters $\boldsymbol{C}$ may be evaluated by solving eq.(8).

4 SOME NUMERICAL RESULTS

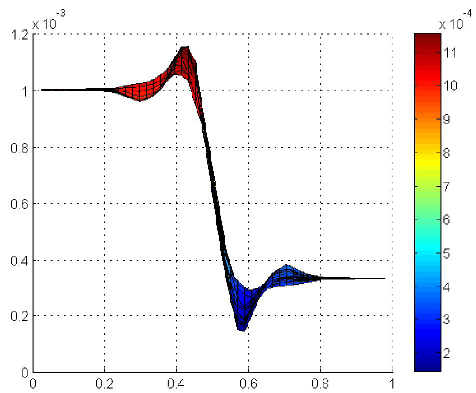
The 2D linear elasticity problem for two-phase composite material is considered in order to verify the numerical homogenisation by meshless FDM and multipoint MFDM solution approaches. The micro scale model is set up based on the RVE technique.

For the first simple benchmark test of MFD star configuration influence, the RVE with two equal part is assumed (Fig. 2). The elastic modules and Poisson's ratios for the left rectangular part are assumed as $E_1 = 1 \cdot 10^5$ MPa, $\nu_1 = 0.1$ and respectively for the right part: $E_2 = 3 \cdot 105$ MPa, $\nu_2 = 0.3$.

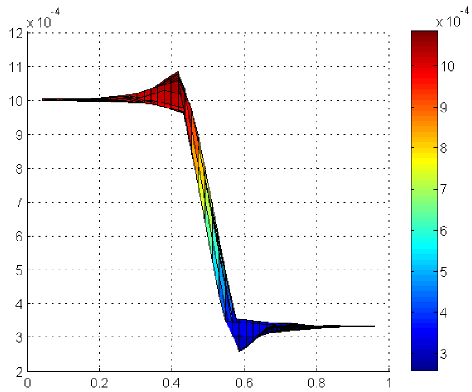


a) b)
Figure 2: The MFD star (stencil) configuration in RVE (test 1)

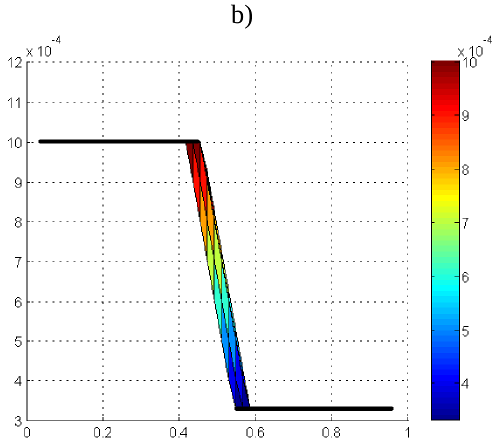
In the case, when the MFD star (stencil) configuration does not correspond to the distribution of the different material part (nodes of the stencil belong to the both type of material, Fig.2b), some oscillations near the boundary of inclusion are observed (Fig. 3a,b). The number of Gauss points in the e.g. Delaunay triangles, and stencil size may have an influence on the amplitude of the oscillations. However, when the MFD star is adjusted to the inclusions distribution (Fig. 2a) – the exact solution has been obtained (Fig. 3c).



a)



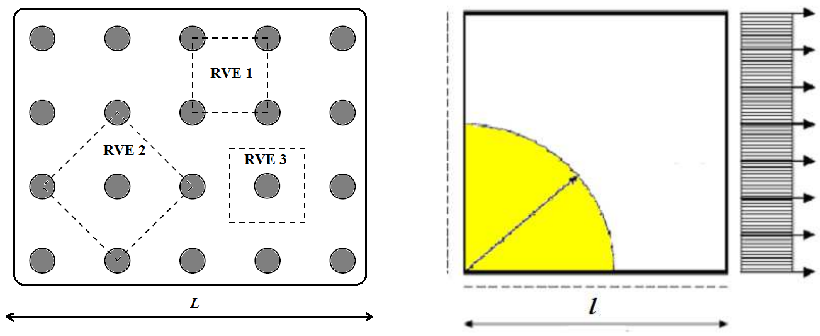
b)



c)

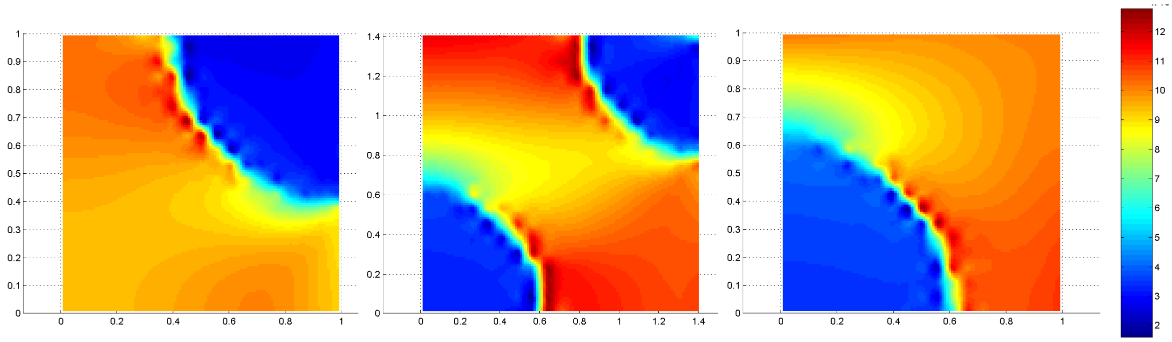
Figure 3: The strain ε_{xx} obtained by meshless FDM for test 1 in the case:
a) stencil does not correspond to the inclusion, 4 Gauss point integration; b) stencil does not correspond to the inclusion, 1 Gauss point integration; a) stencil is adjusted to the inclusion

For the second test, the structure with uniformly distributed circular inclusions with the same radii is assumed. Therefore, heterogeneous material could be represented by one of the RVE models as presented in Fig. 4a. Due to symmetric RVE models, the quarter of the RVE may be considered only. The scheme of such e.g. RVE3 with appropriative boundary conditions is presented in Fig. 4b.



a) b)
Figure 4: Distribution of the inclusions on macro (a) and micro (b) scales

In all cases, the regular uniform meshes are applied in the MFDM solution approach. Numerical results of effective material constants obtained for all types of RVE model are close enough (Fig. 5).



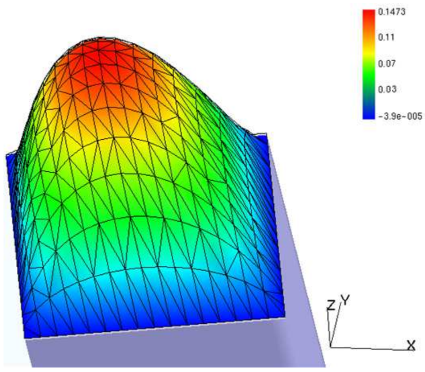
a) b) c)
Figure 5: MFDM results of strain ε_{xx} obtained for RVE1, RVE2, and RVE3

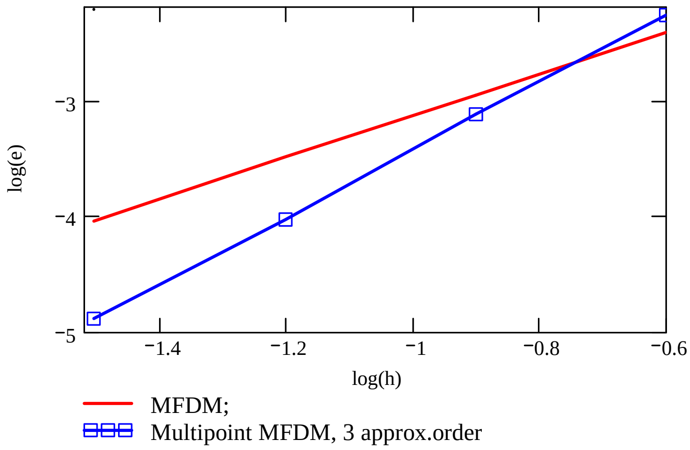
The numerical analysis may be returns to the macro scale after determination of the effective material constants (beside the elastic modulus and Poisson's ratio, the value of the Kirchhoff parameter G may be evaluated also). These effective values homogenize the original heterogeneous material. Consequently, meshless FDM or higher order multipoint solution approach may be applied, e.g. for the de Saint-Venant torsional problem of the heterogeneous prismatic bar with the rectangular cross-section assumed as the next benchmark test. The local formulation in the form of the Poisson's equation with the essential boundary conditions was applied first

$$\begin{cases} \nabla^2\Phi = -2G\theta, & \text{in} \quad \Omega \\ \Phi = 0, & \text{on} \quad \partial\Omega \end{cases}, \tag{10}$$

followed by variational form, where Φ – is the Prandtl stress function, $G\theta$ – torsional stiffness, Ω – domain of the bar cross-section.

The comparison of the MFDM and higher order multipoint MFDM convergence rates is presented in Fig. 6.





a) b)

Figure 6: Twisting of square cross-section prismatic bar: a) Prandtl stress function and b) its solution convergence rate for series of regular meshes. The exact error for the standard meshless FDM, and multipoint MFDM 3-rd approximation order

5 FINAL REMARKS

Formulation and some features of the meshless FDM and its higher order extension – the multipoint meshless FDM for the numerical homogenization problem of heterogeneous materials with periodic structure was presented. The research has been focused on the two-scale analysis based on the single representative volumetric element RVE. The stencil configuration influence was investigated. Several tests confirmed, that adjusting of the MFD star to the inclusion distribution may have an influence on the solution in terms of the meshless FDM. The effective values of the tensor of elastic material parameters were determined for the three RVE types. Results for different RVE types were compared with each other at the micro level. The analysis of the convergence results of the MFDM and multipoint MFDM at the macro level confirmed the better quality of the solution obtained by using the higher order extension of the meshless FDM.

Although obtained so far results are encouraging, it is only the early stage of the research. Therefore, further research is planned.

Acknowledgment

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