Introduction to the numerical homogenization by means of the Meshless Finite Difference Method with the Higher Order Approximation

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Abstract

Paper focuses on application of the Meshless Finite Difference Method (MFDM) solution approach and its selected extensions to the numerical homogenization of the heterogeneous material**.** The most commonly used method of computer modeling for the multiscale problem (at both the macro and micro (RVE) levels) is the Finite Element Method (FEM)**.** However, this fact does not mean that one should not search for the alternative, perhaps more efficient approaches, especially based on the meshless discretization. The aim of this paper is to present a problem formulation for numerical homogenization based on the extended algorithm of the Meshless (Generalized) FDM. The Higher Order Approximation (HOA), which is applied here, is based on the correction terms of the simple meshless difference operator. Those terms produce the improved higher order solution, without necessity of providing additional unknowns to both cloud of nodes and MFD operator. The HO solution may be used e.g. for a-posteriori error estimation of superior quality, when compared with the existing estimation techniques.
The paper is illustrated with simple tasks of 2D linear theory of elasticity, which highlight benefits of the considered approach towards more complex problems of mechanics.

Keywords: error estimation, finite element methods, finite difference methods, homogenization, meshless methods, multiscale problems, higher order approximation

1. Introduction

The most commonly applied computational method for numerical analysis of the multiscale problems is the Finite Element Method FEM [1]. However, searching for new alternative approaches is still justified. Especially investigated here is the solution approach based upon the meshless discretization. The aim of this work is the presentation of the homogenization problem formulations [1], based on the solution algorithm of the Meshless (Generalized) Finite Difference Method (MFDM, [2]). Its testing on simple 2D problems of the linear elasticity as well as signalization of its benefits in more complex problems of mechanics are also considered.

In the first part of the paper, presented are features of the basic MFDM algorithm for analysis of the boundary value problems of mechanics. Highlighted are those steps of the algorithm, which significantly differ from the element-based formulation and are typical for the MFDM solution approach. In addition, some generalizations and extensions will be presented, which are the result of the scientific work in the recent years (higher order approximation, a-posteriori solution error estimation, adaptation techniques, the estimation of the solution convergence).

Though the meshless formulation of the homogenization problem is general, numerical analysis was carried out here only for the selected group of 2D mechanical problems. The following assumptions were adopted:

- heterogeneity of the material is periodic,
- determination of the effective material constants (Young modulus E for the tensile test and Kirchhoff modulus G for the shear test) is performed only once at the micro-level, regardless of the subsequent numerical analysis at the macro level,
- materials with linear elasticity,

The scope of numerical analysis include

- the algorithm for the Higher Order MFDM [3] at the macro and micro levels, effective for any irregular groups of nodes (including also the regular meshes), generated a-priori or as a result of the analysis of adaptation approach,
- tests for various types of the heterogeneity location in the RVE,
- tests for different techniques of numerical integration in the MFDM (grid of triangles and rectangles),
- postprocessing of the nodal values with higher order approximation based on the correction terms of the meshless difference operator,
- comparison of results obtained from both the FEM (linear triangular elements and bilinear rectangular elements) and the MFDM solution approaches, on selected regular meshes and irregular clouds of nodes,
- tests on the sets of regular meshes, with the solution convergence estimation,
- tests on irregular clouds of nodes, taking into account the heterogeneous distribution of inclusions,
- comparison of the effective material values obtained after numerical homogenization with those calculated for the heterogeneous material for increasingly dense clouds of nodes, computed by means of the appropriate averaging technique.

The presentation also includes a summary of the original author's software (Matlab environment) and indication of the directions for further analysis.

2. Meshless Finite Difference Method

The basic MFDM solution approach [2] consists of several basic steps, which are listed below

- nodes generation and modification,
  - domain partition (Voronoi tessellation and Delaunay triangulation),
  - domain topology determination,
- MFD star selection and classification,
- local MWLS approximation,

- mesh generation for the numerical integration (for global formulations only),
- generation of MFD operators,
- MFD discretization of boundary conditions,
- generation and solution of MFD equations,
- postprocessing by the MWLS,

Several extensions of the basic MFDM solution approach are also investigated [3]. Among them one may distinguish

- higher order approximation, provided by correction terms of the simple MFD operator,
- a-posteriori error estimation,
- adaptive solution approach.

3. A-posteriori error estimation based on the Higher Order approximation

In several previous works [3,4], proposed was a new original concept of raising approximation order, without necessity of providing additional degrees of freedom into the simple MFD operator. Instead, considered are additional higher order terms [3], which come from the Taylor series expansion of the simple MFD operator coefficients. Besides the HO derivatives, they may also contain singularity or discontinuity terms. These HO derivatives may be calculated using appropriate formulae composition and the already known basic MFD solution. They are applied as the correction terms to this MFD operator, modifying the right hand side of the MFD equations only.

Improved HO solution may be applied in a-posteriori error estimation as the superior quality reference solution [3]. Reference solution is required in all types of estimators instead of the exact solution, unknown in the most practical cases.

HO reference solution provides error estimation of the $2p$-th order, where p denotes the basic approximation order considered and, as the opposite to the well-known estimators, it does not need so much computational effort. It may be applied in both the meshless and element-based types of domain discretizations and function approximations [4].

4. Problem formulation at the macro-level

At the macro level assumed was the heterogeneous material with rectangular cross section with the inclusions spaced periodically. Determination of the shear stresses in a twisted prismatic bar is posed in the local formulation through the Prandtl stress function F. The cross section of dimensions 0.1 m x 0.1 m is applied. The radius of a circle-shaped inclusions equal to 0.003 m provides a required separation of scales.

The heterogeneous material will be replaced by the homogeneous equivalent medium with the effective material constant (here, Kirchhoff modulus G). Its computation will be performed at the micro level (single RVE), using the tensile or the shear test. Shear test is sufficient in this case, however it limits the possible wider use of the effective parameters for the other problems of elasticity.

5. Problem formulation at the micro-level

For the testing purposes, three different locations of the inclusions in the Representive Volume Element (RVE) were considered. Assumed plane stress (shear or tensile test) of linear elastic problem is represented by a set of following equations:

- equilibrium equations (without mass forces) and the stress boundary conditions,
- constitutive equations,
- geometric equations with the displacement conditions,
- continuity equations at the border of two materials.

Both local (typical also for classical FDM) and variational formulations (typical also for the FEM) were considered here. The variational formulation is derived from the local one and additionally involves domain and boundary integrations.

6. Numerical examples

Fig.1 presents the comparison of the effective material constant (G_{eff}) for the homogeneous material with the ones averaged on the macro-level for the heterogeneous material on the set of more and more denser clouds of nodes. The effective value G_{eff} , obtained by means the MFDM analysis, proves to be very close to the averaged value of G for the heterogeneous material, obtained for the very dense cloud of nodes.

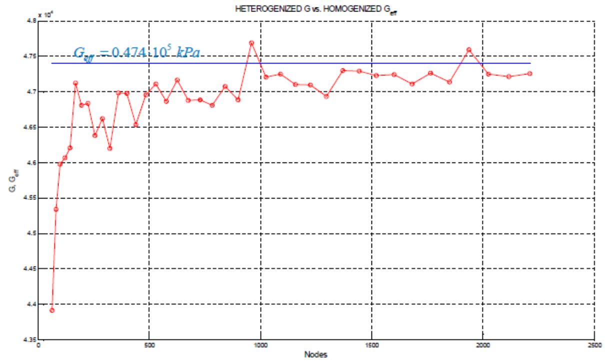

Figure 1: Comparison the average values of the shear modulus (G) for the set of more and more denser cloud of nodes with the homogenized one obtained from the RVE analysis.

7. Final remarks

All results obtained so far are very encouraging. However, it is only an interesting starting point and the very beginning of the research. The main task is the development of the meshless FDM approach for those multiscale mechanical problems, which are currently analysed by means of the FEM (e.g. 3D and non-linear problems, including plasticity). Analysis of real engineering problems is planned as well.

References

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