

## Parallel fast multipole boundary element method applied to computational homogenization

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### Abstract

In the present work, a fast multipole boundary element method (FMBEM) and parallel computer code for 3D elasticity problems was developed and applied to numerical homogenization of solid containing spherical voids. The system of equation was solved by using the GMRES iterative solver. The boundary of the body was discretized by using quadrilateral serendipity elements with adaptive numerical integration. Operations related to single iteration, performed by traversing the corresponding tree structure upwards and downwards, were parallelized by using the OpenMP standard. The assignment of tasks to threads was based on the assumption that the tree nodes at which the moment transformations are initialized can be partitioned into disjoint sets of equal or approximately equal size and assigned to the threads. The achieved speedup as a function of number of threads was examined.

*Keywords: fast multipole boundary element method, 3D linear elastostatics, computational homogenization, parallelization, OpenMP*

### 1. Introduction

The main advantage of the boundary element method (BEM) is that in many engineering problems, only discretization of boundary of the analysed domain is sufficient [1]. Also, the method is considered accurate in problems with stress concentration. In this work, a modern BEM version, the fast multipole BEM (FMBEM) is applied, that is based on the fast multipole method [3]. The method is characterized by reduced computational complexity in comparison to the conventional BEM with quadratic, or higher order order, complexity. In the FMBEM, the system of equations is solved iteratively and complexity of single iteration is linear or quasi-linear [6]. Modern computers with multi-core CPUs give possibility to parallelize computer codes. Basic approaches are parallelization by using the MPI (characterized by distributed memory) and OpenMP (characterized by shared memory) standards. In the paper [5] an MPI parallel FMBEM version was developed and applied to analysis of fiber reinforced composites on a 32-processor cluster. However, achieved speedup was not examined. In [2], FMBEM for the Laplace equation, parallelized by using OpenMP and another standard, Cluster OpenMP, that supports OpenMP and allows distributed memory computers, was presented. In the present work, an OpenMP parallelization scheme based on partitioning nodes of FMBEM tree structure is proposed. Such approach is simple to implement. In numerical example, a model of porous material, with cubic arrangement of spherical voids, is analysed and the speedup is examined.

### 2. Parallel version of the FMBEM

The idea of FMBEM is based on hierarchical clustering of collocation points and boundary elements (Figure 1) and distribution of potentials over the clusters. The clustering process is mapped with a tree structure with the whole domain corresponding to root at level 0. Tree nodes at the highest level, leaves, correspond to the smallest clusters. The potentials are integrals depending on fundamental solutions and boundary quantities -

displacements and tractions, that occur in the boundary integral equation [1, 6]. This idea is realized by the application of multipole expansions for far-field potentials. Coefficients of the expansions - multipole moments - are dependent on quantities related to clusters of integration points. Centers of the multipole moments are shifted to centers of larger groups (moment-to-moment translation, M2M) and transformed into moments of local expansion (multipole-to-local translation, M2L). Centers of the local moments are shifted to centers of smaller clusters (local-to-local translation, L2L) and to each collocation point. Near-field potentials are calculated directly as in the conventional BEM. The system of equation is solved iteratively. Single iteration involves the following operations for the calculation of matrix-vector product:

- calculation of near-field potentials by using coefficients stored in matrices, that are calculated directly,
- calculation of the multipole moments for leaves,
- M2M translations with downward pass,
- M2L translations,
- L2L translations with upward pass,
- evaluation of the boundary integrals by using the local series.

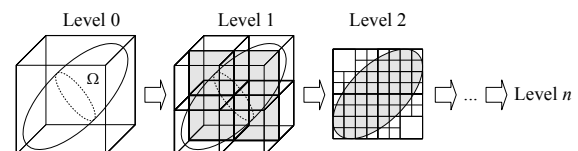


Figure 1: Clustering boundary elements and nodes

In parallel computations, the tree structure is partitioned in order to define tasks that are assigned to threads. The partitioning is realized by two lists, that are built for each thread, that

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contain pointers to nodes at which the above operations are initialized. In particular, the operations (a), (b), (c) and (f), from the previous paragraph, are performed by using the List 1 (that contains pointers to leaves), and operations (d) and (e) by using List 2 (that contains pointers to nodes on level 2). The lists and corresponding tree nodes are shown in Figure 2.

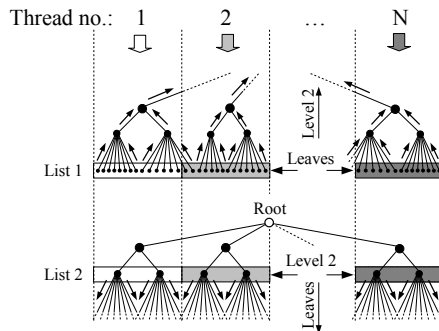


Figure 2: Moment transformation parallelization scheme

### 3. Numerical example

Computational homogenization of a solid with cubic arrangement of identical spherical cavities was considered. Representative volume element (RVE) with  $5 \times 5 \times 5$  cavities, and porosity 0.4, was modelled (Figure 3). The RVE was a cube of 1 mm edge length. The parameters of the solid material were: Young's modulus  $E = 2 \cdot 10^5$  MPa and Poisson's ratio  $\nu = 0.3$ . Each wall of the cube was divided into array of  $16 \times 16$  quadratic elements. The total number of elements of each model was equal to 13 536, the total number of nodes 40 860, and the number of DOF 122 580. The expansion degree was set to 12. The maximum number of tree level was set to 4. The GMRES tolerance was set to  $10^{-6}$ . The number of GMRES iterations was equal to 50. The analysed material is characterized by the cubic symmetry due to the arrangement of cavities, and has three independent elastic constants that can be represented e.g. by bulk modulus and two shear moduli. Full set of the constants can be computed by two homogenization tests. In this example, only one test was performed, with linear displacement boundary conditions corresponding to extension of the model along single axis [8]. The full set of computed elastic constants compared to other results can be found in [7]. The FMBEM analysis provided effective elastic constants with relative difference of few per cent in relation to analytical models. A workstation with AMD Opteron 6272 CPU, 2.10 GHz (16 cores), with 16 GB RAM was used.

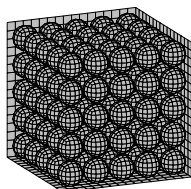


Figure 3: Interior of the discretized RVE model

In Figure 4, achieved speedup, compared to linear speedup and Amdahl's law approximation with parameter  $p = 0.96$  [4], is presented. The value of  $p$  indicates the part of the total time spent by single processor that can be done in parallel. The proposed approach is characterized by simple implementation and can give acceptable results. In [2], the speedup obtained by OpenMP for

the solution of the system of equations, that is strictly related to the single iteration speedup, was about 5 for 16 threads.

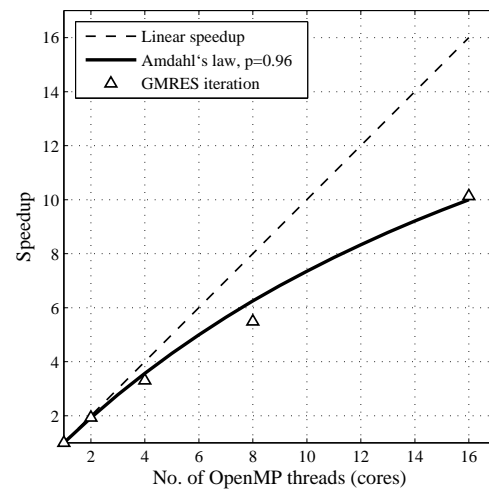


Figure 4: Parallel performance of single GMRES iteration

### 4. Conclusions

The presented FMBEM parallelization approach is based on the assumption that the amount of work for each thread can be estimated only by partitioning nodes on two levels of the tree, i.e. the level 2 and the highest level (leaves). The method can be applied to the efficient analysis of linear elastic structures of complex geometry, e.g. representative volume elements of non-homogeneous materials in computational homogenization.

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