BULLETIN OF THE POLISH ACADEMY OF SCIENCES
TECHNICAL SCIENCES, Vol. 68, No. 2, 2020
DOI: 10.24425/bpasts.2020.131847

On speeding up nano- and micromechanical calculations for irregular systems with long-range potentials

L. RYBARSKA-RUSINEK*, E. REJWER, and A. LINKOV

Rzeszów University of Technology, ul. Powstańców Warszawy 12, 35-959 Rzeszów, Poland

Abstract. Irregular systems with long-range interactions and multiple clusters are considered. The presence of clusters leads to excessive computational complexity of conventional fast multipole methods (FMM), used for modeling systems with large number of DOFs. To overcome the difficulty, a modification of the classical FMM is suggested. It tackles the very cause of the complication by accounting for higher intensity of fields, generated by clusters in upward and especially in downward translations. Numerical examples demonstrate that, in accordance with theoretical estimations, in typical cases the modified FMM significantly reduces the time expense without loss of the accuracy.

Key words: nano- and micromechanics, long-range interaction, fast multipole methods, cluster intensity.

1. Introduction

In nano- and micromechanics, numerical simulation unavoidably leads to the need to consider multiple pair-wise interactions between discrete particles (in nano-mechanics), or elements which appear after discretization of partial differential equations for a continuous medium (in micromechanics). Direct accounting for each of interactions would lead to immense time expense. Thus in practice, the interactions are divided on those within an area containing close neighbors (short-range interactions), and those including elements beyond this area (long-range interactions). For rapidly decreasing potentials of Lennard-Jones type, merely the first group is of essence [9, 10, 15]. Then interactions involve merely quite a limited number of close neighbors, the interaction matrix is low-populated and well-developed methods for such matrices (e.g. [21, 26]) are available and widely used. They reduce the computational complexity to the order of the number N of the system DOF. This makes the time expense acceptable even if N is large.

However, for Coulombian and gravitational potentials in nano-mechanics, and for kernels (potentials), corresponding to fundamental solutions of Laplace or Kelvin type in boundary integral equations (BIE) of continuum mechanics, the long-range interactions cannot be neglected. To account for them with non-excessive time cost, special methods are developed (see, e.g. [2, 5, 14, 23, 24]). Such are methods of Ewald's type [23], employing Fourier transform, and, in a general case, fast multipole methods (FMM), initiated by Greengard and Rokhlin [5] and further developed in analytical (A-FMM) (e.g. [14, 17–19]) and kernel independent (KI-FMM) (e.g. [2, 12, 13, 24, 25]) forms. FMM are equally applicable to physically discrete systems (in nano-mechanics) and to discrete systems, arising after spatial discretization of BIE for a continuous media (in micromechanics). For certainty, the following discussion is performed in terms of continuum mechanics.

In the both cases, a discretized system may be strongly irregular due to the presence of clusters of field concentration. Then the number of translations, performed on up and downward travels a hierarchical tree, and consequently the total time expense for the translations, becomes unacceptable. The objective of the paper is to develop a general, simple and easily implemented means to drastically reduce the number of translations of any FMM, when a system is strongly irregular.

We suggest an improvement of the classical FMM, employing the very cause of the difficulty, which is the presence of clusters with high intensity of sources. To this end, we evaluate the intensities of objects and compare them when performing up- and downward translations on iterations of solving the system. Translations from objects of relatively small intensity are excluded from execution.

The structure of the paper is as follows. In Section 2, the essence of the problem and the main suggestion are presented. It is noted that for homogeneous, in particular regular, systems, all the intensities are the same, and a FMM works in a usual way. In contrast, for a system with significant difference of intensities, the number of translations is unavoidably reduced. From general considerations it appears that in limit all the translations may be excluded what suggests that the gain may be quite significant. Section 3 contains general comments on numerical realization of the improvement suggested. It explains that the implementation requires just complementing a computational program of any FMM with a simple subroutine(s) evaluating intensities and comparing them with a threshold. In Section 4, illustrative examples are given to reveal the extent of possible decrease in the number of translations in practical calculations. They show that indeed in typical cases of systems with clusters, the number of translations and consequently the time expense for their execution drastically decreases. Brief conclusions are summarized at the end of Section 4. They emphasize that the

*e-mail: rybarska@prz.edu.pl

Manuscript submitted 2019-09-23, revised 2019-12-23, initially accepted for publication 2019-12-27, published in April 2020

implementation of the improvement suggested is quite simple and requires quite small changes in a code of a conventional FMM. For a system without clusters, the calculations are automatically performed as usual.

2. Essence of the problem and the main suggestion

Consider a conventional FMM, analytical or kernel independent. The concepts and terminology, used in the following discussion, are those explained in the works [14, 24, 25]. The key idea of a FMM consists of removing the complexity N^2 of matrix-to-vector multiplications, performed on iterations of solving the system of equations. The number N of DOFs in evaluations of the complexity appears now in the first degree as $O(N)$ instead of $O(N^2)$. Then the complexity is actually defined by multiply repeated up- and downward runs, each of which requires performing translations. The complexity of an individual translation is of order p^2, where p is the number of expansion terms in the A-FMM, or the number of nodal values of equivalent densities in the KI-FMM. For a scalar potential, the number p is at least 10 in 2D problems; it is at least 100 in 3D. Although the complexity of an individual translation is not high, one needs to perform M_T translations on each of M_{IT} iterations. Thus the total complexity is of order $p^2 M_T M_{IT}$. It becomes unacceptable, if the number of translations is too large. In the product $p^2 M_T M_{IT}$, each of the factors may be minimized by, respectively, (i) developing special methods of matrix-to-vector multiplication, (ii) using improved preconditioners and/or initial guess, and (iii) reduction of the number M_T of translations. Each of these items has been a subject of special researches. The reduction of the complexity p^2 of individual translations, in some cases, may be achieved by SVD acceleration [2, 24] or by using *ad hoc* methods in particular cases. For instance, as shown in the paper [6], Coulombian potential in 3D may be represented by repeated integral evaluated via specially designed quadrature rules. This reduces the complexity from p^2 to nearly p, while the great number of terms in the quadrature rules notably decreases the computational efficiency of the method.

The second path (using improved preconditioner and/or initial guess) refers mostly to boundary element methods (BEM), which require iterations to find unknown densities. It is strongly dependent on a particular potential (kernel of a boundary integral) and on a particular problem (e.g. [16]).

The third way (reducing the number M_T of translations) suggests means less sensitive to the form of a potential than the two previous. When there is an occasion, it may be employed together with them. Thus it is of importance to develop approaches, which reduce the number of translations. From now on, we focus on this topic.

In any FMM, the greatest number of translations is performed on the bottle-neck stage of a downward run. These are M2L translations on each hierarchical level for each box belonging to this level. The classical definitions of M2L translations, interaction and *V* lists (e.g. [14, 24]) imply that the number of M2L translations to a cell B on some level of a hierarchical tree equals to the number of entries in its *V*-list. The number of entries is maximal when there are no empty cells in a tree (this is the case for homogeneous distribution of sources). In this case, *V*-lists introduced in [24] (see also [25]) for non-uniform distributions, coincide with the interaction lists, considered in [14] for nearly uniform distributions. Then the interaction list of a cell B includes all the cells, which belong to the neighbors of the B *parent*, but which are not neighbors of B itself. In Fig. 1, the contour of the cell B is shown by bold solid line; the contour of its parent by thinner solid line; and contours of other cells by dashed lines. The cells of the B's interaction list are marked by crosses. From Fig. 1, it is easy to infer that in 2D, the number of such cells equals to $(5^2 - 3^2) + (7^2 - 5^2)/2 - 1 = 27$. Similarly, in 3D, the maximal number of cells in an interaction list of a cell B equals to $(5^3 - 3^3) + (7^3 - 5^3)/2 - (7 - 1)3 = 189$. Therefore, the maximal number N_{M2L} of M2L translations is $N_{M2L} = 27$ in 2D and $N_{M2L} = 189$ in 3D (see also, e.g. [22]). The maximal numbers of other translations (M2M and L2L) for each parent on each hierarchical level is 4 in 2D and 8 in 3D. This explains why M2L translations take the greatest part of the time expense on up and downward runs.

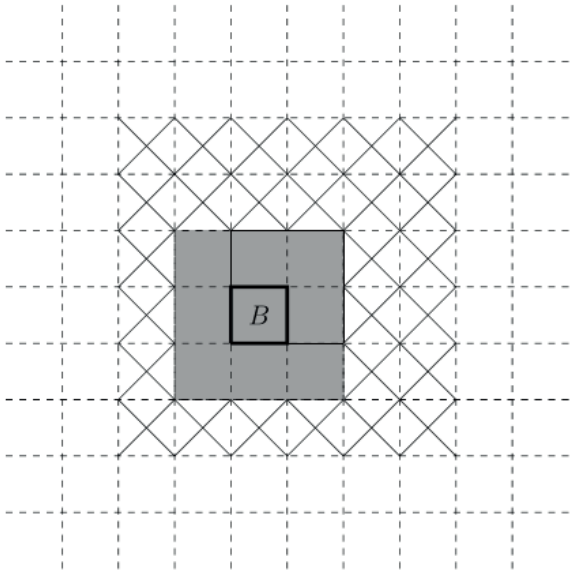

Fig. 1. Types of objects around a box B on its hierarchical level. Grey: the box B and its neighbors. White with crosses: objects in interaction list of B (require M2L translations). White: objects, whose influence is accounted for by the parent of B

The simplest general approach to reduce the number of M2L translations consists of exclusion from translations those cells of an interaction list, which are sufficiently far from the center of the cell's parent (e.g. [1, 7, 22]). The influence of the excluded cells is translated to the parent of the cell considered. This method, called the level-skip M2L, reduces the utmost number of M2L translations in 3D from 189 to 119 (e.g. [22]). Such reduction is available for any distributions of

locations and intensities of sources. It may be performed before, simultaneously or after employing some approach tending to reduce the number of translations when distributions are inhomogeneous. In particular, for the cases, when distribution of source locations is strongly inhomogeneous, an approach, able to reduce the number of M2L translations, is suggested in [4] with the aim to simplify parallel computations. The approach employs asymmetric building a hierarchical tree by dividing branches onto cells, containing the equal number of sources, instead of the conventional dividing onto cells of the same sizes. While the locations of cells may be arbitrary, the method assumes that their intensities are the same. An extension of the method to sources of various intensities would unavoidably lead to rebuilding the hierarchical tree when the intensities are changed on iterations of a BEM. Thus, it is of essence to reduce the number of translations for cases when the distribution of intensities is inhomogeneous, as well. An approach to reach this objective without rebuilding a hierarchical tree may employ the following considerations.

For a homogeneous distribution of sources, all M2L translations are to be performed when using a conventional FMM. However, for inhomogeneous spatial distribution of sources, some of the well-separated cells are empty, and they do not enter interaction lists and, consequently, they do not participate in translations. Note, that an empty cell may be considered to be a cell of zero intensity. Clearly, a cell may be neglected, as well, when its intensity, while non-zero, is small enough (say, goes to zero in limit). In a classical FMM, a cell of arbitrary small intensity still participates in translations. Our suggestion consists in excluding a cell from translations, if its intensity, being non-zero, is relatively small. As clear from the discussion above, in some cases, the number of M2L translations for an object may be diminished to zero.

For a system with clusters, the total portion of cells with relatively small intensity, may be significant. Then their exclusion from M2L translations will provide similarly significant reduction of the time expense for the bottle-neck operation. This is the key concept of our paper.

It remains to strictly define (i) the measure of a cell intensity, and (ii) a criterion to conclude which intensity is small enough to exclude its bearer from translations. These definitions may be problem dependent. From physical considerations, it is clear that for a A-FMM, a proper measure of the cell intensity is zero-order moment. In a KI-FMM, it corresponds to the integral from the equivalent density over the equivalent surface. What concerns with the criteria for exclusion a cell from M2L translations for a given box, it has to account for comparative intensities of (i) the parent of the box (e.g. on Fig. 1, the box bounded by thin continuous lines), (ii) other cells in the same interaction list and (iii) cells in the U list (the box and its neighbors).

Comment. An approach to cut off the area of strong influence in dependence on the intensity of the source has been successfully used in the paper [20]. It served to reduce the time expense for calculations of stresses, induced by a large group of already activated flaws (possible sources of seismic events), at locations of flaws, which may be activated by the stresses. In this case, the linear size of the activated flaw was chosen as a measure of intensity to assign the cut-off radius of its influence.

3. Computational implementation

Computational implementation of the improvement suggested is illustrated by considering a plane harmonic problem for a piece-wise homogeneous medium with arbitrary interface conditions on contacts of structural elements (Fig. 2). The complex variable singular and hypersingular BIE for this class of problems, derived in [3], are, respectively

$$Re\left(-\frac{1}{2\pi}\int_L\left[\Delta q_n ln(\tau - z)ds + i\frac{\Delta(kT)}{\tau - z}d\tau\right]\right) = \\ = \frac{1}{2}\left(k^+T^+(z) + k^-T^-(z)\right), \tag{1}$$

$$Re\left(-\frac{e^{i\alpha_z}}{2\pi}\int_L\left[ie^{-i\alpha_\tau}\frac{\Delta(q_n/k)}{\tau - z} + \frac{\Delta(T)}{(\tau - z)^2}\right]d\tau\right) = \\ = \frac{1}{2}\left(q_n^+(z)/k^+ + q_n^-(z)/k^-\right), \quad z \in L \tag{2}$$

where L is the total boundary of the system of blocks (the contact between surfaces of adjacent blocks is treated as a single line, in which thermal and mechanical values may experience discontinuity); $z = x + iy$, $z \in L$ is the complex coordinate of a field point; τ is the complex coordinate of an integration point; the symbol Δ in front of a value, denotes its jump across the contour; T is the potential; q_n is the normal component of the flux at an element of L with the normal n; k is the conductivity ($k \geq 0$); $\alpha_z(\alpha_\tau)$ is the angle between an element dz ($d\tau$) and the x-axis; the upper index "plus" ("minus") refers to the side, with respect to which the normal n is outward (inward). The A-FMM to solve (1) in frames of the CV-BEM is developed and described in details in [19].

For certainty, the discussion below is given in terms of a thermal problem. Thus the potential T corresponds to the temperature, the flux q is the heat flux and k is thermal con-

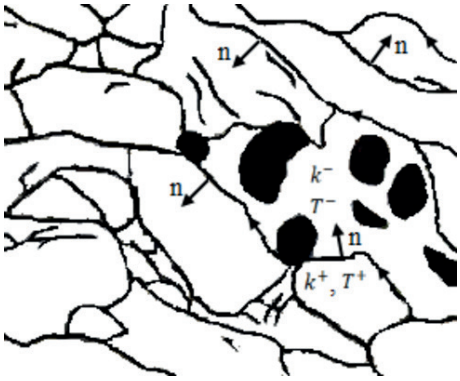

Fig. 2. Piece-wise homogeneous blocky structure

ductivity. The computer code presented in [19] is complemented with simple subroutines evaluating the number of M2L translations and comparing intensities of cells. In accordance with Section 2, the intensities of cells are found as zero-order moments, which are factors at the kernel of the lowest order at infinity. This kernel is $log(z - z_c)$ in the singular equation (1) and $1/(z - z_c)$ in the hypersingular equation (2) with z_c being the center of an object of the hierarchical tree. Thus for the hypersingular equation, used in numerical examples, the intensity of a leaf-cell is defined as

$$M = \sum_{j=1}^{m} \int_{L_j} \Delta q_n dt \approx \sum_{j=1}^{m} \sum_{s=1}^{k} c_s^j \Delta q_s^j$$

where m is the number of boundary elements in a leaf, L_j is the contour of the j-th element in the leaf, c_s^j are the weights of a quadrature rule used for integration over L_j, Δq_s^j are the nodal values of the density on L_j. For a parent-cell on any level, its intensity is evaluated as the sum of intensities of its children.

Computational implementations for 3D problems and KI-FMM follow the same pathway as that sketched above for a representative 2D problem solved by the complex variable A-FMM. Specifically, for any A-FMM in both 2D and 3D, the path stays exactly the same. What concerns with KI-FMM (in both 2D and 3D), all the calculations are also performed as usual, except for evaluation of intensities, used to exclude translations from objects with relatively small intensity. For a KI-FMM, the intensity, corresponding to zero-order moment, is given by the integral

$$M_B = \int_{S_{Be}} q_{Be} dS \tag{3}$$

where S_{Be} is the equivalent surface of an object B, q_{Be} is the equivalent density on the surface S_{Be}. In particular, the sketched line with the definition (3) is used in the example 3 of Section 3. This example refers to 3D problems for an elastic medium with cracks. The problems are solved by KI-FMM with a hypersingular potential, defining far-fields of stresses. In these problem, the unknown values are displacement discontinuities (DD) on crack surfaces. Then the equivalent densities q_{Be} in (3) have the meaning and dimension of equivalent DD.

Comment. In practical calculations, it may happen that although the exact values of moments (in A-FMM), or densities (in KI-FMM), corresponding to the final solution are high, their approximate values stay small on a number of successive iterations after starting an iterative process. This occurs, in particular, when starting from the commonly used simplest initial guess of zero initial values. Then the gain, reached by neglecting relatively weak neighbors, is lost; it appears only after a sufficient number of iterations. Therefore, to use the improvement to utmost extent, it is reasonable to start iterations with initial values, which better approximate the solution than the zero-values guess. A better initial approximation may be obtained by finding it as the solution of a problem close to the considered problem, but in contrast with that, has low populated matrix. For example it may be a system with the matrix whose non-zero entries correspond to nodes merely in leaves and their neighbors.

4. Numerical results and conclusions

Consider examples for plane problems of steady heat flow in infinite and finite regions with cracks. The cracks are thermally non-conductive, so that the normal component q_n of the flux on their surfaces is zero $(\Delta q_n = q_n^+ - q_n^- = 0)$, while the temperature is discontinuous $(\Delta T = T^+ - T^-)$. In these cases, equation (2) is sufficient to solve a problem. For certainty, the conductivity is set unit $(k = 1)$.

Example 1. Consider the system with distinct domination of clusters represented by two vertical large cracks of the length $2l$ and 62 vertical small cracks of the length $0.04l$ with centers uniformly placed in the area around clusters. The centers of large cracks are at the distance $4l$ along the x-axis and the distance $2l$ along the y-axis (Fig. 3). The flux at infinity has the direction of the x-axis $(q_x^\infty = q = 1, q_y^\infty = 0)$. By superposition, the problem is reduced to that with zero flux at infinity, while the normal components of the flux on cracks become $q_n^+ = q_n^- = -qn_x$, where n_x is the x-th component of the unit normal to a crack. The discontinuities $\Delta q_n = 0$ and $\Delta T = T^+ - T^-$ on crack surfaces do not change. The equation (2) is sufficient for finding the discontinuity ΔT on each crack for a given flux $q_n^+ = q_n^- = -n_x$ at its surfaces. In the example considered, $n_x = 1$; then $q_n^+ = q_n^- = -1$.

In numerical experiments, each of cracks was represented by 4 boundary elements with 3 nodes each, what corresponds to second order approximation of densities. Thus the total number of unknowns was 768. The parameters of the A-FMM were set in accordance with results of the paper [19]: maximal number of nodes in a leaf was 4; the CV series employed in translations

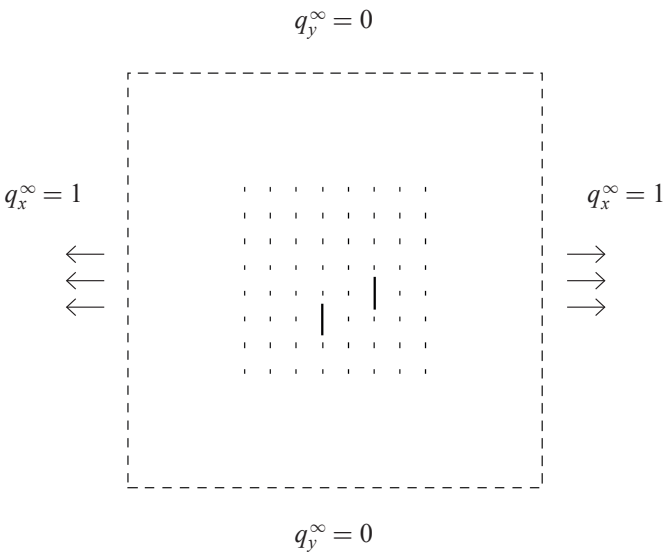

Fig. 3. Irregular systems of cracks set uniformly in an infinite region

were truncated to the 15th term. This yielded the number of levels equal to 4, and the number of real unknowns, found in each of translations, equal to $p = 30$. Thus the typical complexity of a translation is $p^2 = 900$. An iteration was performed by using GMRES procedure. The assigned tolerance was 10^{-4}.

Starting from the commonly used simplest guess of zero initial values, solving the problem to the accuracy accepted required 70 iterations. On each of the iterations the number of M2L translations was 2630. The solution for the temperature discontinuity ΔT gave 0.1248 and 0.1249 at the center of the left and right large cracks, respectively. For small cracks, the discontinuity ΔT at their centers was in the narrow range from 0.0021 to 0.0029. The magnitudes of zero-moments were of order $2 \cdot 10^{-3}$ for leaves containing clusters, while for the remaining leaves it was much less being of order $5 \cdot 10^{-5}$. When starting from zero-values initial guess, the differences between absolute values of ΔT on large and small cracks on first iterations were negligible. Still, the differences of zero-moments for large and small cracks became quite distinct on the iterations much before the end of the iterative process. Many other numerical simulations have confirmed that the differences in moments become much more evident in iterations than the differences in absolute values of densities. This justifies the definition of the intensity, accepted in Section 2 for A-FMM, which associates it with zero-moments.

The notable contrast in zero-moments of objects (both leaves and cells), belonging to the same level of the tree, suffices using the approach suggested in Section 2 for diminishing the number of M2L translations. In the case considered, the simplest criterion for exclusion from translations is as follows. A cell is excluded if its intensity is less than an assigned threshold of the average intensity of all cells entering the same interaction list. For the threshold 0.1, the criterion appears quite safe and it is assumed in calculations discussed. In practice, it neglects far-fields, translated by M2L procedures, of those objects which do not contain clusters.

With this criterion, the number M_T of M2L translations decreased from 2630 to merely 52 on each of iterations. The resulting values of ΔT became 0.1267 for the large cracks (error 1.5%) and stayed practically unchanged for small cracks, being in the range from 0.0021 to 0.0030 at their centers. Thus, as expected, the loss of the accuracy was insignificant, while the time expense for M2L translations reduced 50-fold.

In this example, the size of small cracks is nearly two orders less than the size of large cracks. Thus it may be expected that when the number N of unknowns, defined by the presence of many small cracks, grows, the number of M2L translations would grow proportionally to N. This refers to M2L translations performed both conventionally and with the approach suggested. As a result, the relative reduction in the number of translations should stay actually unchanged. Indeed, our calculations with growing number of unknowns (2000, 6000 and 18 000) have shown proportional growth of the number of translations (5148, 18 590 and 65 836). The relative reduction stayed on the level mentioned (some 50-fold).

Note that the example refers to infinite area with evident domination of clusters. It is quite favorable for reduction of M2L translations, because there are no external boundaries, which themselves present clusters. The opposite case, when the region is finite and the presence of its boundaries notably restricts the possibility to reduce the number of M2L translations, is studied in Example 2.

Clearly, a reduction of the number of translations depends also on the intensity threshold assigned. Specifically, for infinite threshold, translations will be excluded at all; then the accuracy of calculations may become unacceptable. In the opposite extreme case of zero threshold, all the translations of a conventional FMM will be performed; consequently, the accuracy will be that of the conventional FMM. For a threshold equal to the greatest of compared intensities, the number of translations is between these extremes depending on a particular distribution of compared intensities; in particular, for a homogeneous system, there will be no reduction. Evidently, a proper choice of the criteria for exclusion depends both on distribution of sources in the system considered and on required accuracy of calculations of local fields. Thus, as mentioned in Section 2, a proper choice is problem-dependent and, as usual in such cases, it should be left to a perspective user to assign it as an input parameter. Still, also as usual, general recommendations may be made for sufficiently wide particular classes of problems. We illustrate the influence and proper choice of the threshold some later, when discussing Example 3.

Example 2. Consider steady heat flow in a square region containing randomly seeded small cracks and two clusters. The sizes of small and large cracks are the same as in the previous example (respectively, $0.04l$ and $2l$). The square side is $A = 16l$. The number of small cracks is 198. Their centres are distributed with the uniform density function along the axes x, y parallel to the square sides. The angles of normals with the x-axis are also distributed randomly with uniform density function in the interval $[0, \pi]$. The angle of the normal to the x-axis for the both large cracks is $\pi/4$ (Fig. 4). As above, the flux through

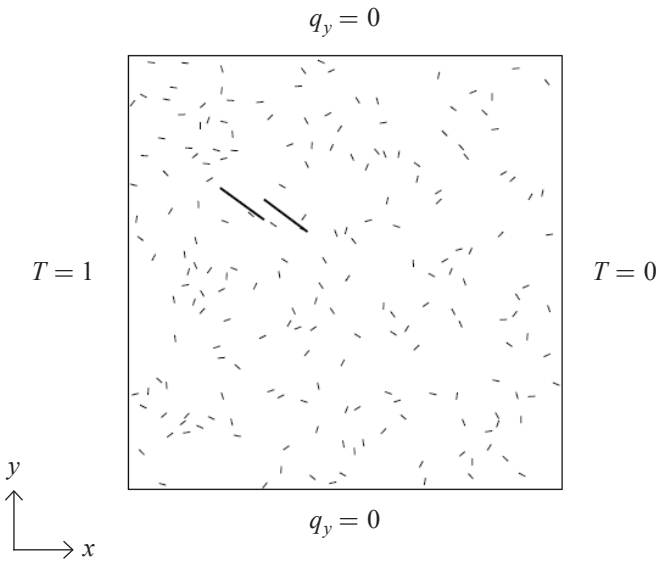

Fig. 4. Irregular systems of cracks set uniformly in an infinite region

cracks surfaces is zero. The mixed boundary conditions correspond to the homogenization problem of finding the effective conductivity of a representative volume with cracks. Specifically, we prescribe constant temperature $T_l = 0$ and $T_r = 1$ at the left and right vertical sides of the square, respectively; and zero fluxes through the horizontal sides. Each side of a square is represented by 30 straight boundary elements of the length $0.53l$. Each of them has 3 nodes providing the second order density approximation. The total number of unknowns is 2760. The maximal number of nodes in a leaf is set 6. This yields the number of levels equal to 4. Other parameters of the A-FMM (the number of expansion terms, complexity of a translation, tolerance for GMRES) are the same as in the previous example.

In the case considered, areas of high intensity include not only the large cracks but also the square sides. The total number of M2L translations is now 4228; solving the problem requires 720 iterations when starting from zero initial values. The quite large number of iterations is explained by the combined influence of the poor initial guess and mixed boundary conditions. Specifically, assigning zero fluxes at horizontal boundaries, implies that, in contrast with Example 1, the correct order of unknown values (assumed zero by initial guess), is not reached on the first iteration; now it is reached rather slowly. The values of ΔT at centers of large cracks are 0.08178 and 0.07988 for the left and right crack, respectively. The total fluxes through the left and right side of the square are 0.98969 and 0.99133; the difference between them is 0.00164. Since for an exact solution, the difference should be zero, this implies that the relative integral error of the flux is on the level of 0.2%.

Neglecting inputs of small intensities leads to reduction of M2L translations from 4228 to 1514, that is 2.5-fold. The number of iterations stays the same. There is no significant changes in the calculated quantities: the values of ΔT differ from those, evaluated without reduction of the translations, merely in the fourth significant digit, both for large and small cracks. There is also no changes in the total flux through the vertical sides of the square; this implies that there is no difference in the effective conductivity defined by the total flux. We see that even in the case quite unfavorable for reducing the number of M2L translations, there is a noticeable gain without loss of the accuracy.

Similar to the first example, the size of small cracks is much less than that of large ones. Thus, again, increasing the number of small cracks has led to proportional growth of the number of M2L translations both for conventional and improved FMM. Like in Example 1, the relative reduction stayed actually unchanged (about 2.5-fold).

Example 3. The two previous examples referred to 2D problems and to cases of small cracks with sizes much (50-fold) less than the size of large cracks. To illustrate the performance of the approach in 3D, we consider an elasticity problem for a cluster represented by a large rectangular crack with the unit short side $(a_L = 1)$ and the longer side $5a_L$. The crack is located in an infinite medium with the elasticity modulus $E = 10^4$ MPa and the Poisson's ratio $\nu = 0.25$. Fifty small square cracks with the sides $a_S = 0.5a_L$ are seeded in the vicinity of the large crack

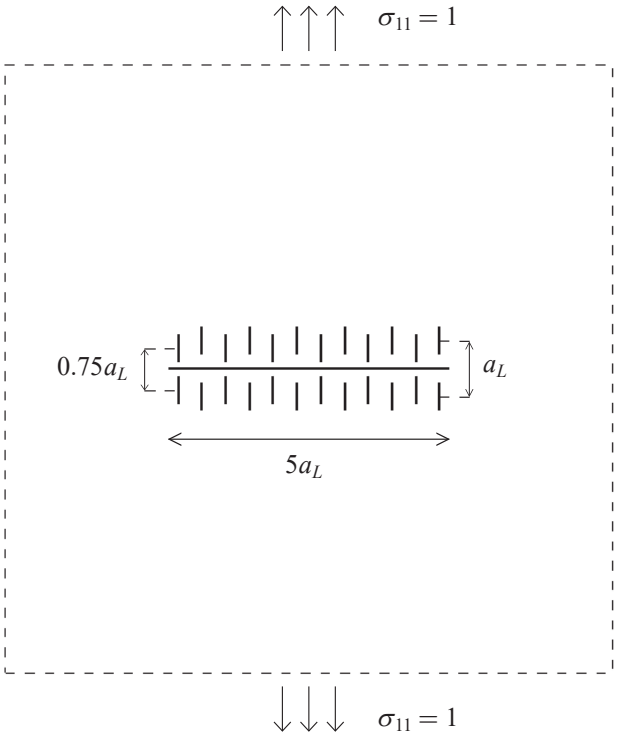

Fig. 5. Vertical cross-section of the systems of cracks through the middle of the large crack

in the rectangular parallelepiped of sizes $5a_L \times a_L \times a_L$ symmetrically about the center of the large crack. The uniaxial tension $\sigma_{11} = 1$ MPa acts at infinity in the direction orthogonal to the plane of the large crack. The vertical cross-section through the middle of the large crack is shown in Fig. 5.

The hypersingular BIE for 3D problems of the kind and the BEM for them are given in [8, 11]. The resulting algebraic system is solved by the kernel independent FMM suggested in [24] (see also [25]). The large crack is represented by 320 square boundary elements; each of small cracks is represented by 16 square elements. With three unknown displacement discontinuities at each boundary element, the total number of unknowns is $3\,(320 + 50 \times 16) = 3360$. When applying the FMM, the assigned maximal number of elements in a leaf was taken 20. Then for the problem considered, the number of levels in the oct-tree was 6; the total number of cells was 202; the total number of M2L translations was 4306; and the *average* number of entries in a *V*-list was 22.

In contrast with two previous examples, the short side of the large crack is merely 2-fold longer than the sides of small cracks. This impels using more restrictive rule for assigning cut-off intensities to reduce the number of M2L translations. We exclude some of the M2L translations in a quite restrictive, while safe and general, way by assigning the maximal relative error ε, caused by the reduction. The reduction is executed as follows.

On an iteration step of the FMM, when performing the upward run, we calculate current intensity q of each cell (leaf or branch). These intensities are used on the downward run

when performing M2L translations to each cell on each level starting from the level 3 (or 2, if using the level-skip method). For the cell, we analyze intensities q_i ($i = 1, \ldots, N_V$) of N_V cells belonging to its V-list. We arrange q_i in the order of non-increasing intensities:

$$q_1 \geq q_2 \geq \cdots \geq q_{NV} \tag{4}$$

(commonly, q_i may be assumed positive with changing the sign when appropriate). Then the total intensity Q of the far-field, translated by N_V translations M2L, is $Q = \sum_{i=1}^{N_V} q_i$. When abridging the sum to N_a first terms, the approximate intensity of the far-field is $Q_a = \sum_{i=1}^{N_a} q_i$, and the absolute error ErQ_a of the approximation is the sum of remaining terms $ErQ_a = \sum_{i=N_a+1}^{N_V} q_i$, when $N_a < N_V$, and $ErQ_a = 0$ when $N_a = N_V$. In view of (4), for an assigned relative error ε of the far-field, the relative error of the approximation Q_a will not exceed ε when

$$ErQ_a < \varepsilon Q. \tag{5}$$

The inequality (5) defines a simple algorithm for excluding translations from cells of relatively small intensities. It consists of successive summation of intensities q_i, ordered according to (4), in inverse order: from the smallest intensity q_{NV}. The summation is continued till (5) is met. The critical intensity q_a, starting from which the inequality (5) is violated, defines the threshold q_a and the tolerance $\delta = q_a/Q$, corresponding to the assigned relative error ε. We may safely exclude M2L translations from those cells of the V-list, whose intensities are less than the threshold q_a. The error of the far-field will not exceed ε.

Underline, that the criterion described is quite conservative, because an error of M2L translations may have insignificant influence on the accuracy of final results, as compared with the influence of L2L translations. Consequently, for particular problems, it is possible to assign rather large relative error ε (up to 0.75 and even 1) by performing just a few tests with successively growing values of ε. (Recall that $\varepsilon = 1$ corresponds to exclusion all M2L translations of far-fields to the given cell).

For the example considered, three values of ε have been used: $\varepsilon = 0.1$; 0.5; 0.75. With these values, the total number of M2L translations decreased from 4306 (for the conventional FMM) to, respectively, 2230, 830 and 384. Accordingly, the time for their executions was reduced 2-fold, 5-fold and 11-fold. Notably, even for $\varepsilon = 0.75$, the final calculated openings (both on large and small cracks) were practically the same as those obtained by the conventional FMM. This implies that in problems of the type considered, quite large value of ε may be used to reach notable reduction of the time expense for M2L translations without loss of the accuracy of final results.

Conclusions. In all the tests with the improved FMM, the accuracy of the final results was actually the same as that of the conventional FMM. This confirms that the improvement suggested is of value for solving large-scale problems for irregular systems. Emphasize that its implementation is quite simple and requires rather small changes in a code of conventional FMM. For a system without clusters, the calculations are automatically performed as usual.

Acknowledgements. The first two authors gratefully acknowledge support of the work, co-founded by the ITHACA project PPI/APM/2018/1/00045 financed by NAWA, and its recommendation by the 6th Conference on Nano- and Micromechanics. The third author expresses special gratitude for the support of the National Science Centre, Poland (no. 2015/19/B/ST8/00712). We also highly appreciate the valuable comments of anonymous reviewers.

References

[1] M.S. Bapat and Y.J. Liu, "A new adaptive algorithm for the fast multipole boundary element method", *CMES: Comput. Model. Eng. Sci*. 58, 161–184 (2010).

[2] Y. Cao, L. Wen, and J. Rong, "A SVD accelerated kernelindependent fast multipole method and its application to BEM", *WIT Transactions on Modelling and Simulation* 56, 431–443 (2013).

[3] A. Dobroskok and A. Linkov, "CV BEM for 2D transient thermo-(poro-)elastic problems concerning with blocky systems with singular points and lines of discontinuities", *Int. J. Eng. Sci*. 48, 658–669 (2010).

[4] S. Engblom, "On well-separated sets and fast multipole methods", *Appl. Num. Math*. 61, 1096–1102 (2011).

[5] L. Greengard and V.J. Rokhlin, "A fast algorithm for particle simulations", *J. Comput. Phys*. 73, 325–348 (1987).

[6] L. Greengard and V.J. Rokhlin, "A new version of Fast Multipole Method for the Laplace equation in three dimensions", *Acta Numer*. 6, 229–269 (1997).

[7] N.A. Gumerov and R. Duraiswami, "Fast multipole methods on graphics processors", *J. Comput. Phys*. 227, 8290–8313 (2008).

[8] D. Jaworski, A.M. Linkov, and L. Rybarska-Rusinek, "On solving 3D elasticity problems for inhomogeneous region with cracks, pores and inclusions", *Comput. Geotech*. 71, 295–309 (2016).

[9] M. Kmiotek and A. Kucaba-Piętal, "Influence of slim obstacle geometry on the flow and heat transfer in microchannels", *Bull. Pol. Ac.: Tech*. 66(2), 111–118 (2018).

[10] A. Kordos, and A. Kucaba-Piętal, "Nanovortex evolution in entrance part of the 2D open type long nanocavity", *Bull. Pol. Ac.: Tech*. 66(2), 119–125 (2018).

[11] A.M. Linkov, "Real and complex hypersingular integrals and integral equations in computational mechanics", *Demonstr. Math*. XXVIII (4), 759–769 (1995).

[12] A.M. Linkov, E. Rejwer, and L. Rybarska-Rusinek, "On solving continuum-mechanics problems by fast multipole methods", *Dokl. Phys*. 62(8), 400–402 (2017).

[13] A.M. Linkov, E. Rejwer, and L. Rybarska-Rusinek, "Torsional rigidity of a bar with multiple fibers", *Mech. Solids* 52(4), 452–456 (2017).

[14] Y. Liu, Fast Multipole Boundary Method. Theory and Applications in Engineering, *Cambridge University Press, Cambridge*, 2009.

[15] H. Margenau and N.R. Kestner, Theory of Intermolecular Forces. (ed. D. Ter Haar). *Pergamon*, 1969.

[16] A.P. Peirce and E. Siebrits, "A dual mesh multigrid preconditioner for the efficient solution of hydraulically driven fracture problems", *Int. J. Numer. Methods Eng*. 63, 1797–1823 (2005).

[17] J. Ptaszny, "Parallel fast multipole boundary element method applied to computational homogenization", *AIP Conference Proceedings* 1922, 140003 (2018).

[18] J. Ptaszny and M. Hatłas, "Evaluation of the FMBEM efficiency in the analysis of porous structures", *Eng. Comput*. 35(2), 843–866 (2018).

[19] E. Rejwer, L. Rybarska-Rusinek, and A. Linkov, "The complex variable fast multipole boundary element method for the analysis of strongly inhomogeneous media", *Eng. Anal. Boundary Elem*. 43, 105–116 (2014).

[20] L. Rybarska-Rusinek, E. Rejwer, and A. Linkov, "Speeded simulation of seismicity accompanying mining and hydrofracture", *Eng. Comput*. 35(5), 1932–1949 (2018).

[21] E.B. Tadmor and R.E. Miller, Modeling Materials: Continuum, Atomistic and Multiscale Techniques, *Cambridge University Press, Cambridge*, 2011.

[22] Y. Wang, Q. Wang, et al. "Graphics processing unit (GPU) accelerated fast multipole BEM with level-skip M2L for 3D elasticity problems", *Adv. Eng. Software* 82, 105–118 (2015).

[23] W.K. Winnett and C.P. Nash, "Ewald's method for calculating lattice sums in ionic crystals", *Comput. Chem*. 10(3), 229–237 (1986).

[24] L. Ying, G. Biros, and D. Zorin, "A kernel-independent adaptive fast multipole method in two and three dimensions", *J. Comput. Phys*. 196(2), 591–626 (2004).

[25] L. Ying, "Fast algorithms for boundary integral equations", Multiscale Modeling and Simulation in Science (eds. B. Engquist, P. Lötstedt, O. Runborg), *Springer-Verlag Berlin Heidelberg*, 139–193, 2009.

[26] O.C. Zienkiewicz, R.L. Taylor, and J.Z. Zhu, The Finite Element Method: Its Basis and Fundamentals, 6-th ed. *Elsevier Butterworth – Heinemann*, 2005.