Acceleration Methods for the Calculation of Results in Boundary Element Modeling

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Abstract – **One of the most widely used methods for numerical modeling of physical processes is the boundary element method (BEM). Compared to the well-known finite element method (FEM), main advantage of BEM is the reduced dimension of the problem. Discretization is only required at the boundary between the materials, therefore, mesh generation in the computational domain becomes significantly simplified. One of the problems that complicate practical application of BEM is great computational costs in calculating the characteristics of the field inside the computational domain based on the solution obtained. This is due to integrating over the entire boundary required in the conventional method in order to obtain the result. This paper addresses the study of a possibility of accelerating such calculations via parallelization and vectorization and using the fast multipole method. The efficiency of the proposed methods is investigated. The results are obtained by solving the problem of magnetic field calculation in the operating area of the C-shaped dipole magnet.**

Index Terms – **Numerical modeling, boundary equations, boundary element method, fast multipole method, vectorization.**

I. INTRODUCTION

DESIGNING MODERN sophisticated devices such as particle accelerators is practically impossible without the use of numerical modeling. It provides an opportunity to calculate the characteristics of physical processes, i.e. electromagnetic or thermal, occurring in the device. Such physical processes are usually described by systems of partial differential equations.

One of the most widely used methods for solving these systems is the finite element method (FEM) [1, 2, 12, 14]. It makes it possible to effectively take into account non-linearity and heterogeneity of the coefficients of equations, however, it requires the mesh to be constructed in the whole computational domain.

Another well-known method is the boundary element method (BEM) [8, 11]. As compared to FEM, the main advantage of BEM is that meshing is needed only at the interface between the materials, which significantly simplifies the process of mesh constructing in the computational domain and eliminates the error of approximation inside subdomains. One of the problems that complicate the usage of BEM is high computational costs of calculating of the solution values at points located within subdomains, as it requires integration along the entire boundary of the subdomain. Another problem of the boundary element method is an inefficient treatment of non-linearity and heterogeneity. In such cases, the coupled FEM-BEM method can be used [9], so that linear subdomains are approximated by boundary elements and non-linear subdomains – by finite elements.

II. PROBLEM DEFINITION

One of the problems encountered in the numerical simulation is the need for processing the results. The most simple and obvious processing is computing the solution value at the desired point of the computational domain. In the case of the finite element method it is enough to determine the finite element that contains the point, calculate the values of the local basis functions at this point and sum the products of each basis function value by its respective weight. In case of boundary elements, as mentioned above, each computational point requires evaluation of the integrals over the entire boundary of the subdomain containing this point. It is obvious that this procedure is time consuming, so this paper is concerned with the issue of accelerating the calculation of results in boundary element modeling.

III. THEORY

A. Solution Representation in BEM

To obtain the solution of the Laplace's equation, BEM uses the representation of a harmonic function as a sum of single and double layer potentials [15]:

$$u(\mathbf{r}') = \int_{\partial\Omega} u^*(\mathbf{r},\mathbf{r}') \frac{\partial}{\partial \mathbf{n}_\mathbf{r}} u(\mathbf{r})\, d\Gamma_\mathbf{r} - \int_{\partial\Omega} \frac{\partial}{\partial \mathbf{n}_\mathbf{r}} u^*(\mathbf{r},\mathbf{r}') u(\mathbf{r})\, d\Gamma_\mathbf{r}, \quad (1)$$

where $\partial\Omega$ is the boundary of the subdomain of the computational domain containing point $\mathbf{r}'$, $u^*(\mathbf{r},\mathbf{r}')$ is the fundamental solution of the Laplace's equation, which is given by

$$u^*(\mathbf{r},\mathbf{r}') = \begin{cases} \dfrac{1}{2\pi} \ln \dfrac{1}{|\mathbf{r}'-\mathbf{r}|}, & \text{in 2D,} \\ \dfrac{1}{4\pi |\mathbf{r}'-\mathbf{r}|}, & \text{in 3D.} \end{cases} \quad (2)$$

After applying the boundary element discretization [11], from (1) we obtain the following expression:

$$u(\mathbf{r}') \approx \sum_{i=1}^{M} p_i \int_{\partial\Omega} u^*(\mathbf{r},\mathbf{r}') \varphi_i(\mathbf{r})\, d\Gamma_\mathbf{r} - \sum_{j=1}^{N} q_i \int_{\partial\Omega} \frac{\partial}{\partial \mathbf{n}_\mathbf{r}} u^*(\mathbf{r},\mathbf{r}') \psi_j(\mathbf{r})\, d\Gamma_\mathbf{r}, \quad (3)$$

where $\{\varphi_i\}$, $i = 1..M$ are the basis functions used to approximate the fluxes through the boundary, $\{\psi_j\}$, $j = 1..N$ are the basis functions used to approximate the values on the boundary, p_i, q_j are the weights of decomposition of the flux and the solution by basis functions φ_i and ψ_j respectively.

B. Acceleration methods

Let us call the method for calculating the boundary element solution values according to the formula provided in the preceding paragraph a *direct* method. There are some methods to reduce the costs of calculating the integrals over the entire boundary of the subdomain needed in the direct method. The first method involves accelerating the direct method using the vectoriza-

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tion of calculations. The second one is based on the fast multipole method.

It should be noted that all methods mentioned above, including the direct method, can further be accelerated by parallelizing computations for individual computational points.

C. Vectorization

It is obvious that the integrals can be calculated numerically for all of calculation points that do not lie directly on the boundary of subdomains. After applying the quadrature formulas to (3), $u(\mathbf{r}')$ can be found as follows

$$u(\mathbf{r}') \approx \sum_{i=1}^{M} p_i \sum_{k=1}^{K} \omega_k u^*(\mathbf{r}_k, \mathbf{r}') \varphi_i(\mathbf{r}_k) - \\ - \sum_{j=1}^{N} q_i \sum_{k=1}^{K} \omega_k \frac{\partial}{\partial \mathbf{n}_{\mathbf{r}_k}} u^*(\mathbf{r}_k, \mathbf{r}') \psi_j(\mathbf{r}_k), \tag{4}$$

where $\{\omega_k\}$ and $\{\mathbf{r}_k\}$ are the weights and points of the quadrature respectively, $k = 1..K$.

Since it is usually necessary to determine the value of the solution not at one but at several points, it is effective to change the order of summation and compute independent from the point calculations beforehand

$$\Phi_k = \omega_k \sum_{i=1}^{M} p_i \varphi_i(\mathbf{r}_k), \quad \Psi_k = \omega_k \sum_{j=1}^{N} q_i \psi_j(\mathbf{r}_k). \tag{5}$$

In the result we obtain the following formula

$$u(\mathbf{r}') \approx \sum_{k=1}^{K} \left[u^*(\mathbf{r}_k, \mathbf{r}') \Phi_k - \frac{\partial}{\partial \mathbf{n}_{\mathbf{r}_k}} u^*(\mathbf{r}_k, \mathbf{r}') \Psi_k \right]. \tag{6}$$

Vectorization, in parallel computing, is a kind of parallelization of the program, in which the scalar operations are replaced by operations on arrays (vectors) that handle all of the elements of a vector at one point in time. Such operations are called SIMD-instructions (Single instruction – multiple data). They enable the parallelism at the data level.

One of the modern implementations of SIMD-instructions is AVX (Advanced Vector Extensions). It is an extension of the x86 instruction system for Intel and AMD microprocessors [6].

In the process of evaluating the formula (6), it makes sense to apply the vectorization to the calculation of values $u^*(\mathbf{r}_k, \mathbf{r}')$ and $\frac{\partial}{\partial \mathbf{n}_{\mathbf{r}_k}} u^*(\mathbf{r}_k, \mathbf{r}')$ for a number of quadrature points $\mathbf{r}_k$ simultaneously, and also for the following operations on Φ_k and Ψ_k.

Because realistic problems usually do not require the accuracy of the solution being of more than 5 significant digits, it is permissible to use real numbers in single precision.

The study of the possibility of accelerating the boundary element method using OpenMP and AVX instruction is given in the paper [13].

D. The Fast Multipole Method

The fast multipole method is an algorithm developed by L. Greengard and V. Rokhlin, and was originally intended for speeding up the calculation of long-range interactions in solving the N-body problem. It is based on the representation of the fundamental solution of the Laplace's equation in the form of a multipole expansion, which allows grouping sources located close to each other and treating them as one [4]. Nowadays, the fast multipole method usually is used in conjunction with the boundary element method [3, 5, 10].

Let us provide a brief derivation of the multipole expansion of $u(\mathbf{r}')$ from a form described in formula (6). The multipole expansion of $\frac{1}{|\mathbf{r}' - \mathbf{r}|}$ is given by [3]

$$\frac{1}{|\mathbf{r}' - \mathbf{r}|} \approx \sum_{l=0}^{P} \sum_{m=-l}^{l} R_l^{m*}(\mathbf{r}) I_l^m(\mathbf{r}'), \tag{7}$$

where $R_l^m(\mathbf{r})$ и $I_l^m(\mathbf{r})$ are regular and irregular spherical harmonics respectively, P is a number of harmonics, determining the accuracy of decomposition. A detailed exposition is given in the article by L. Greengard and V. Rokhlin [3].

Applying the obtained expansion to (6) we get the multipole expansion of $u(\mathbf{r}')$:

$$u(\mathbf{r}') \approx \frac{1}{4\pi} \sum_{l=0}^{P} \sum_{m=-l}^{l} I_l^m(\mathbf{r}') \sum_{k=1}^{K} \left[R_l^{m*}(\mathbf{r}_k) \Phi_k - \frac{\partial}{\partial \mathbf{n}_{\mathbf{r}_k}} R_l^{m*}(\mathbf{r}_k) \Psi_k \right]. \tag{8}$$

Note that the expression for the internal sum is independent of r', and, thus, may be calculated once for all computational points:

$$M_l^m = \frac{1}{4\pi} \sum_{k=1}^{K} \left[R_l^{m*}(\mathbf{r}_k) \Phi_k - \frac{\partial}{\partial \mathbf{n}_{\mathbf{r}_k}} R_l^{m*}(\mathbf{r}_k) \Psi_k \right], \tag{9}$$

$$u(\mathbf{r}') \approx \sum_{l=0}^{p} \sum_{m=-l}^{l} I_l^m(\mathbf{r}') M_l^m. \tag{10}$$

Since the area where the calculations of results should be performed is rarely remote enough from all of the points of quadrature, it makes sense to represent them in a hierarchical clustering based on their spatial layout. In this case, each cluster should build its own decomposition, in which the origin of coordinates is a center of the cluster.

To calculate the expansion in clusters with subsidiaries, it is more efficient to use the formulas named Multipole-To-Multipole for calculation instead of direct computation. They are described in detail in the article by L. Greengard and V. Rokhlin [3].

As it was mentioned before, the accuracy of the expansion is determined by the number of harmonics. Ten harmonics are enough for the relative error to be of the order of 10^{-6} for the problem described.

IV. EXPERIMENTAL RESULTS

The experimental results were obtained by solving the problem for the C-shaped dipole magnet shown in Fig. 1. Computational points were located in the working area of the magnet.

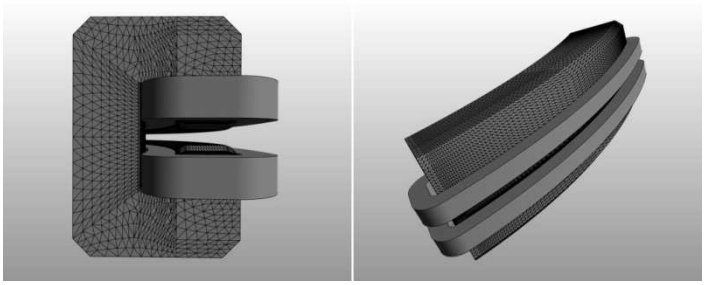

Fig. 1. C-shaped dipole magnet

Fig. 2 shows the dependence of data preparation time and calculation time on the number of computational points for the direct method, vectorization of the direct method (float4) and the multipole method (10 harmonics).

The possibility of further accelerating computations by means of parallelization for individual computational points was also investigated. Fig. 3 shows the computation time for obtaining the solution values in 20,000 points for the sequential and parallel versions of algorithms. Parallelization was carried out in a system with shared memory on the processor Intel Core i7-3770K.

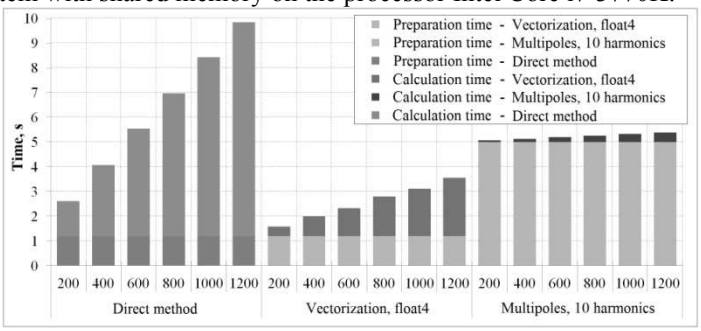

Fig. 2. Preparation and computation times for various numbers of points

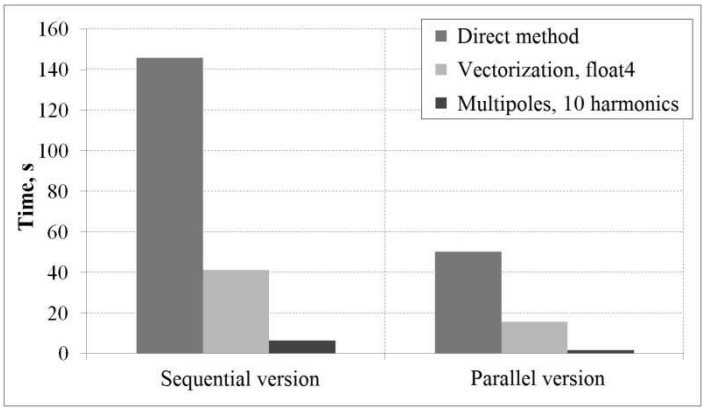

Fig. 3. Calculation time in 20000 points

V. DISCUSSION OF RESULTS

The results of computational experiments show that in case of a small number of points it is not profitable to use the fast multipole method due to the long data preparation time. The use of vectorization speeds up the computation by 4 times compared to the direct method. When the number of computational points becomes more than 1500, the use of multipole becomes reasonable. Fig. 3 shows that for such number of points that the preparation time can be neglected, the use of the parallel fast multipole method can reduce the total computation time by two orders of magnitude.

VI. CONCLUSION

The methods presented make it possible to significantly accelerate the calculation of solution values in given points for boundary element modeling. For a small number of points, it is efficient to use vectorization and parallelization, however, for a large number of points, the parallel fast multipole method is profitable.

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