Fast Multipole Boundary Element Method for Simulation of Composite Materials

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Summary

The simulation of 2D elastic solid containing a large number of inclusions is presented using fast multipole BEM. A scheme of similar sub-domain approach is also applied for the case of identical circular inclusions. Generalized minimum residual method (GMRES) is adopted as an iterative solver for the equation system. The number of inclusions in numerical example computed on one PC reached more than 1,000 by the combination of above-mentioned algorithms. Numerical results show that the fast multipole BEM is applicable to large scale simulation of certain composite materials.

Introduction

Simulation of composite materials has been investigated by more and more researchers. Among the numerical methods to get effective elastic properties of composite materials, BEM is particularly suitable for certain structures that contain many inclusions because of dimension reduction and high accuracy [1]. But conventional BEM is not suitable for large scale problems. The coefficient matrix formed by BEM is dense and sometimes asymmetric. Conventional solution needs $O(N^3)$ operations and $O(N^2)$ memory, where N is the number of DOF. Fortunately, both can be reduced now to $O(N)$ with the help of fast multipole method (FMM).

FMM was first introduced by Rokhlin in 1985 as a fast solver for potential problems[2]. Because of the potential of FMM for solution of large scale problems, fast multipole BEM has been studied by researchers of different fields. Several $O(N\log N)$ and $O(N)$ algorithms for elasticity problems are reported in literature[3,4]. Recently, further improvement of the efficiency of FMM, the new version FMM[5], is finished by using so-called diagonal forms and exponential expansion.

In this paper, the new version of fast multipole BEM and similar sub-domain approach[1] are applied to simulate 2D elastic solid with a large number of arbitrarily or regularly distributed identical circular inclusions. The results of effective elastic properties of such composite materials are obtained by numerical test.

Scheme of Fast Multipole BEM for 2D Elasticity

The boundary integral equation for 2D elasticity without body force is written as:

$$c_{\alpha\beta}(x)u_\beta(x) + \int_\Gamma T^*_{\alpha\beta}(x,y)u_\beta(y)d\Gamma(y) = \int_\Gamma U^*_{\alpha\beta}(x,y)t_\beta(y)d\Gamma(y) \tag{1}$$

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where x and y stand for source point and field point respectively; $x, y \in \Gamma$. $\alpha, \beta = 1, 2$; $c_{\alpha\beta}(x)$ is related to the geometry at point x; u_α, t_α are boundary displacement and traction respectively; $U^*_{\alpha\beta}(x, y)$, $\mathrm{T}^*_{\alpha\beta}(x, y)$ are kernel functions for 2D elasticity.

The basic idea of fast multipole BEM consists of four main steps. In Fig.1, the contribution of far-field integral of field point y to source point x is first shifted to y_0, then from y_0 to y_1, from y_1 to x_0 and finally from x_0 to x_1.

In this paper, the scheme of fast multipole BEM for 2D elasticity in our previous work [6] is modified and new detailed formulations of four main steps are given below.

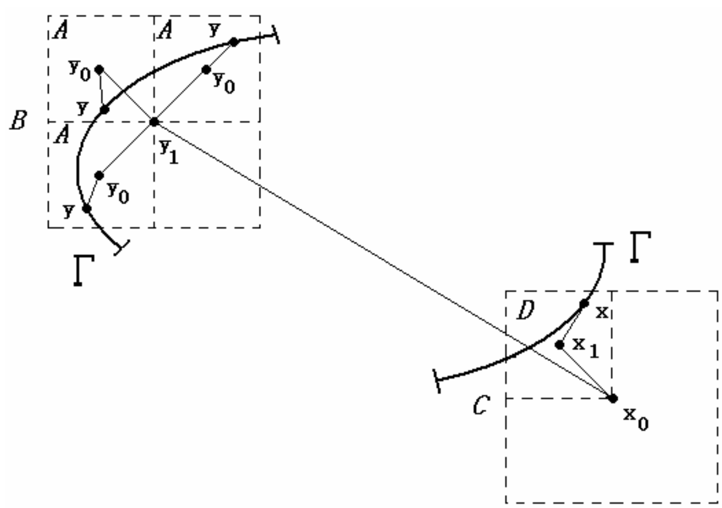

Fig.1 main steps of fast multipole BEM

The first step of fast multipole BEM is the far-field Taylor expansion of kernels with respect to the field point y around a selected point y_0, which is the center of a small square box ***A*** containing y (Fig.1). ***A*** is far enough from source point x, that is, each field point y in ***A*** satisfies $|y - y_0| \le |x - y_0|/2$. Let the kernels be represented by $\psi(x, y)$, which can be expanded to the following complex Taylor series:

$$\psi(x, y) = \sum_{k=0}^{\infty} \frac{1}{k!} \psi^{(k)}(x, y_0)(y - y_0)^k \tag{2}$$

Expanding the kernel, the detailed Taylor series of $H(x)$, which denote the integral $\int_{\Gamma_f} U^*_{\alpha\beta}(x, y) t_\beta(y) d\Gamma(y)$, are shown in Eq. (3). There are six items used in the previous work[6] for expansion; and they are simplified using only one half items now.

$$
\begin{aligned}
H(x) = & \sum_{k=0}^{\infty} \mathrm{Re}\left[f(x-y_0,k) c_f(y_0,k) \right] + \sum_{k=1}^{\infty} \mathrm{Re}\left[f^{(r)}(x-y_0,k) c_{fr}(y_0,k) \right] \\
& + \sum_{k=1}^{\infty} \mathrm{Re}\left[f^{(i)}(x-y_0,k) c_{fi}(y_0,k) \right]
\end{aligned} \tag{3}
$$

where [3]

$$
f(x,k) = \begin{cases} \ln(x), k=0 \\ \dfrac{1}{x^k}, k=1,2,\ldots \end{cases} \qquad f^{(r)}(x,k) = \frac{\mathrm{Re}(x)}{x^k}, \quad f^{(i)}(x,k) = \frac{\mathrm{Im}(x)}{x^k}, k=1,2,\ldots \tag{3a}
$$

Series $c(y_0,k)$, called multipole moments, are only related to integral of y. They are calculated only once and can be used for different source point x to obtain $H(x)$.

Another integral $\int_{\Gamma_f} T^*_{\alpha\beta}(x,y) u_\beta(y) d\Gamma(y)$ can be expanded similarly.

The second step of fast multipole BEM is the shift of multipole to multipole moments. Point y_1 is the center of a larger box ***B*** containing the initial box ***A*** (Fig.1). Replacing y_0 by y_1, $H(x)$ can be rewritten similarly to Eq.(3). The new multipole moments $c(y_1,k)$ can be obtained by the old ones, $c(y_0,k)$.

The third step of fast multipole BEM is the shift of multipole to local moments. Point x_0 is the center of a box ***C*** containing source point x, and box ***C*** is as the same size as ***B*** (Fig.1). By expanding the kernels with respect to source point x around x_0, another Taylor series, called local expansion, is obtained:

$$
\begin{aligned}
H(x) = \sum_{k=0}^{\infty} \Big\{ & \mathrm{Re}\left[(x-x_0)^k d_n(x_0,k) \right] + \mathrm{Re}\left[\mathrm{Re}(x-x_0)(x-x_0)^k d_{nr}(x_0,k) \right] \\
& + \mathrm{Re}\left[\mathrm{Im}(x-x_0)(x-x_0)^k d_{ni}(x_0,k) \right] \Big\}
\end{aligned} \tag{4}
$$

where the new series $d(x_0,k)$ are called local moments. They can be obtained by the multipole moments $c(y_1,k)$.

The forth step of fast multipole BEM is the shift of local to local moments. Point x_1 is the center of the smaller box ***D*** containing source point x, and box ***D*** is ***C***'s child (Fig.1).

Replacing x_0 by x_1, $H(x)$ can be rewritten similarly to Eq.(4). The new local moments $d(x_1, k)$ can be obtained by the old moments $d(x_0, k)$.

A tree structure is used to get both multipoles and local moments recursively. In each iterative step of GMRES, matrix-vector product is replaced by operation on the tree, which only costs $O(N)$.

In new version of fast multipole BEM, the third step is replaced by another three new steps. Because the basic idea of new version fast multipole BEM for 2D elasticity is introduced briefly in literature [7] and the formulation of new version is similar to that of this paper, they are not listed here.

Numerical Results

Results of numerical tests are presented below. All numerical tests are taken on a PC with Pentium IV (1.8GHz) and 1GB memory.

Example 1: To verify accuracy of fast multipole BEM for large scale problems, the comparison of two periodical structures subjected boundary loads proportional to their edge length respectively is made: Sub-structure of these two structures is a square plate of 1×1 mm with a circular inclusion of radius 0.3mm in the center, as shown in Fig. 2(a). The former structure consists of 2×2 sub-structures, 4 inclusions, 26,880 DOF, subjected on outer boundary with given normal displacement u_n=0.0002mm, as shown in Fig. 2(b). The latter consists of 40×40 sub-structures, 1,600 inclusions, 544,000 DOF, subjected with given normal displacement u_n =0.004mm. The material properties are: matrix $E_b = 200$MPa, $\nu_b = 0.3$, inclusions $E_i = 400$MPa, $\nu_i = 0.3$.

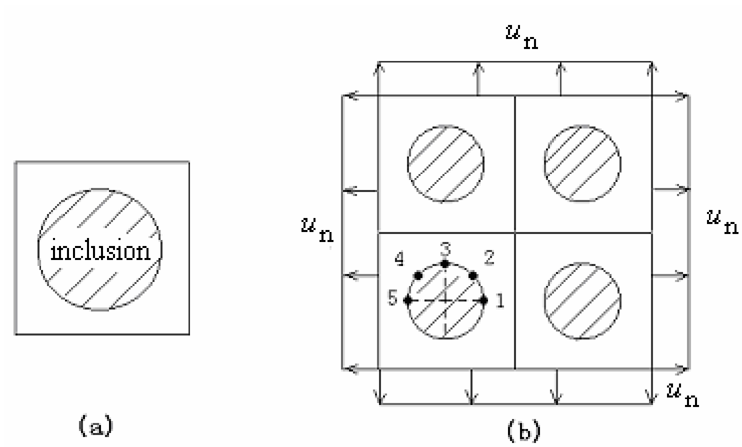

Fig.2 sub-structure and periodic structure with inclusions

In Table 1, results at some selected points in Fig. 2(b) on the boundary of two corresponding inclusions that belong to 2×2 and 40×40 structures respectively are compared. The difference between them is approximately 1×10^{-5}.

Table 1 Comparison of displacement and traction of some selected points

Selected point		1	2	3	4	5
Displacement $u_n(\text{mm})\times10^{-5}$	2×2	6.0619	10.0911	5.6697	−4.3262	−14.3269
	40×40	6.0619	10.0910	5.6697	−4.3262	−14.3268
Traction $t_n(\text{MPa})\times10^{-2}$	2×2	7.94244	7.68617	7.94238	7.68618	7.94237
	40×40	7.94238	7.68614	7.94239	7.68614	7.94239

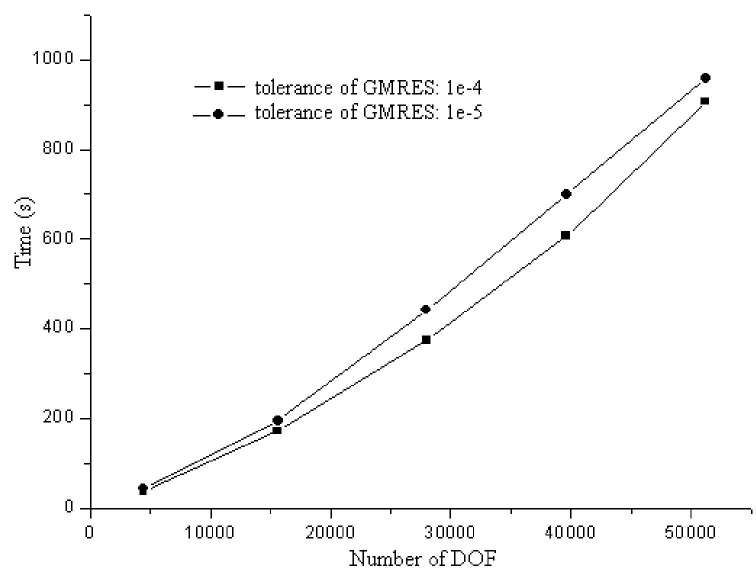

Fig.4 Time cost versus different number of DOF and tolerance of GMRES

Table 2 Effective volume moduli of different number of inclusions

Number of inclusions	10	50	100	150	200
Number of DOF	4,400	15,600	28,000	39,600	51,200
Effective volume modulus (MPa)	239.5	239.7	239.6	239.6	239.6
Effective volume modulus using IDD (MPa)					242.3

Example 2: 2D elastic solids with different number of arbitrarily distributed identical circular inclusions are simulated and time costs are shown in Fig.4. Results of effective volume moduli are listed and compared with an analytic solution of interaction direct deviation method (IDD) [8] in Table 2. The volume ratio of inclusions to whole region is fixed to be 0.2. The material properties are: matrix E_b= 200 MPa, ν_b = 0.3, inclusions E_i = 1000MPa, ν_i = 0.3.

Conclusions

In this paper, a new version of fast multipole BEM combined with similar sub-domain approach is applied for simulation of certain 2D composites containing a large number of inclusions. Numerical results show that the presented algorithm is efficient for certain large scale simulations. The further investigation will be extended to the simulation of 3D composites with inclusions.

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