A Novel Approach for Volume-Integral Evaluation in the BEM

Jian Ding* and Wenjing Ye**

Woodruff School of Mechanical Engineering, Georgia Institute of Technology
771 Ferst Dr., Love 316, Atlanta, GA 30332, USA
*gte731s@prism.gatech.edu, **wenjing.ye@me.gatech.edu

ABSTRACT

For non-homogeneous or nonlinear problems, a major difficulty in applying the Boundary Element Method (BEM) is the presence of volume integrals in the boundary integral formulation. In this paper, we describe a novel approach for evaluating these volume integrals without volume discretization of the problem domain. Based on this approach, an accelerated BEM solver for Poisson equations using only surface discretization has been developed. Case studies have been performed and results have been compared with analytical solutions.

Keywords: Poisson equation, BEM, volume integral, fast algorithm.

1. INTRODUCTION

The need for efficient solutions to problems with complex 3-D geometries, such as those encountered in microelectromechanical systems (MEMS), has led to the development of fast algorithms. Based on the accelerated Boundary Element Method (BEM) [1,2], fast solvers for electrostatic problems [3], Stokes problems [4], etc. have been developed and applied successfully in solving practical problems [5]. However, to date most applications of the BEM have been limited to linear and homogeneous problems. For non-homogeneous or nonlinear problems, a major difficulty in applying the BEM is the presence of volume integrals in the boundary integral formulation (BIE). One common approach for treating the volume integrals is to perform a volume discretization [6,7]. Unless the nonlinearity exists only in a small region, such an approach loses the major advantage of the BEM – the need of only surface discretization. In this paper, we describe a novel approach for evaluating volume integrals resulted from either a nonlinear problem or a non-homogeneous problem without volume discretization of the problem domain.

The key idea of the proposed approach is to use the 3-D uniform grid, which was initially constructed to accelerate the surface integration [1], to perform the volume integration. This grid is independent of the problem domain. The only requirement is that the grid must encompass the problem domain. Detailed description is given in the section that follows. The advantage of the proposed approach is twofold: (1) volume discretization of the problem domain is avoided and (2) the 3-D uniform grid can also be used to accelerate the volume integration.

Based on this approach, an accelerated BEM solver for Poisson equations using only surface discretization has been developed. Results from the fast Poisson solver are compared with analytical solutions. The convergence of the proposed approach as well as its efficiency and accuracy are demonstrated.

2. THE PROPOSED APPROACH

For the purpose of clarity, we use the Poisson equation to illustrate the proposed approach. The general form of the Poisson equation reads

\[ \nabla^2 u = b, \]  

where \( u \) is the unknown function and \( b \) is the non-homogeneous term. The equivalent integral formulation is given as following:

\[
\begin{align*}
    u(x) &= \frac{\partial G(x,y)}{\partial n(y)} u(y) dS(y) - \int \frac{\partial u(y)}{\partial n(y)} G(x,y) dS(y) \\
    &= \int_B b(y) G(x,y) dv(y), \quad x \in \partial \Omega.
\end{align*}
\]

In (2), \( G(x,y) \) is the Green’s function of the Laplace operator,

\[ G(x,y) = \frac{1}{4\pi r}, \]  

where \( r = |x-y| \).

\( n(y) \) is the normal vector at the field point \( y \) and \( \Omega \) is the problem domain. The volume integral on the right-hand side of (2) requires volume discretization of \( \Omega \) if a standard method is employed. In this work, we propose to use the uniform 3-D FFT grid, which was set initially for accelerating the surface integration [1], to perform the volume integration (see Fig.1). This is done by defining \( \tilde{b}(y) = b(y) \) if \( y \in \Omega \) and \( \tilde{b}(y) = 0 \) if \( y \in B \setminus \Omega \), where \( B \) is a set of cubes consisted by the FFT grid. Thus, the volume integral in (2) \( \int_B b(y) G(x,y) dv(y) \) is replaced by a volume integral performed on the grid, i.e., \( \int_B \tilde{b}(y) G(x,y) dv(y) \).
The precorrected-FFT accelerated technique for surface integrals [1] can be extended to accelerate the volume integration. The implementation of acceleration is similar to that of surface integrals, that is, the volume integral is separated into two parts, nearby interactions and far-field interactions. The nearby interaction is calculated directly. The far-field interactions are calculated approximated using the Fast Fourier Transform.

2.1 Nearby interactions

A major difficulty in calculating nearby interactions is the evaluation of singular integrals, i.e., integrals correspond to the case when the evaluation point \( \mathbf{x} \) is on the cube (see Fig.2(a)). Due to the singularities of the integrands, standard Gauss quadrature (GQ) will not give accurate results. We employed a “projection + transformation” scheme to accurately evaluate the singular integrals. As illustrated in Fig. 2, the cube is first separated into several prisms according to the surface panels on the cube (projection).

For the singular prism (i.e., the one with the evaluation point, Fig.2(b)), it is further separated into three smaller prisms, each with the evaluation point as one of its vertices (Fig.2(c)). A transformation similar to the one in [8] is then performed to remove the singularity (Fig.2(d)) and Gauss quadrature is employed to evaluate the resulted non-singular integrals. High accuracy can be achieved by using high-order Gauss quadrature.

This “projection-transformation” scheme not only can remove the singularities associated with the integrands, but also can be applied to problem domains with irregular boundaries.

2.2 Far-field interactions

Since the volume integrals that we deal with are of convolution form, the precorrected-FFT technique can be used to speed up the evaluation. To do so, a projection of the density functions (\( \hat{b} \) in the Poisson equation case) onto the surrounding grid points (marked with subscript \( g \)) is done first. Once the grid densities have been calculated, the FFT technique is employed to compute the convolution on the grid. The results are then interpolated back to the evaluation point. This procedure is summarized in the equation shown in (3).

\[
\int_{B_i} G(x,y) b(y) dv(y) \approx \sum_{g} G_g(x,y_g) \int_{B_g} b(y) w_g(y) dv(y)
\]

where \( B_i \) is the \( i \)-th cube and \( w_g \) is the projection operator to \( g \)-th grid point. In the examples presented in this paper, the volume integral \( \int_{B_g} b(y) w_g(y) dv(y) \) is evaluated using 3D Gauss quadrature since the integrand is a non-singular function and \( B_i \) is a regular shaped domain. \( w_g \) is obtained through a transposed polynomial interpolation scheme [1,9] which only involves information of the relative position of the projection point to the grids geometry. For cubes that are either within or outside the problem domain (\( \Omega \)), the relative position of Gauss points to the grid points are the same therefore the projection operators \( w_g \) are the same for these cubes. Thus, for a given order of Gauss quadrature, a normalized unit cube can be used to represent these cubes and \( w_g \) can be pre-computed and stored to achieve some efficiency.

Figure 2. (a) A cube with the evaluation point on the surface; (b) Projection: the cube is separated into two prisms; (c) Singular prism: it is separated into three smaller prisms; (d) Transformation: prism 1 is transformed into the cube in (e).
2.3 Numerical implementation

The integral equation shown in (2) was solved using a boundary element method together with the precorrected-FFT acceleration technique. A piece-wise constant collocation scheme is used to discretize the integral equations. The surface of the structure is discretized into $n$ small panels. On each panel, $u$ and $\partial u/\partial n$ are assumed to be constant. A system of equations for the panel unknowns is then derived by insisting that the integral equations are satisfied at each panel centroid. The result is a linear system which relates the known quantities ($u$ and $d$ in our example) to the unknown quantities ($q_u$ and $q_n$), as in Equation (4)

$$G \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_n \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix} + F \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}.$$  (4)

In (4), the load vector $d$ consists of the volume integrals shown in (2). The linear system in (4) was then solved using the iterative method, GMRES [10] and accelerated using the precorrected-FFT technique [5].

3. RESULTS AND DISCUSSION

3.1 Singular case

The proposed approach (projection + transformation) for handling singular volume integrals was tested by evaluating $\int_\Omega \frac{1}{\| \mathbf{x} - \mathbf{y} \|} d\mathbf{v}(\mathbf{y})$ on the singular prism shown in Figure 2(b). Results are given in Table 1 together with those obtained by applying Gauss quadrature directly without removing the singularity (direct Gauss quadrature scheme).

Table 1. Results of $\int_\Omega \frac{1}{\| \mathbf{x} - \mathbf{y} \|} d\mathbf{v}(\mathbf{y})$ on the singular prism shown in Fig. 2(b) using the “projection-transformation” scheme

<table>
<thead>
<tr>
<th>Order of GQ</th>
<th>Convergence of proposed method</th>
<th>Convergence of direct Gauss quadrature scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>6.13402</td>
<td>7.15768</td>
</tr>
<tr>
<td>10</td>
<td>6.86821</td>
<td>9.14612</td>
</tr>
<tr>
<td>15</td>
<td>6.87066</td>
<td>9.44576</td>
</tr>
<tr>
<td>19</td>
<td>6.87047</td>
<td>9.39324</td>
</tr>
<tr>
<td>Comment</td>
<td>Converged using $O(19)$ GQ</td>
<td>Not converged using up to $O(100)$ GQ</td>
</tr>
</tbody>
</table>

From Table 1, with order of 19, the result obtained by the “projection + transformation” scheme converges to at least 4 digits while the direct Gauss quadrature scheme fails to converge even with order of 100. This indicates the singularity of the integrand has been successfully removed by the proposed approach.

3.2 Results for volume integral

The accuracy and efficiency of the proposed approach (i.e., the nearby interactions are calculated directly and far-field interactions are computed using the precorrected-FFT technique) for volume integral evaluation ($\int_\Omega \frac{1}{\| \mathbf{x} - \mathbf{y} \|} d\mathbf{v}(\mathbf{y})$) were tested on the domain shown in Figure 3. Results, compared with those obtained from direct calculation (i.e., without the acceleration), are shown in Tables 2 and 3 respectively. The FFT cubes were constructed using the grid points (shown in Figure 3).

Table 2. Results of $\int_\Omega \frac{1}{\| \mathbf{x} - \mathbf{y} \|} d\mathbf{v}(\mathbf{y})$ on the singular prism shown in Fig. 2(b) using “projection-transformation” scheme

Case 1 is for the domain with 300 surface panels and case 2 is for a 1200 surface-panel-discretization. The two cases use different numbers of FFT cubes. More cubes are used in case 2 to speed up the computation. By increasing the order of Gauss quadrature for both singular case and non-singular cases, converged results are obtained. The results shown in Tables 2 and 3 are obtained using $O(18)$ and $O(14)$ GQ for case 1 and case 2 respectively in singular interaction evaluation and $O(2)$ GQ for non-singular interactions. It is clear that error introduced by the acceleration is very small and saving in the computational cost is significant. Also, the more FFT cubes used, the more efficient the computation.
Table 2. Accuracy of the proposed approach for volume integration (acceleration vs. direct).

<table>
<thead>
<tr>
<th></th>
<th>Direct integration</th>
<th>Proposed approach with pFFT acceleration</th>
<th>Relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0.871063</td>
<td>0.871867</td>
<td>0.092%</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.819738</td>
<td>0.819828</td>
<td>0.011%</td>
</tr>
</tbody>
</table>

Table 3. Computational time (in seconds) of proposed approach for volume integration.

<table>
<thead>
<tr>
<th></th>
<th>Direct integration</th>
<th>Proposed approach with pFFT acceleration</th>
<th>Acceleration percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>73.234</td>
<td>74.969</td>
<td>2.37%</td>
</tr>
<tr>
<td>Case 2</td>
<td>97.391</td>
<td>114.36</td>
<td>17.42%</td>
</tr>
</tbody>
</table>

3.3 Application example—Poisson problem

Based on the proposed approach, a 3-D Poisson solver has been developed. This solver was tested on a specific equation of

\[ \nabla^2 u = 1. \]  \tag{5} \]

The boundary conditions are prescribed according to those indicated in Figure 4. The corresponding analytical solution to this problem is

\[ u = \frac{x^2}{2}, \quad \frac{\partial u}{\partial n} = x \cdot n_x. \]  \tag{6} \]

Figure 4. Case study of the Poisson solver: \( \nabla^2 u = 1 \).

Table 4 gives the simulation results and comparison with the analytic solution. The efficiency and accuracy of the proposed approach have been demonstrated. It should be pointed out that the error shown in Table 4 contains error introduced from volume integration as well as from surface integration. In fact, the total error in this example is dominated by the error introduced by surface integration, which is around 12% for the 300 surface-panel-discretization case and 9% for the 1200 surface-panel-discretization case.

Table 4. Performance of the Poisson solver based on the proposed approach: errors (measured in L2-norm which is calculated as \[ \sum_{i=1}^{N} \left( \int \left( \frac{\partial u}{\partial n} \right)^2 ds \right) ds \] , obtained by comparing the simulation with analytical solutions) and CPU time.

<table>
<thead>
<tr>
<th>Error # of surface panels</th>
<th>300</th>
<th>1200</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct integration</td>
<td>13.55%</td>
<td>8.18%</td>
</tr>
<tr>
<td>(no-acceleration)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>pFFT-approach</td>
<td>13.58%</td>
<td>8.19%</td>
</tr>
<tr>
<td>(with acceleration)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Time savings percentage</td>
<td>3.59%</td>
<td>36.8%</td>
</tr>
<tr>
<td>(acceleration vs. direct)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

5. CONCLUSIONS

In this paper, we described an efficient numerical approach to compute volume integrals present in the boundary integral formulations of non-homogeneous or nonlinear problems. A “projection-transformation” scheme is used to improve the accuracy of the evaluation of singular interactions. For non-singular interactions, 3D Gauss quadrature combined with precorrected-FFT technique results in significant time savings while maintaining a good accuracy. A 3-D Poisson problem was solved using the developed fast solver. The efficiency and accuracy of the proposed approach have been demonstrated.

REFERENCES