Fast BEM Solution for Coupled 3D Electrostatic and Linear Elastic Problems

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ABSTRACT

This paper presents the development of a precorrected-FFT accelerated linear elastic Boundary Element Method solver that can be coupled with existing BEM solvers for electrostatic and Stokes Flow problems. The resulting coupled solvers are mesh consistent—requiring a single mesh for all domains. A number of test cases are evaluated with the linear elastic solver, as well as a coupled electrostatic-structural plate bending problem. performance of the accelerated solver is very good, approaching $\mathcal{O}(N \log N)$ for CPU time and memory expense for most test cases. Accuracy is reasonable, but for some problems highly refined meshes may be required to achieve this.

Keywords: boundary element method, linear elasticity, precorrected-FFT, coupled problems

1 Introduction

In order to support the continued growth of Micro- and Nanosystems, efficient modeling techniques—capable of solving complex coupled systems—are needed. One modeling solution that addresses some of the issues of microsystem modeling is the Boundary Element Method (or BEM, detailed descriptions may be found in many references e.g. [2]). The characteristic advantage of the BEM is the reduction in dimensionality of the problem by one. This can result in a significantly smaller mesh and system of equations than would result from domain based methods (Finite Difference or Finite Element). This advantage is most dramatic in problems with infinite or semi-infinite domains—common in the study of potential flow (fluids, electrostatics, magnetic, heat transfer, soil mechanics, and microsystems).

Although smaller, the systems of equations resulting from the BEM formulation are also fully dense, offsetting some of the computational benefits of the reduced system size. Recent developments of matrix compression techniques, such as Fast Multipole Method (FMM) [5, 7], panel clustering [6], precorrected-FFT (or PFFT) technique [4,8], wavelet-like method [3], have done much to overcome this drawback of the BEM. This paper presents the development of a precorrected-FFT BEM solver for mesh mesh-consistent coupled 3D electrostatic-structural analyses (mesh-consistency meaning the same mesh is used for multiple analysis domains). This avoids many of the difficulties encountered in hybrid FEM/BEM solver (usually FEM for structural domain, BEM for electrostatic or fluid domain) especially translation of mesh solutions between analysis domains and mesh deformation [1].

2 Integral Equations

The BEM is an integral method—thus requiring an an integral form of the governing equations. For 3D linear elasticity this formulation is

$$\begin{aligned} u_j(\boldsymbol{\xi}) &= \int_S \left[t_i(\boldsymbol{x}) G_{ij}(\boldsymbol{x}, \boldsymbol{\xi}) - F_{ij}(\boldsymbol{x}, \boldsymbol{\xi}) u_i(\boldsymbol{x}) \right] \mathrm{d}S(\boldsymbol{x}) \\ &\quad + \int_V \boldsymbol{\psi}(\boldsymbol{z}) G_{ij}(\boldsymbol{z}, \boldsymbol{\xi}) \, \mathrm{d}V(\boldsymbol{z}) \end{aligned} \tag{1}$$

This study uses constant plane triangular elements and neglects any body forces ($\phi(z)$), allowing the discretized form of the integral equation to be simplified as follows:

$$\mathrm{c}\boldsymbol{u}^p = \sum_{q=1}^{N} \left\{ \begin{array}{l} \left[\displaystyle\int_{\Delta S_q} \mathrm{G}^{pq} \, \mathrm{d}S_q \right] \boldsymbol{t}^q \\ \qquad - \left[\displaystyle\int_{\Delta S_q} \mathrm{F}^{pq} \, \mathrm{d}S_q \right] \boldsymbol{u}^q \end{array} \right\} \tag{2}$$

where t_i and u_i are tractions and displacements, respectively, S and V are the surface and volume over which the integrations are performed (volume integration is only necessary in the case of body forces), and

$$\mathrm{G}^{pq} = G_{ij}(\boldsymbol{x}^q, \boldsymbol{\xi}^p) \tag{3}$$

$$\mathrm{F}^{pq} = F_{ij}(\boldsymbol{x}^q, \boldsymbol{\xi}^p) \tag{4}$$

are the kernel functions with respect to field point p and load point q. Integration is with respect to $\boldsymbol{x}$ over the surface ΔS of the boundary element [2]. The "free term" coefficient matrix, c, arises from dealing with the singular F kernel integral (i.e. when $\boldsymbol{x} = \boldsymbol{\xi}$) and for constant plane elements is defined as:

$$\mathbf{c} = \begin{cases} 1/2\,\mathrm{I} & \text{if } \boldsymbol{\xi} \in S \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

where I is the identity matrix.

The definitions of the fundamental solutions (also referred to as kernel or Green's functions) $G_{ij}(\boldsymbol{x},\boldsymbol{\xi})$ and $F_{ij}(\boldsymbol{x},\boldsymbol{\xi})$ for linear elasticity are given by:

$$G_{ij}(\boldsymbol{x},\boldsymbol{\xi}) = \frac{1}{8\pi(1-\nu)}\frac{1}{r}\left[(3-4\nu)\delta_{ij} + \frac{y_i y_j}{r^2}\right] \tag{6}$$

$$F_{ij}(\boldsymbol{x},\boldsymbol{\xi}) = -\frac{1}{16\pi(1-\nu)}\frac{1}{r^2}\left[\begin{array}{l}(1-2\nu)\left(n_j\frac{y_i}{r} - n_i\frac{y_j}{r}\right) \\ +\left(\frac{3y_i y_j}{r^2} + C_4\delta_{ij}\right)\frac{y_k}{r}n_k\end{array}\right] \tag{7}$$

with $\boldsymbol{x}$ designated the "load" (or "source") point and $\boldsymbol{\xi}$ the "field" (or "evaluation") point, $y_i = \xi_i - x_i$, $r^2 = y_i y_i$ [2].

The appropriate discretized integral formulation and kernel function for 3D electrostatics are given by

$$\phi^i = \sum_{j=1}^{N}\left\{\left[\int_{\Delta S_j} G^{ij}\ \mathrm{d}S_j\right] q^j\right\} + \phi_\infty \tag{8}$$

and

$$G^{ij} = G(\boldsymbol{\xi}^i, \boldsymbol{x}^j) = -\frac{1}{4\pi\epsilon}\frac{1}{r} \tag{9}$$

with the same r, $\boldsymbol{x}$, and $\boldsymbol{\xi}$ as previously defined [10], ϵ is the permittivity of the medium, and q is the charge density. In free space, $\epsilon = \epsilon_0 = 8.85419$ pF/μm. For conductors the panel tractions, $\boldsymbol{t}$, can be calculated directly from the panel charges:

$$\boldsymbol{t} = -\frac{q^2}{2\epsilon}\boldsymbol{n} \tag{10}$$

where $\boldsymbol{n}$ is the outward normal of the panel. For a meaningful solution charge conservation must also be enforced:

$$Q_{total} = \int_S q\ \mathrm{d}S = 0 \tag{11}$$

3 Implementation

The linear elastic BEM solver presented here builds on previous PFFT implementations. Constant elements allow analytical evaluation of singular and non-singular panel integrations, transparent transfer of data between coupled models and simplify any mesh deformation. The collocation scheme is used (Equations (2), (8), and (11)) requiring the boundary conditions to be satisfied at certain nodes of each panel (for constant elements, boundary conditions are satisfied at the centroid of each panel). This leads to a linear system of equations that is solved using the GMRES iterative method coupled with the precorrected-FFT acceleration technique. The basis of acceleration techniques (PFFT, FMM, etc.) is that far-field interactions may be approximated, rather than calculated directly.

Figure 1 illustrates the procedure for computing the far-field interactions—interaction between two panels (p and q) with panel p being the evaluation panel and panel q being the source panel. First, the density function (displacement, traction, or charge density) of the source panel is projected onto the surrounding grid points by a transposed polynomial interpolation [11] (Step 1). A FFT technique is then employed to compute the matrix-vector products on the grid points by convolving the projected grid-point densities with the corresponding kernels (Green's function) (Step 2). Finally the matrix-vector product on the evaluation panel is extrapolated from the products on the surrounding grid points via polynomial interpolation (Step 3). For a detailed description of the precorrected-FFT technique, readers are referred to [9, 11].

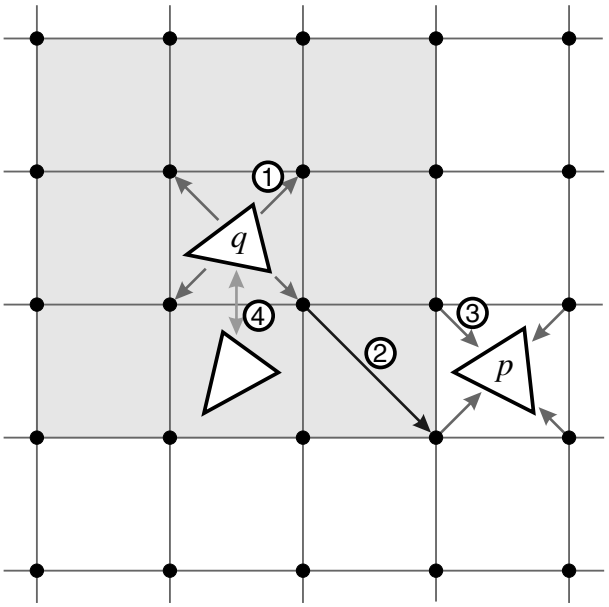

Figure 1: Diagram illustrating the steps of the precorrected-FFT: superposed uniform grid, projection (1), convolution (2), interpolation (3), and direct interactions (4).

Near-field interactions are evaluated in the conventional manner: integrating the kernel functions over the panels to populate the near-field portions of the system matrix and multiplying them with the density functions on the source panels (Step 4). These integrals are evaluated analytically to ensure the greatest accuracy possible. The contributions of the near- (direct) and far-field (PFFT) are then summed together to approximate the matrix-vector product for that iteration.

In theory, the PFFT technique can reduce the computational expense (memory and CPU time) from $\mathcal{O}(N^2)$ (for the unaccelerated setup and iterative solution of the BEM) to $\mathcal{O}(N \log N)$ for most problems. A simple relaxation scheme was used for the coupled electrostatic-structural solver.

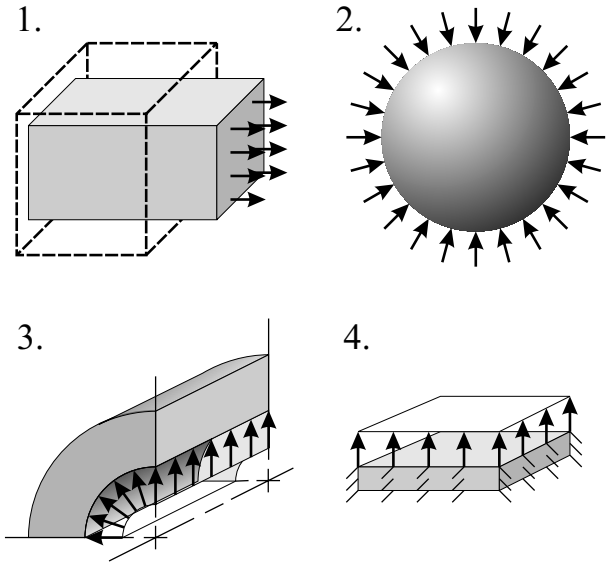

Figure 2: Case Studies: 1. Axially loaded bar, 2. hydrostatically loaded sphere, 3. thick-walled pressure vessel, 4. plate bending (uniform and coupled electrostatic loading)

4 Performance

A number of different case studies (see Fig. 2) were used to evaluate the performance of the PFFT linear elastic solver. Table 1 briefly summarizes some of these results. (Material properties are for polysilicon: $E = 165$ GPa, $\nu = 0.33$.) In general the PFFT has slightly higher error than the direct solution for a given mesh. However, the PFFT is capable of solving much more refined meshes than a direct solver as both memory requirements and CPU times significantly reduced—allowing improved accuracy and performance. Figs. 3 and 4 present the the percent error and CPU cost (respectively) for the axially loaded bar case—illustrating the accuracy and performance ($\mathcal{O}(N \log N)$ vs. $\mathcal{O}(N^2)$ CPU time trends). Similar results (accuracy and performance) were obtained from the hydrostatically loaded sphere pressure vessel, and plate bending problems. The solution of the pressure vessel takes advantage of the ability of the BEM to directly calculate (rather than interpolate) the solution (displacement or stress) at any point internal to the body, based on the solution at the surface. The displacements of three internal points and the inner and outer surfaces were compared to a converged finite element model, with very good agreement.

A common micromechanical feature is a membrane (or plate) subject to a pressure—either atmospheric or the result of electrostatic potential. As such, this is an ideal test case for mesh consistent coupled solutions. For the pressure loading case the boundary conditions consisted of clamped edges and a uniform pressure ap-

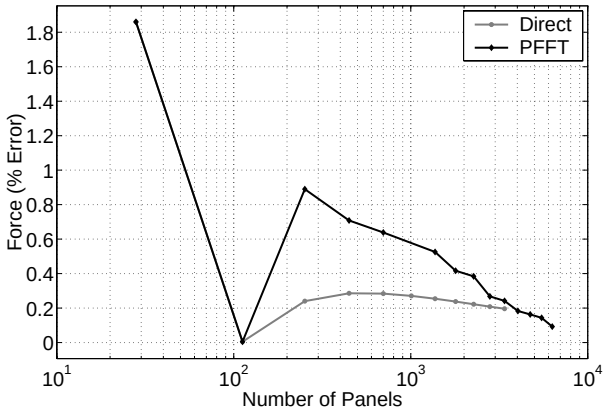

Figure 3: Percent Error vs. mesh size for Direct and PFFT linear elastic BEM solver

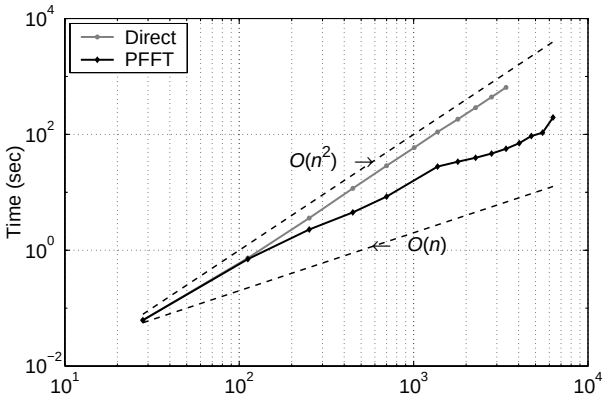

Figure 4: CPU time vs. mesh size for Direct and PFFT linear elastic BEM solver

Table 1: Results of Case Studies (cases as illustrated in Fig. 2)

Case	Error Type	Error
1[a]	Percent error of reaction force	0.092%
2[b]	Percent RMS error with reference to effective pressure	0.365%
3[c]	Average error of displacement at radial locations	1.967%
4[d]	Percent error of maximum displacement	6.967%
4[e]	Percent error of maximum displacement	2.093%

[a]Bar $L = 3$ µm, $W = H = 1$ µm, $d = 0.003$ µm, 6300 elements
[b]Unit Sphere (1 µm) subject to uniform compressive deflection of 1 nm, 12288 elements
[c]$R_o = 25$ µm, $R_i = 10$ µm, $P_o = 0$ MPa, $P_i = 100$ MPa, 1568 elements
[d]$L = W = 10$ µm, $T = 1$ µm, $P = 100$ MPa uniform, 30720 elements
[e]$L = W = 10$ µm, $T = 1$ µm, $Gap = 2.25$ µm, $V = 10$ kV, 30720 elements

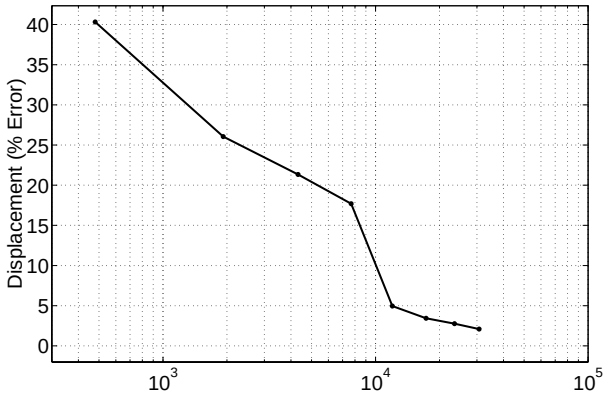

Figure 5: Convergence of coupled electrostatic-structural plate bending problem with mesh refinement.

plied to the upper surface of the plate. A large number of elements were needed to achieve reasonable results reaching a minimum error of less that 7% (converged FEM used as the reference solution) revealing some of the weakness of the BEM in dealing with bending problems. For the coupled problem, the tractions resulting from the electrostatic solution are applied to the structural problem and the resulting displacement field solution used to "morph" the electrostatic mesh. The morphed mesh is then used to again solve for the electrostatic traction and the process repeated in a relaxation scheme until a desired level of convergence is achieved. The solution is compared to results from a coupled analysis using CoventorWare™and achieved an error of less than 2% (with 30720 elements, see Fig. 5). (No convergence study was performed on the CoventorWare™solution and this may explain the apparently lower error of the coupled solution).

5 Conclusions

In this paper we have presented the BEM formulation for 3D linear elasticity and electrostatics and discussed the implementation of the BEM with constant elements and the precorrected-FFT acceleration technique. A number of test cases have been evaluated producing reasonably good accuracy. Computational efficiency is improved significantly by the PFFT technique with relatively small increase in error. Furthermore much more refined meshes can be analyzed than are possible with unaccelerated BEM. The solution of a coupled electrostatic-structural plate bending problem shows promise for the PFFT BEM as a useful tool in micro- and nanoscale modeling.

Acknowledgements

This work builds on previous BEM implementations for capacitance extraction (FastCap [8]) and Stokes Flow (FastStokes) [11].

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