A DIFFERENTIAL ALGEBRAIC FRAMEWORK FOR THE FAST INDIRECT BOUNDARY ELEMENT METHOD

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Abstract

Beam physics at the intensity frontier must account for the beams' realistic surroundings on their dynamics in an accurate and efficient manner. Mathematically, the problem can be expressed as a Poisson PDE with given boundary conditions. Commonly, the Poisson boundary value problem is solved locally within many volume elements. However, it is known the PDE may be re-expressed as indirect boundary integral equations (BIE) which give a global solution [1]. By solving the BIEs on M surface elements, we arrive at the indirect boundary element method (iBEM). Iteratively solving this dense linear system of form $Ax = b$ scales like $O(m_{\text{iterations}}M^2)$. Accelerating with the fast multipole method (FMM) can reduce this to $O(M)$ if $m_{\text{iterations}} \ll M$. For N evaluation points, the total complexity would be $O(M) + O(N)$ or $O(N)$, $N = M$. We have implemented a constant element version of this fast iBEM based on our previous work with the FMM in the differential algebraic (DA) framework [2]. This implementation is to illustrate the flexibility and accuracy of our method. A future version will focus on allowing for higher order elements.

INTRODUCTION

High intensity charged particle beams have been applied in an ever-growing number of areas. Modern scientific, medical, and industrial applications require precise control and/or high beam quality than conventional methods allow. For future system designs, it is imperative to simulate the forces due to self fields in large scale models, where pairwise summation scales like $O(N^2)$. It is known the forces due to the surroundings become important for higher current. Modern simulations must account for both effects to some application dependent tolerance.

Conventional simulation codes solve the Poisson PDE locally within small volume elements. In general, these local solutions are less accurate far from the origin, with little control on the error bounds. Discretized volume methods are ill-suited to model the forces due to the surroundings in beam physics applications, where the beam is assumed to be far away from the surroundings.

Using Green's identities, we may reformulate the PDE as boundary integral equations (BIEs). The BIEs guarantee a global solution matching the boundary conditions with well bounded error [1]. Solving the BIEs on the discretized boundary gives a dense, nonsymmetric matrix equation of type $Ax = b$ with size M boundary elements. This is known as the boundary element method (BEM) [1]. Iteratively solving this matrix equation would then scale like $O(M^2)$ due to the matrix-vector product. The fast multipole method can be used to accelerate the BEM, ideally scaling like $O(M)$ [3].

In previous work, we implemented the fast multipole method (FMM) for space charge using differential algebraic (DA) methods [2,4]. Ideally, the FMM scales like $O(N)$ and is well-bounded by Taylor's theorem [3]. For preliminary studies, we accelerate the constant element BEM using our FMM implementation with multipole order p. When solving the system matrix, we started with a lower order FMM, multipole order $\frac{p}{2}$ in our iterative solver to precondition the system. We then ran at the prescribed order to reach our final tolerance. In this work, we compare results obtained from the analytical solution for a perfectly conducting thin spherical shell and the conventional BEM. We also show results for an elliptic cylindrical shell using our implementation. We work with arbitrary units for simplicity.

IMPLEMENTATION SETUP

We chose the indirect formulation of the boundary integral equations with the ansatz that a unique solution exists [1]. For further details, readers may refer to [1,3]. We split the BVP into Poisson type, $\Delta\phi(\mathbf{x}) = \rho(\mathbf{x})$ in the interior, $\mathbf{x} \in \Omega_-$, with open boundary conditions and Laplace type, $\Delta\psi(\mathbf{x}) = 0$, on the boundary, $\mathbf{x} \in \Gamma$ and solve the Laplace equation for the appropriately modified boundary conditions. As our first trial, we choose the single layer potential with Dirichlet BCs. For the interior Dirichlet problem, our BIE is,

$$\psi(\mathbf{x}) = \int_{\Gamma(\mathbf{y})} G(\mathbf{x},\mathbf{y})\sigma(\mathbf{y})\mathrm{d}\Gamma(\mathbf{y}) \quad \mathbf{x} \in \Omega_- \tag{1}$$

Our discretized BIE for constant elements is,

$$\psi_i = I_{ij}\sigma_j \quad \mathbf{x} \in \Gamma \tag{2}$$
$$I_{ij} = G(\mathbf{x}_i,\mathbf{y}_j)\int_{\Gamma(\mathbf{y}_j)} \mathrm{d}\Gamma(\mathbf{y}_j)$$

Where $G(\mathbf{x},\mathbf{y})$ is the Green's function.

Simulation parameters are given in Table 1. The sample particles for the spherical shell were given a uniform distribution and constrained to $|\mathbf{r}| \leq 0.02$. The sample particles for the cylindrical shell were also given a uniform distribution and constrained to $\sqrt{r_x^2 + r_y^2} \leq 0.054$ and $-0.05 \leq r_z \leq 0.05$. Since we are interested in the boundary effects on a charged particle beam, we evaluated the potentials at the sample particle positions.

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Table 1: Simulation Parameters

No. of particles	1000
Species	Proton
FMM order	12
Inside sphere	$\|\mathbf{r}\| \leq 0.02$
Inside cylinder	$\sqrt{\mathbf{r}_x^2 + \mathbf{r}_y^2} \leq 0.054, -0.05 \leq \mathbf{r}_z \leq 0.05$

PERFECTLY CONDUCTING SPHERE

We use the perfectly conducting sphere as an analytical check. From the image charge method [5], the potential due to a point charge q inside a sphere of radius R with constant potential Φ_0 is

$$\Phi(\mathbf{x}) = \left[\frac{q}{|\mathbf{x}-\mathbf{y}|} - \frac{Rq}{y\left|\mathbf{x} - \frac{R^2}{y^2}\mathbf{y}\right|}\right] + \Phi_0 \qquad (3)$$

We discretized a sphere with $\Phi_0 = 0$, centered at the origin as shown in Fig. 1. We have included the unit normals to show the orientation of the boundary elements. The discretization parameters are shown in Table 2. The relative error between the discretized surface area and the actual surface area is given as a measure of the discretization accuracy.

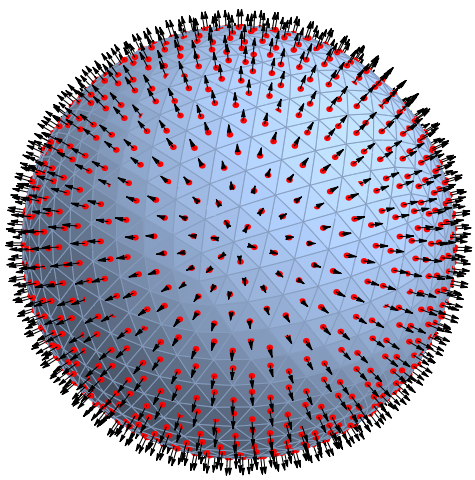

Figure 1: Discretized spherical shell with 1280 elements and its outward normals at the element centroids.

Table 2: Sphere Parameters, $R = 0.1$

No. of elements	Area relative error
80	7.17×10^{-2}
320	1.88×10^{-2}
1280	4.76×10^{-3}
5120	1.19×10^{-3}

We collected the total potentials at the sample particle positions from our FMM accelerated BEM (FMBEM) and compared it with the conventional BEM and the analytical result. As shown in Fig. 2 and Fig. 3, the relative error is drastically reduced as no. of elements increases.

The discrepancy between the analytical result and convention BEM is mainly due to the discretization error. Figure 4 compares the relative error between the conventional BEM and the FMBEM with 5120 elements at multipole order 12. The inexact matrix-vector products computed by the FMM for the iterative solver still contribute a small discrepancy, suggesting reduction from multipole order.

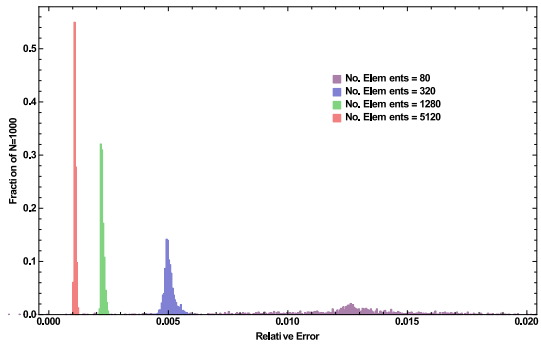

Figure 2: Relative error in computed potentials inside the conducting spherical shell between analytical vs conventional BEM. Distributions for $M = 80, 320, 1280, 5120$ elements are shown.

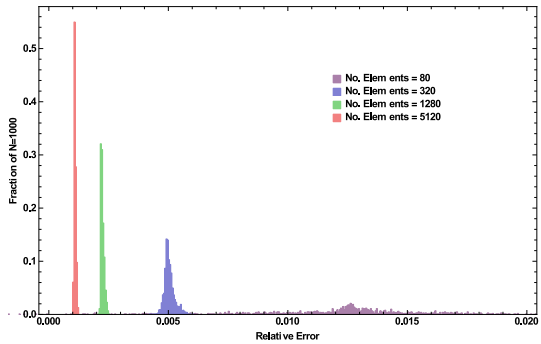

Figure 3: Relative error in computed potentials inside the conducting spherical shell between analytical vs fast multipole accelerated BEM. Distributions for $M = 80, 320, 1280, 5120$ elements are shown at multipole order 12.

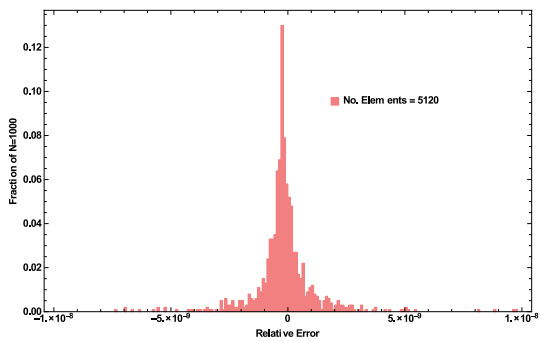

Figure 4: Relative error in computed potentials inside the conducting spherical shell between the conventional BEM vs fast multipole accelerated BEM. The distribution for $M = 5120$ elements is shown at multipole order 12.

We next studied the discrepancy between the conventional BEM and FMBEM as a function of multipole order. We show the results in Fig. 5. The relative error decreases with multipole order because the inexact matrix vector products in the iterative solver become more accurate. Figure 5 suggests

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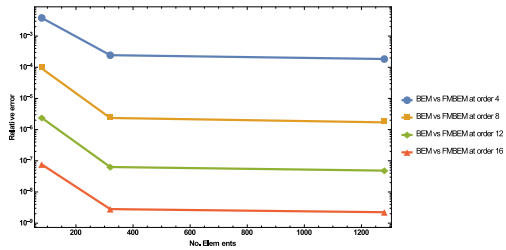

Figure 5: Relative error between the BEM and FMBEM vs. no. of elements and multipole order. We see good performance as multipole order increases.

for constant elements, we need extremely high multipole order to achieve machine accuracy. We hope to address this by allowing for high order elements.

CYLINDRICAL SHELL

We have shown our implementation gives good results with high number of elements and multipole order. To test our implementation on a more practical problem without a known analytical solution to the authors at this time, we computed the potentials inside an elliptic cylinder due to a bunch. We discretized an elliptic cylinder with $\Phi_0 = 0.6$ along the wall and $\Phi_0 = 0$ at the endcaps, shown in Fig. 6. The unit normals show the orientation of the boundary elements. The cylinder parameters are given in Table 3, with the relative error in surface area to show the discretization accuracy. The cylinder was placed between $z = -0.2$ and $z = 0.7$.

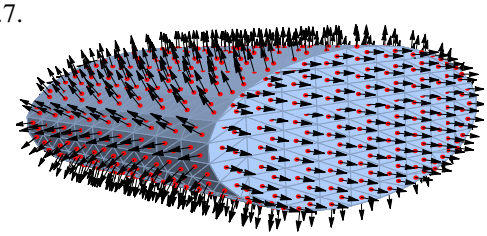

Figure 6: Discretized cylindrical shell with 876 elements and its outward normals at the element centroids.

Table 3: Cylinder Parameters, $R_x = 0.2$, $R_y = 0.5$, $L = 0.9$

No. of elements	876
Area relative error	3.49×10^{-3}
Φ_0 on wall	0.6
Φ_0 on endcaps	0

We placed a weak constant potential on the walls and zero potential on the endcaps. We show the self-potentials and the potentials due to the boundary at the particle positions in Fig. 7.

We see the potentials are grow towards the center of the bunch, suggesting a dominant outward force, aka space charge force. We see some asymmetry from the boundary contribution since the endcap at $z = -0.2$ is closer.

CONCLUSIONS

We have successfully combined our differential algebraic fast multipole method with the constant element boundary element method. We have shown convergence with number of elements and multipole order. We have presented the potentials on a bunch inside an elliptic cylinder with constant potential on the walls. For this particular case, the effect due to the particles is dominant. There is much room for improvement and optimization in this implementation. We will next focus on the high-element-order fast multipole-accelerated boundary element method.

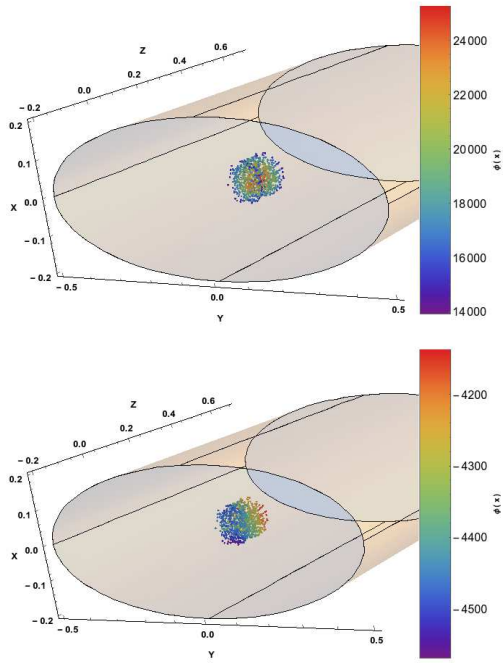

Figure 7: Potentials at the sample particles inside an elliptic cylindrical shell. The sum of the potentials is highest inside the bunch, dominated by the self potentials. Top: Self potentials. Bottom: Potentials due to the boundary.

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