Exact solutions to model surface and volume charge distributions

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Abstract. Many important problems in several branches of science and technology deal with charges distributed along a line, over a surface and within a volume. Recently, we have made use of new exact analytic solutions of surface charge distributions to develop the nearly exact Boundary Element Method (neBEM) toolkit. This 3D solver has been successful in removing some of the major drawbacks of the otherwise elegant Green’s function approach and has been found to be very accurate throughout the computational domain, including near- and far-field regions. Use of truly distributed singularities (in contrast to nodally concentrated ones) on rectangular and right-triangular elements used for discretizing any three-dimensional geometry has essentially removed many of the numerical and physical singularities associated with the conventional BEM. In this work, we will present this toolkit and the development of several numerical models of space charge based on exact closed-form expressions. In one of the models, Particles on Surface (ParSur), the space charge inside a small elemental volume of any arbitrary shape is represented as being smeared on several surfaces representing the volume. From the studies, it can be concluded that the ParSur model is successful in getting the estimates close to those obtained using the first-principles, especially close to and within the cell. In the paper, we will show initial applications of ParSur and other models in problems related to high energy physics.

1. Introduction

Gaseous ionization detectors exhibit a complex array of physics processes. Numerical simulation is an important tool to understand these detectors at the device level. Extensive simulation is used to analyze the performance and characteristics of existing detectors and to improve their design. With the advent of Micro-Pattern Gas Detectors (MPGD), the importance of simulation has grown further. These detectors have intricate patterns of micron-order dimensions that makes their geometries of an essentially three-dimensional nature. While this design aspect serves the purpose for which they are used, namely excellent rate capability, spatial, temporal and energy resolutions, analysis of these detectors has become difficult due to the mentioned features. In addition, for almost all the gaseous ionization detectors, there are problems related to space charge accumulation that are extremely difficult to handle computationally. For example, even geometries as simple as the resistive plate chambers (RPC) in their various design variations, that are also the detector of choice for a large variety of experiments, can be significantly affected by space charge. Wire chambers, such as drift tubes, or multi-wire
proportional chambers, all suffer from this problem that severely limits their usage in present high luminosity experiments, their upgrades and new experiments being planned for the future.

During recent times, a simulation framework for gaseous detectors have been developed by the RD51 collaboration in which Garfield [1] has played a central role. Garfield simulates transport, amplification and signal induction in ionization detectors, and provides links to codes that compute parameters necessary for this computation. For example, interface is provided to Heed for calculating primary ionization and cluster formation [2], to Finite Element Method (FEM) codes such as Ansys and Boundary Element Method (BEM) codes such as neBEM for computing the electromagnetic field [3, 4], and to Magboltz for estimating Townsend, attachment coefficients and transport properties [5]. Among these tools, neBEM is a recently formulated BEM toolkit [6, 7] that has the distinct advantage of being able to truly represent charge distributions on elements of rectangular and triangular shapes and incorporate their effects while solving the electromagnetic field problems involving 3D geometries of arbitrary complexity. In this brief report, we will restrict ourselves to demonstrating the accuracy of neBEM while computing electric field for an MPGD with complex geometry. In addition, preliminary use of this approach to solve problems related to volume distribution of charges will also be presented.

2. The neBEM toolkit and its applications

Some of the features expected in a field-solver handling gaseous detectors in general, and MPGDs, in particular, may be listed as its ability to handle large length scale variations (meter to microns), to provide potential and field at arbitrary locations within a volume of interest, to model devices with arbitrary complexity in terms of geometrical shape and material components. The neBEM approach was developed with these aims and it has been reasonably successful in achieving its goals [8]. In what follows, we will briefly discuss the approach and discuss its ability to solve electromagnetic field in one of the MPGDs.

The potential can be obtained by solving the Poisson’s equation adopting the BEM approach, among other possibilities.

\[ \nabla^2 \phi(\mathbf{r}) = -\rho(\mathbf{r})/\varepsilon_0 \]

The solution yields the distribution of charges which is obtained through the satisfaction of a given potential configuration. The potential \( \phi(\mathbf{r}) \), for a point charge \( q \) at \( \mathbf{r}' \) is known to be

\[ \phi(\mathbf{r}) = \frac{q}{4\pi\varepsilon_0|\mathbf{r} - \mathbf{r}'|} \]

Superposition holds for a general charge distribution and leads to

\[ \phi(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')d\mathbf{v}'}{4\pi\varepsilon_0|\mathbf{r} - \mathbf{r}'|} = \int G(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}')d\mathbf{v}' \]  

where, the free space Green’s function for the Laplace operator in three dimensions is given as

\[ G(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi\varepsilon_0|\mathbf{r} - \mathbf{r}'|} \]

Similarly, a general charge distribution yields a field

\[ \mathbf{E}(\mathbf{r}) = -\nabla \Phi \]

or,

\[ \mathbf{E}(\mathbf{r}) = -\nabla \left( \int G(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}')d\mathbf{v}' \right) \]
Thus,

\[ \vec{E}(\vec{r}) = \int \frac{\rho(\vec{r}') (\vec{r} - \vec{r}') dv'}{4\pi \epsilon_0 |\vec{r} - \vec{r}'|^3} \]  

(2)

The boundary conditions are specified in a form suitable for a given problem. The conditions can be Dirichlet (known potential values), Neumann (known field values, or other known conditions normal to an interface) or Robin / Mixed (mixture of Dirichlet and Neumann) on the material boundaries / interfaces. The following integral equation of the first kind can be easily set up if we consider only the Dirichlet problem at present, for ease of discussion,

\[ \phi(\vec{r}) = \int_{\text{vol}} G(\vec{r}, \vec{r}') \rho(\vec{r}') dv' \]  

(3)

Here, the potential at a point \( \vec{r} \) is \( \phi(\vec{r}) \), the charge density at an infinitesimally small volume \( dv' \) is \( \rho(\vec{r}') \), while the permittivity of free space is \( \epsilon_0 \). In order to solve the problem, we need to find \( \rho(\vec{r}) \) as a function of space. This solution needs to be capable of yielding the known distribution of \( \phi(\vec{r}) \). Potential and field at any point in the computational domain can be obtained as soon as the charge distribution on the boundaries and all the interfaces has been solved.

In order to apply the BEM technique, the first step is to discretize the boundaries and interfaces of a given problem. The shape of the discretized elements can be arbitrary, but the most common are rectangular or triangular. Between these two, the triangular elements offer more flexibility and can be used to model geometries of any variety for the both FEM and BEM. The charge distribution on the discretized elements that satisfies eq. 3 are solved for, once meshing is over. A large number of solution approaches exist, among which the constant element collocation approach is one of the most popular. In this zero-th order formulation, the charge distribution on each element is assumed to be uniform and equivalent to point charges located at the centroid of the elements. This approach provides a good optimization between accuracy and computational complexity.

This approximation, although popular due to reasons mentioned above, lead to numerical and physical singularities that can lead to grossly inaccurate results. As a result, a very large number of BEM formulations have been developed to deal with issues related to specific problems. The neBEM approach was developed to provide a formulation that could deal with many of the issues together. This was achieved by the use of symbolic integration to arrive at exact close-form analytical expression for potential and field due to singularities distributed on rectangular and triangular elements [6, 7]. While this cannot be elaborated here, we will demonstrate efficacy of the approach by comparing its results with that of FEM for an MPGD with a complex shape.

Micro Wire Detector (MWD), one among the MPGDs, is a lithographically produced cathode mesh of square holes on one side of a kapton foil and anode strips on the other, running along the middle axis of cathode mesh holes. The kapton is used so that it provides a mechanical joint between the cathode mesh of square holes and the anode strips. The detailed structure of this detector has been described in [9]. For the calculations using neBEM, the same geometry has been used here. However, the shape of kapton foil has been considered rectangular for the present studies, instead of trapezoidal in [9]. A drift plane with a voltage 1.11kV has been considered which is 785 mm away from anode strip following [9].

As an example of extremely difficult situation, field along a line around the anode just 1 micron away from the surface is considered here 1(b) [9]. Sampling of field values for neBEM has been considered to be as small as 0.1 micron. In addition, it should be noted that no smoothing or filtering has been applied as post-processing. From fig. 2(a), sharp rise in the field values is observed at all the four edges while smooth variation of field is observed on each of the four surfaces. Field values are found to decrease sharply once the points are beyond anode surfaces. FEM computation is significantly more jagged and is clearly unable to produce correct results near and at the edges.
The effect of discretization has also been studied in relation to this problem. In the earlier computation, we had used 20 elements to represent the top surface and 10 elements on the side surface. The elements were made successively smaller towards the edges. In order to study effect of using coarse discretization, we also used larger elements of fixed size, only 3 elements each to represent both top and side surfaces. Although there is significant difference between the results, the overall trend is represented well by the larger elements, as shown in fig. 2(b). It is important to note that there is no jaggedness (at 0.1 micron sampling) despite the use of unreasonably large elements.

There may be several reasons that lead to the difference between the results obtained using neBEM and FEM. In order to impose periodicity on the geometry, we have considered a 33 matrix of microwire units for neBEM, instead of invoking symmetry. The Neumann boundary condition has been used on the side boundaries of the FEM computational domainIn [9] in order to fulfill the same requirement. The potential and field at any arbitrary point using neBEM have been obtained using the closed form analytic influence coefficients have been used. This is the principal reason leading to the smooth solution obtained using neBEM.
3. Particles on Surface - ParSur

Algorithms used for the evolution of a charge cluster in three dimensions involves huge computational expenditure. Drastic simplifying assumptions are made in order to reduce the magnitude of the expenses. It has been found that numerical simulation of reduced dimensions (1.5D or 2D) can reproduce most of the essential features of the evolution of a cluster. However, for even more realistic simulations, we need to develop more accurate, but efficient models and tools. In recent times, space charge problems in 3D have been successfully analyzed using the popular Particle-in-Cell (PIC) model. This model has been applied to a wide variety of fields, including plasma physics, solid and fluid mechanics and several other areas of science and technology [?]. It has its own set of problem which includes computational expenditure, particle discretization errors, fixed-grid formalism. Thus, we need to look for a better model in order to study the problem of cluster evolution in a gas detector.

As has been discussed above, it is easy for neBEM to represent distributed surface charges. So, the present approach involves the representation of a given volume by a set of surfaces. The evolving volume charge distribution is smeared on the various surfaces depending on their proximity to them. This leads to the name of the approach, Particles-on-Surface (ParSur). Once the smearing is over, it is easy to estimate precisely the effect of charge distributed on any given rectangular or triangular surface using the analytic expressions of neBEM. Using ParSur, the effect of space charge is expected to be simulated accurately. Below, we have presented results from a brief study on very simple implementations of both PIC and ParSur and made a brief comparison.

![Figure 3: Effect of volume distribution of ions and electrons (a) Potential (b) Field](image-url)
To begin with, we have considered a simple rectangular volume filled with ions and electrons. The number of charged particles is large and they are randomly placed within the volume as shown in fig. ???. The potential and field of this volume distribution of charges have been estimated using the approaches discussed above and by the exact method, i.e., by summing up the influence of each and every charge within the volume. The comparison in fig. 3(a) and fig. 3(b) shows that the ParSur approach is significantly closer to the exact values in both the cases.

Finally, we have considered a volume filled with charges of only one sign - either positive or negative. In this case, unlike in the earlier one, the potential and field does not get cancelled on an average. In figs. 4(a) and 4(b), it is once again clear that the estimates made by ParSur follows the trend shown by the exact curve.

![Figure 4: Effect of volume distribution of electrons only](a) Potential (b) Field

4. Conclusion

We have introduced the neBEM approach for solving problems related to charge distributions. Based on close-form exact solutions, this approach has been developed as a toolkit and has been used to solve many problems related to nuclear or particle physics detectors. One such example involving micro-wire detectors has been presented and compared with FEM solutions to illustrate the efficacy of the approach. Finally, simple problems related to volume charge distributions have been solved using several approaches, among which results from ParSur, a model based on the neBEM approach, has been presented. It has been found that the new model is quite capable in estimating potential and field for these simple volume distributions. In future, ParSur will be developed further to address problems related to detector space charge accumulation problems.

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