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A domain-decomposition method to implement electrostatic free boundary conditions in the radial direction for electric discharges ☆

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ABSTRACT

At high pressure electric discharges typically grow as thin, elongated filaments. In a numerical simulation this large aspect ratio should ideally translate into a narrow, cylindrical computational domain that envelops the discharge as closely as possible. However, the development of the discharge is driven by electrostatic interactions and, if the computational domain is not wide enough, the boundary conditions imposed to the electrostatic potential on the external boundary have a strong effect on the discharge. Most numerical codes circumvent this problem by either using a wide computational domain or by calculating the boundary conditions by integrating the Green's function of an infinite domain. Here we describe an accurate and efficient method to impose free boundary conditions in the radial direction for an elongated electric discharge. To facilitate the use of our method we provide a sample implementation. Finally, we apply the method to solve Poisson's equation in cylindrical coordinates with free boundary conditions in both radial and longitudinal directions. This case is of particular interest for the initial stages of discharges in long gaps or natural discharges in the atmosphere, where it is not practical to extend the simulation volume to be bounded by two electrodes.

Program summary
Program Title: `poisson_sparse_fft.py`
Program Files doi: http://dx.doi.org/10.17632/x7f6czrnsh.1
Licensing provisions: CC By 4.0
Programming language: Python
Nature of problem: Electric discharges are typically elongated and their optimal computational domain has a large aspect ratio. However, the electrostatic interactions within the discharge volume may be affected by the boundary conditions imposed to the Poisson equation. Computing these boundary conditions using a direct integration of Green's function involves either heavy computations or a loss of accuracy.
Solution method: We use a Domain Decomposition Method to efficiently impose free boundary conditions to the Poisson equation. This code provides a stand-alone example implementation.

1. Introduction

Despite their prevalence in industry and in nature, electric discharges still hold many unknowns. For example, we do not yet understand precisely how a lightning channel starts, how it advances in its way to the ground or how exactly are bursts of X-rays produced as it progresses [1]. This is partly due to the short time and length scales involved in such processes which, combined with their jittery behavior, prevents the use of many diagnostic techniques. Due to these limitations, much of what we know about electric discharges comes from computer models which, at least within a simulation, are predictable and reveal arbitrarily small scales.

Consider streamer simulations. Streamers are thin filaments of ionized air that precede most electric discharges in long gaps at atmospheric pressure. The main challenge for simulating streamers is the wide separation between length scales: whereas the total length of the streamer channel at atmospheric pressure ranges from about one to some tens of centimeters, the ionization of air molecules is mostly confined to a layer thinner than one millimeter. Despite this difficulty, there are many numerical codes that explain most of the observed properties of streamers [2–7]. In the past decades these models have gradually improved and successfully overcome many of the challenges posed by streamer physics. However, they are still computationally intensive and often require days of runtime to produce meaningful simulations.

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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In this work we look at one of the problems behind these long running times: the large aspect ratio of a single-channel discharge. Whereas the width of an atmospheric-pressure streamer is at most about one centimeter, its length spans many times this extension. In order to minimize the amount of work performed in a simulation, one strives to adapt the computational domain to the dimensions of the streamer, which means using a narrow cylindrical domain with a diameter only slightly larger than the streamer width. However, in such a narrow domain the electrostatic interaction between separate points in the channel is strongly affected by the boundary conditions imposed on the electric potential at the outer boundaries.

One approach to avoid this artifact while keeping a narrow domain around the streamer is to calculate the boundary values of the potential by direct integration of the electrostatic Green's function in free space [3,8–11]. These values are then imposed as inhomogeneous Dirichlet boundary conditions in the solution of the Poisson equation. In a cartesian grid with M cells in the radial direction and N cells in the axial direction the direct integration of the Green's function at each of the N nodes in the external boundary requires about MN^2 operations. Since the work employed by fast Poisson solvers scales as $MN\log(MN)$ (MN for multigrid solvers), the computation of boundary values by direct integration may easily dominate the work employed in the electrostatic calculations. This is mitigated in part by using a coarse-grained charge distribution in the integration. However, in that case there is a tradeoff between the degree of coarsening and the minimal radial extension of the domain required for a tolerable error.

Beyond this common approach used to solve Poisson's equation in electric discharges, some other methods have been developed. A family of these methods has been built upon the idea of the decoupling of local and far-field effects [12] and the computation of the boundary potential by means of a potential generated by a set of screening charges located in the outer surface of the computational domain [13]. Based on these two methods mentioned above, reference [14] uses a domain decomposition approach to exploit parallel computing capabilities; first, Poisson's equation subject to unbounded boundary conditions is solved in a set of disjoint patches. As a second step a coarse-grid representation of the space charge is obtained and Poisson's equation is again solved in a global coarse-grid whose solution is used to communicate far-field effects to local patches. Finally, Poisson's equation is solved in a fine grid using boundary conditions computed from the coarse-grid solution corrected with local field information.

A different family of methods uses the convolution with Green's function subject to free boundary conditions. They manage the singular behavior of Green's function by either regularizing it [15], or by replacing the singular component to the integrand of the convolution by an analytical contribution [16]. These methods have achieved an order of convergence greater than two.

Here we adapt to the cylindrical geometry of electric discharges the domain-decomposition method described by Anderson [17] (see also [18] for a review of similar techniques). As we discuss below, this method requires two calls to the Poisson solver but otherwise the leading term in its algorithmic complexity follows the scaling of the Poisson solver itself. Therefore for large grid sizes our approach is more efficient than the direct integration method. Furthermore, as we do not reduce the resolution, we do not introduce any numerical error in addition to the discretization error of the Poisson equation. We believe that the method we present is simple enough that it can be easily implemented on top of any existing streamer simulation code. To aid in this task we provide a standalone example in Python.

Some applications may also require free boundary conditions for the z-direction: for example, when the discharge develops far from the electrodes. In those cases one may also reduce the computational domain in the longitudinal direction while the core of the simulation remains inside the computational domain. We have considered this topic of interest in Appendix A where we have applied the domain decomposition method to obtain free boundary conditions also in the longitudinal direction. This extension requires an extra solution of Poisson's equation.

Note that streamers are not the only type of discharge that typically exhibits a large aspect ratio and that therefore our scheme is also applicable to other processes such as leaders and arcs.

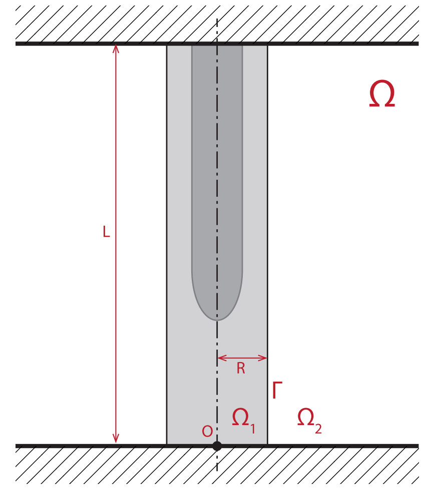

Fig. 1. Geometry of the discharge considered in this work. An elongated channel propagates between two conducting electrodes. The space between these electrodes, Ω is divided into two domains: the inner domain Ω_1 is our computational domain and contains all the space charge. The outer domain Ω_2 extends indefinitely outwards from the external boundary of Ω_1 and does not contain any space charge. The cylindrical surface Γ is the common boundary between Ω_1 and Ω_2.

2. Description of the method

2.1. Domain decomposition

The most convenient decomposition of the domain strongly depends on the problem at hand. The decomposition we present here is suitable for elongated discharges and probably some other applications but the procedure and the highlighted ideas are not restricted to this particular scheme.

We consider the geometry sketched in Fig. 1, where an elongated, cylindrically symmetrical streamer propagates between two planar electrodes. With minimal changes, our scheme can be extended to more complex geometries commonly employed in streamer simulations, such as protrusion–plane, protrusion–protrusion and sphere–plane. The electrostatic potential ϕ satisfies the Poisson equation with appropriate boundary conditions:

$$\begin{aligned} \Delta\phi &= f \quad \text{in} \quad \Omega, \\ \phi &= g \quad \text{on} \ \partial\Omega, \end{aligned} \tag{1}$$

where $f = -q/\epsilon_0$, with q being the charge density and ϵ_0 the vacuum permittivity. In principle an arbitrary boundary condition, here denoted by g, can be applied to the upper and lower electrodes. However, to simplify our discussion we limit ourselves to the most common case where $g = 0$, meaning $\phi = 0$ at $z = 0$ and $z = L$ (to impose a potential difference V between the two electrodes we simply add $\phi_{\text{inhom}} = zV/L$ to the solution of the homogeneous problem). The domain Ω is the space between the two electrodes, formally defined as

$$\Omega = \left\{x \equiv (\rho, \theta, z) \in \mathbb{R}^3 / 0 \le \rho, 0 \le \theta < 2\pi, 0 \le z \le L\right\}. \tag{2}$$