Pseudo-spectral 3D simulations of streamers with adaptively refined grids

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A three-dimensional code for the simulation of streamers is introduced. The code is based on a fluid model for oxygen-nitrogen mixtures that includes drift, diffusion and attachement of electrons and creation of new charge carriers through impact ionization and photo-ionization. The electric field created by the space charges is solved self-consistently. The code assumes that the streamer geometry is not far from an axisymmetric configuration and it is therefore possible to apply a relatively coarse discretization in the angular coordinate. The other two coordinates are represented in adaptively refined grids, allowing a fine resolution of the space-charge layer. In order to take advantage of multiprocessor machines, a pseudo-spectral method (applying discrete Fourier transform forth and back at each time-step) was implemented to resolve the angular dependence.

1. Introduction

One generic process of electrical breakdown in large volumes is the streamer: under a high enough electric field an accumulation of electron avalanches can lead to a charge separation and the formation of a thin, curved layer of space-charge that locally enhances the electric field, inducing further ionization events in its vicinity and thus creating a narrow, propagating plasma channel.

The extremely high, localized electric field close to the streamer head creates a focused small region of highly energetic electrons that give streamers their industrial and economic relevance. Since the power provided to the discharge is so accurately focused on a small region, streamers are an efficient method for radical production, pollution removal and surface treatment [1].

In nature, streamers are observed in sprites [2]: bipolar atmospheric discharges that appear at high altitudes above thunderclouds.

The numerical study of streamers faces the challenge of their multi-scale nature [3]: the large difference in length-scales between the thin space-charge layer, where most of the relevant physics takes place, and the much larger streamer body. A numerical simulation needs to resolve with a very high resolution the space-charge layer while not expending too many resources in simulating the remaining large volume. To cope with this difficulty considerable progress has been made in recent years in the development of adaptively refined grids [4].

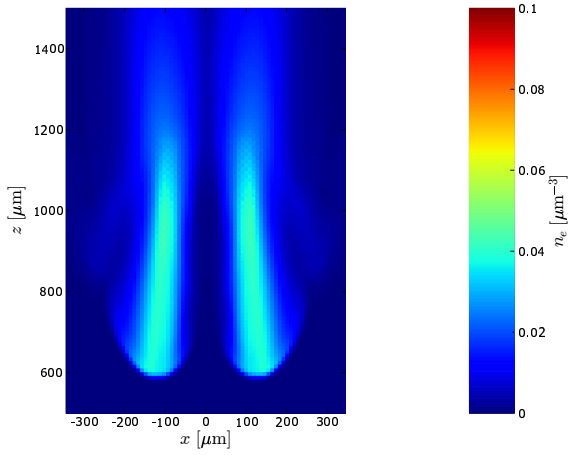

FIG. 1: Electron densities of two adjacent negative streamers in a non-attaching gas such as nitrogen as simulated by the 3D streamer code (see the text for details). Although the repulsion of two close streamers was an expected result, up to our knowledge, this is the first time that a numerical simulation has been able to actually show this phenomenon.

Most of these developments were, however, limited to completely axisymmetric systems due to obvious limitations in the available computational capacity. There are however several topics in streamer physics that are calling for the removal of such limitation. Among them are interacting streamers and the spontaneous symmetry breaking during streamer branching.

Today, the arrival of more powerful hardware has

finally allowed us to remove the assumption of complete cylindrical symmetry from the computational models. This article aims to describe the implementation of such three-dimensional code.

2. Fluid streamer model

We consider a model for streamers in oxygen-nitrogen mixtures that includes electrons and positive and negative ions in which electrons diffuse and drift according to the local electric field $\mathbf{E}$, while ions, due to their much larger mass, are considered immobile. The charge carriers are generated by impact ionization that depends on the local electric field and photoionization by photons emitted anywhere in the gas area, although mainly from the high-field region:

$$\begin{aligned} \partial_t n_e &= \nabla \cdot (n_e \mu_e \mathbf{E}) + D_e \nabla^2 n_e \\ &\quad + S_i + S_{ph} - \nu n_e, \end{aligned} \tag{1}$$

$$\partial_t n_+ = S_i + S_{ph}, \tag{2}$$

$$\partial_t n_- = \nu n_e, \tag{3}$$

where n_e, n_+ and n_- are the electron, positive ion and negative ion densities respectively, D_e is the electron diffusion coefficient and ν is the rate of attachement of free electrons to neutral oxygen molecules. The impact ionization S_i is given by Townsend's approximation,

$$S_i = n_e \mu_e |\mathbf{E}| \alpha(|\mathbf{E}|) = n_e \mu_e |\mathbf{E}| \alpha_0 e^{-E_0/|\mathbf{E}|}, \tag{4}$$

in which α_0 is the ionization coefficient. The photoionization term is given, following the model for oxygen-nitrogen mixtures of Ref. [5], by

$$\tilde{S}_{ph}(\mathbf{r}) = \frac{1}{4\pi} \frac{p_q}{p + p_q} \int_V \frac{\tilde{f}(p|\mathbf{r} - \mathbf{r}'|) \tilde{S}_i(\mathbf{r}') d^3(p\mathbf{r})}{|p\mathbf{r} - p\mathbf{r}'|^2}, \tag{5}$$

where p is the gas pressure, p_q is the quenching pressure of the photoionizing singlet states of nitrogen, which we take to be $p_q = 60\,\mathrm{Torr}$ [6, 7] and $\tilde{f}(p\tilde{r})$ is the absorption function of photoionizing radiation in the wavelength range $980 - 1025\,\text{Å}$ by oxygen molecules [5, 8] (corresponding to $4\pi\psi/p$ in the notation of Ref. [8]).

The electric field $\mathbf{E}$ is determined through Poisson's equation for the electric potential,

$$\nabla^2 \phi = \frac{e}{\epsilon_0}(n_e - n_+ + n_-), \quad \mathbf{E} = -\nabla\phi, \tag{6}$$

where e is the elementary charge.

3. A 3D streamer code

In recent years a set of computational tools was developed to simulate accurately and efficiently the model described in the previous section for axisymmetric systems. A 3D simulation scheme should naturally build on those developments and profit from this know-how. Hence our goal was to produce a streamer simulation code with the following properties:

Adaptive grid refinement. The major problem in numerical streamer simulations is their aforementioned multi-scale nature. An efficient algorithm should have a large resolution for the fine and steep structure of the space charge layer while the complete streamer is also taken into account, albeit at a lower resolution. The model to follow here is the refinement of the grids according to a curvature monitor as described in [4, 9].

Efficient computation of the photoionization source. Calculating the photoionization source can be quite expensive if one naively translates the integral equation (5) into a sum over all pairs of grid-points. A more efficient procedure is possible if one approximates the integral kernel by a carefully selected expansion [10] such that one can reduce the computations to the solution of a set of elliptical partial differential equations which can be solved much faster and fit well into a refinement scheme.

Parallelism. An axisymmetric simulation usually lasts from several days up to several weeks, depending on varoius factors such as the initial conditions and the external field. A 3D simulation would naturally require several times as many computations and hence up to several months if a single processor were to perform all the work. There was therefore a strong pressure towards a parallel code. While the time-integration of the fluid equations (1) in multiple processors is straight-forward to parallelize the solution of the Poisson equation (6) and the calculation of the photoionization term is convenient to work in Fourier space.

We developed a code that fulfills all these requirements at the expense of assuming that during most of its lifetime, the streamer remains close to a cylindrical axis. This approach unfortunately prevents us from simulating very complicated structures, such as a fully branched tree of streamers. However, even in those extremely complicated cases, simple electrostatic arguments can convince us that a consideration of all the branches adds little value to our understanding, since the dynamics is still driven by the small scale physics close to the heads of the streamers, where everything

can again be approximated by an almost cylindrical streamer that moves in a given external field.

The code represents its variables in cylindrical coordinates: $n_{e,i} = n_{e,i}(r, z, \theta)$ and uses locally refined grids in the r, z projection while the grid spacing of the θ variable, $\Delta\theta$ is constant in all the simulated domain. In order to solve the Poisson equation (6) a discrete Fourier transformation is performed on θ:

$$\tilde{\phi}_k(r, z) = \sum_{n=0}^{N-1} \phi(r, z, \theta_n) e^{-ik\theta_n}, \qquad (7)$$

where N is the number of grid cells in the θ direction and $\theta_n = 2\pi n/N$. Then for each separate mode k a Helmholtz equation has to be solved:

$$\nabla^2 \tilde{\phi}_k + \frac{|w_k|^2}{r^2} \tilde{\phi}_k = -\frac{e}{\epsilon_0} (\tilde{n}_{ik} - \tilde{n}_{ek}), \qquad (8)$$

where a tilde ˜ represents the Fourier transform of a quantity and $|w_k|^2 = \frac{2}{\Delta\theta^2}(1 - \cos k\Delta\theta)$.

4. Example: repulsion of two negative streamers in Nitrogen

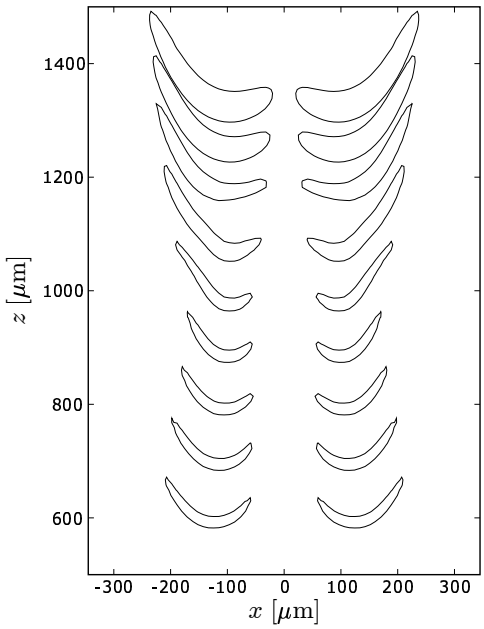

FIG. 2: Equal time steps (separated by $60\,\mathrm{ps}$) of the evolution of the space charge layers of two adjacent streamers. Plotted is the half maximum line of the space charge density on the plane that intersects the centers of both streamers ($y = 0$). The homogeneous background field is $80\,\mathrm{kV/cm}$.

When two streamers are close together their interaction can also be roughly modelled by our code. Therefore a good example and test of the capabilities of the presented code is the simulation of two identical streamers propagating at a close distance in a medium

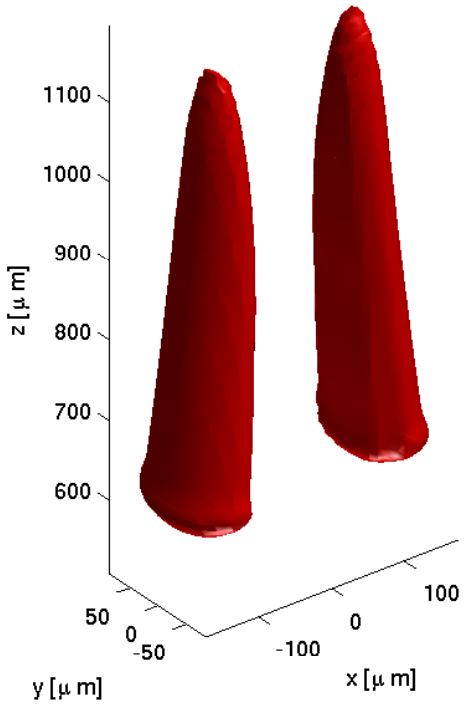

FIG. 3: Surface of constant electron density in an advanced state of the evolution of two adjacent streamers advancing downwards.

with negligible photoionization and attachment, such as pure nitrogen. We selected two seeds at a distance of $115\,\mu\mathrm{m}$ at atmospheric pressure, under a field of $80\,\mathrm{kV/cm}$ pointing upwards and we simulated them with an angular resolution of $\Delta\theta = 2\pi/64$ ($N = 64$).

Figures 1-3 show that the effect of the streamers on each other is a significant repulsion. This, of course, results from the electrostatic repulsion of the charges in their heads.

5. Conclusions and prospect

We have described a code that allows the numerical investigation of streamers under not completely axisymmetric conditions. The code implements adaptive refinement to accurately represent the space-charge layer of a streamer and a pseudo-spectral method and parallel Poisson solver that allows it to benefit from multiple-processor machines.

There are several investigations currently performed with the aid of this code, such as the spontaneous symmetry breaking during the onset of the branching instability and the various ways in which two or several streamers can interact while they are close enough.

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