Simulations of centimeter-scale, atmospheric pressure, positive streamer discharges using EMPIRE-PIC

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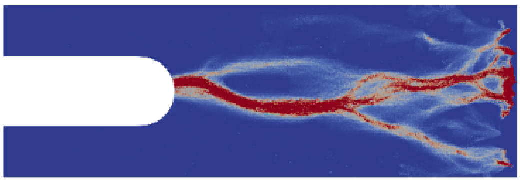
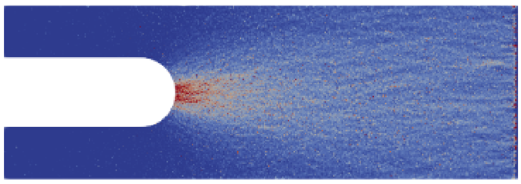
Development of a new particle-in-cell (PIC) code EMPIRE-PIC has enabled simulations of high pressure discharges over wide electrode gaps. This is primarily due to implementation of scalable solvers allowing for 100's of millions of elements, sub-Debye length mesh sizes, and 10's of billions of macro-particles. EMPIRE-PIC allows an unlimited number of species and interaction possibilities, making it suitable for complex plasmas and plasma chemistry. Furthermore, stochastic behavior is intrinsic to the code by allowing random interaction rates. This is particularly important for positive streamer discharges where photo-ionization is a primary streamer propagation mechanism. In this instance it is the photons that photo-ionize secondary species in the gas which in turn generates additional charged particles to be created at random location within the electrode gap. Each of these locations is a source of a new electron avalanche formation and growth of a streamer branch that may or may not connect with the primary branch.

In previous work [3] we established the importance of the mean-free-path (MFP) of photo-ionizing photons. We have shown that the concentration of photo-ionizing gas and thus change in MFP changes the behavior of positive streamer discharge. Namely, that the short MFP photons create a more uniform discharge, while long MFP photons create a filamentary type of streamer discharge. In this work we are going further in establishing the importance of various other simulation parameters such as mesh sizing and particle counts. Comparisons between simulations are performed to determine key drivers in fidelity and accuracy of positive streamer discharges. Examples of two different types of discharge are shown in Figure 1a and 1b.



(a) Example of filamentary discharge. Electron density shown with red representing 10^{20} m^{-3}.



(b) Example of uniform discharge. Electron density shown with red representing 10^{20} m^{-3}.

Simulations presented in this work are of positive discharges between a pin and plate electrode set. In this configuration a pin is the anode and plate a cathode. Tip of the anode is exactly 1 centimeter away from the cathode plate. We apply a constant source of electric field between the two electrodes. For all simulations a voltage of 15 kV is used based on earlier breakdown studies [1]. Surrounding the electrodes is a uniform gas fill at atmospheric pressure. For our simulation we are using a synthetic, argon-like, gas A for which electron collision cross-sections are calculated using established theory [2]. Furthermore, gas A is capable of being in an excited state. When gas A de-excites a photon is released. We also introduce a separate gas B that can interact with these photons and generate an ionized species of gas B which serves as a source of charged species generated randomly through the volume. Gas B concentrations are kept low, nominally 0.01% to 1% of the total volume depending on the simulation and types of effects we choose to investigate. A full list of interactions used in our simulations is shown in (1).

$$
\begin{aligned}
e^- + A &\rightarrow e^- + A^+ + e^- \\
e^- + A &\rightarrow e^- + A \\
A^+ + A &\rightarrow A^+ + A \\
A^+ + A &\rightarrow A + A^+ \\
e^- + A &\rightarrow e^- + A^* \\
A^* &\rightarrow A + \gamma \\
\gamma + B &\rightarrow B^+ + e^-
\end{aligned} \tag{1}
$$

Due to the large computing resources available at Sandia we are able to utilize computations requiring hundreds and even thousands of compute units. Utilizing these resources we were able to demonstrate the effects due to changes in computational parameters. Results of these simulations are used to determine the thresholds on number of macro-particles and the mesh sizes for which streamer discharges are behaving consistently. These thresholds will be used to simulate more complex configurations and larger spatial domain problems.

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