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A PIC based procedure for the integration of multiple time scale problems in gas discharge physics

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ABSTRACT

A efficient PIC technique has been implemented to study the development of electrical discharges during long periods of time. Special motivation is provided by electrical pulsations that develop in very short times but whose repetition period is much longer. The method exploits the existence of different time scales in the electrical discharge to implement a long time-step particle pushing technique both at particle and at mesh levels. The development of a train of hundreds of Trichel pulses, which is a prohibitively long computation with a conventional PIC, has been used to test the validity of the method.
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1. Introduction

Numerical simulation of electrical discharges in gases constitutes a complex task, since the non-linear interplay among ionization, charge density and electric field gives rise to the generation of sharp gradients and propagating shock waves. These facts have motivated the development of different numerical techniques, many of them specially designed to minimize numerical diffusion [1–4]. The pioneer works of Davies et al. [5] used the method of characteristics, which can be easily adapted to the problem of ionization in gases. However, this method required, at least in its original implementation, the interpolation from mesh nodes at each temporal step of the simulation, and did not include any special refinement in order to reduce numerical diffusion. Particularly successful results have been obtained through the use of flux-corrected-transport algorithms with finite differences (FD-FCT). This method is an Eulerian technique that has been optimized to achieve very low numerical diffusion in problems with fronts or shock-like discontinuities [6]. In fact, the Phoenical-FCT method is

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capable of maintaining a steep gradient, without significant distortion, for several thousands of temporal steps (see Fig. 6 in [6]), thus constituting an invaluable tool in the research of corona discharges. Two-dimensional simulation of gaseous discharges have also been also performed using this technique [7,8] and, more recently, the scheme has been successfully extended to two-dimensional and three dimensional geometries by combining FCT with finite element methods [9]. Many other numerical schemes have been applied to the area of gaseous discharges: specially adapted finite-element techniques [10], finite difference Scharfetter–Gummel techniques [4] and, more recently, MUSCL and QUICKEST [11], as well as others techniques [12]. According to the rich bibliography produced, all these methods have been fruitful in fundamental research of transient phenomena in electrical discharges.

Particle-in-cell (PIC) techniques, in spite of being a usual tool in kinetic plasma simulations [13], have not been so widely applied to the simulation of electrical discharges in gases, at least in the drift-diffusion approximation. A modular PIC approach that encompass both fluid and kinetic plasma behavior has been developed by Lapenta et al. [14], who were specially motivated in obtaining the steady-state solutions of DC discharges by solving the time-dependent equations. In a previous work, the authors have also implemented a fluid PIC technique to simulate transient electrical discharges [15]. The proposed implementation included a special treatment of the source/sink terms of particle densities, which improved the precision of the numerical simulation. The PIC technique was then compared with a standard FCT method, and the agreement between both techniques turned out to be remarkable. This is a usual conclusion when comparing PIC with finite difference techniques: for problems that are tractable by finite-difference methods, PIC and FCT give very similar results, but PIC always has a higher computational cost. However, fluid PIC codes, such as FLIP (Fluid-Implicit-Particle) [16], show its potential in specially difficult problems where finite difference methods are not appropriate. In particular, fluid PIC techniques becomes very valuable in the simulation of quasi-stationary states, specially those with large density gradients perpendicular to the flow velocity [17–19].

The goal of this work is to formulate an efficient fluid PIC method to study the development of electrical discharges during long periods of time. PIC methods are particularly adequate for this task, owing to its very low numerical diffusion. The proposed method exploits the existence of very different time scales to implement a long time-step pushing technique [20,21] on computational particles and on virtual node-particles, in a way somewhat inspired in FLIP [16]. The result is a very fast method, capable of simulating electrical pulsations (like Trichel pulses) that usually requires a huge number of computational steps. The proposed technique accelerates PIC calculation to the point of being faster than finite difference techniques.

The paper is organized as follows. In the first section, the basic concepts of the method are reviewed and discussed. In the second section, the long time-step pushing technique is implemented at particle level, and then extended to the grid level in the next section. Finally, in the last section, the problem of the development of a train of Trichel pulses is used to test validity of the method, and a comparison with a conventional PIC method is done.

2. Fundamentals of the method

In the drift-diffusion approximation, the density of species in a one-dimensional electrical gas discharge is governed by a set of continuity equations of the form [6]

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial}{\partial x}(\rho_i(x,t)V_i(x,t)) = S_i(x,t), \quad i = 1,2,\cdots,l, \tag{1}$$

where ρ_i, V_i and S_i represent the number density, the velocity and the source–sink term of the species i, respectively, and l is the total number of species. Typically, this set of equations models the spatio-temporal evolution of an electrical discharge that progresses along a narrow channel in x direction.

The conservation equations for the species densities are coupled to Poisson's equation through the charge density,

$$\nabla^2\phi = -\frac{1}{\varepsilon_0}\sum_{i=1}^{l} q_i\rho_i. \tag{2}$$

where ϕ is the electrical potential, ε_0 is the gas permittivity and q_i is the electric charge of particles of the species i. Poisson's equation must be solved in three dimensions to account for the finite radial extent of the discharge channel [5,22].

As it is well known, PIC methods replace the continuous particle density $\rho_i(x,t)$ with a set of discrete computational particles or *superparticles*. Using the image of these computational particles as "clouds" of physical particles [23], it was show in [15] (see also [24]) the convenience of considering each species density as the product of a density of *fictitious carriers*, N_i, whose number is conserved, and a variable number of physical particles, μ_i,

$$\rho_i(x,t) = N_i(x,t)\mu_i(x,t). \tag{3}$$

With this approach, each equation in (1) splits into two independent equations

$$\frac{\partial N_i}{\partial t} + \frac{\partial}{\partial x}(N_iV_i) = 0, \tag{4}$$

$$\frac{d\mu_i}{dt} = \frac{S_i}{N_i}, \tag{5}$$

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