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Optimizing physical parameters in 1-D particle-in-cell simulations with Python

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ABSTRACT

A particle-in-cell (PIC) simulation tool, OOPD1, is wrapped in the Python programming language, enabling automated algorithmic optimization of physical and numerical parameters. The Python-based environment exposes internal variables, enabling modification of simulation parameters, as well as run-time generation of new diagnostics based on calculations with internal data. For problems requiring an iterative optimization approach, this enables a programmable interactive feedback loop style simulation model, where the input to one simulation is a programmable function of the output of the previous one. This approach is applied to field-emission of electrons in a diode, in order to explore space charge effects in bipolar flow. We find an analytical solution for maximizing the space-charge limited current through a diode with an upstream ion current, and confirm the result with simulations, demonstrating the efficacy of the feedback scheme. We also demonstrate and analyze a modeling approach for scaling the ion mass, which can shorten simulation time without changing the ultimate result. The methods presented can be generalized to handle other applications where it is desirable to evolve simulation parameters based on algorithmic results from the simulation, including models in which physical or numerical parameter tuning is used to converge or optimize a system in one or more variables.

1. Background

There are many problems in particle-in-cell (PIC) simulations where an iterative approach is taken to optimize physical parameters. When the only available interface to the simulation is a high-level graphical user interface (GUI), then a great deal of human interaction is required in the iteration process [1]. This can be highly inefficient when each iteration may take hours or days. Our goal for this work is to develop a programming model where the input and analysis of simulations happen in the same environment (in our case, the Python programming language).

By having the input and analysis exist in the same interface, and that interface being a fully interactive general purpose programming language, we hope to greatly facilitate an automated analysis and feedback-loop-style simulation pattern, where researchers specify an initial simulation, and describe the analysis for determining when to update, change, or halt the simulation, all in the same place and in the same language. Python is just one example of a robust programming language with relatively simple syntax and high portability, which will allow deployment of multi-step algorithms of virtually unlimited complexity in the optimization process, both in terms of analysis and control. Python has been used in other environments to this effect, with great success [2,3].

Field-emission of electrons in diodes is a matter of much interest, another extension of the basic Child–Langmuir system [4]. By adding ion current emitted from the anode, it has been shown that the field-emitted electron current can be enhanced well beyond that predicted by the familiar three-halves law in classical regimes [5]. Here we will expand that earlier work to relativistic energy regimes, and present a high-level approach for optimizing the emitted current via a new Python interface to a low-level simulation code.

2. Model

2.1. The system—bipolar flow

The physical system which we explore is that of field-emitted electrons in the presence of ion current in a one-dimensional diode.

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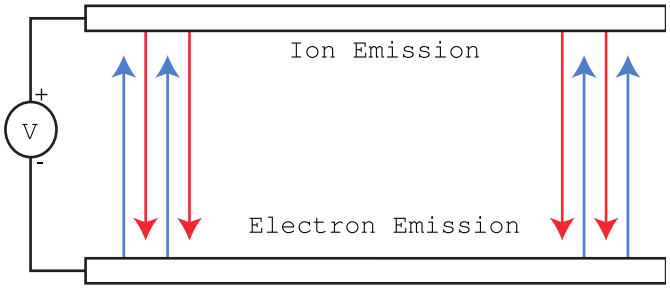

Fig. 1. The diode system. Ions are injected with fixed current, and electrons via field-emission.

A fixed current of ions, with ionization level $Z = 1$, is emitted from the anode at a given current density. Electrons are emitted by field emission, governed by the Fowler–Nordheim equation, as expressed in Eq. (1) [6,7].

$$J = \frac{AE_s^2}{\phi t(y)^2} \exp\left(\frac{-Bv(y)\phi^{3/2}}{E_s}\right) \tag{1}$$

where E_s is the surface electric field, ϕ is the work function, and J is our current density, and t, v, and y are parameters

$$t(y)^2 = 1.1 \tag{2}$$

$$v(y) = 0.95 - y^2 \tag{3}$$

$$y = 3.79 \cdot 10^{-5} \frac{E_s^{1/2}}{\phi}. \tag{4}$$

A fixed DC voltage is applied across the diode, as shown in Fig. 1.

The transmitted electron current is limited by the space charge in the gap [8]. By adding an upstream ion current, some of the space charge is neutralized, and the maximum transmitted current density is increased. Our goal is to determine the maximum electron current limit for a variety of gap distances and voltages.

We can get a steady-state equation for current in the relativistic bipolar diode, by starting with Poisson's equation and the relativistic conservation of energy [9–11]:

$$\nabla^2 \Phi = -\frac{\rho}{\epsilon_0} \tag{5}$$

$$e\Phi = (\gamma_e - 1)\, m_e c^2 + (\gamma_i - 1)\, m_i c^2 \tag{6}$$

where Φ is the potential, ρ is the total charge density, m_e and m_i are their respective masses, e is the magnitude of the electron charge, and γ_e and γ_i are the Lorentz factors for electrons and ions, respectively. Eq. (6) balances potential energy ($e\Phi$) with the kinetic energy contributions ($(\gamma - 1)\, mc^2$) of both electrons and ions at each point in the diode, where

$$\gamma_e = \frac{1}{\sqrt{1 - v_e^2/c^2}} \tag{7}$$

is a function of the velocity (v_e) for each species, which is in turn a function of position in the diode. Adding the relationship of current to charge density,

$$\rho = \rho_e + \rho_i, \tag{8}$$

where the current density J_i is

$$J_i = \rho_i v_i \tag{9}$$

and the electron current density is

$$J_e = \rho_e v_e, \tag{10}$$

a solution combining these with Eq. (1) can be derived [12]:

$$J_e = \frac{\epsilon_0 m_e c^3}{2ed^2} \left\{ \int_1^{\gamma_{e0}} \left[(\gamma_e^2 - 1)^{1/2} + q\Gamma + \frac{\epsilon_0 e}{2m_e c J_e} E_s^2 \right]^{-1/2} d\gamma_e \right\}^2, \tag{11}$$

where Γ collects the relativistic factors

$$\Gamma = \left[(\gamma_i + 1)^{1/2} (\gamma_{e0} - \gamma_e)^{1/2} - (\gamma_{i0} + 1)^{1/2} (\gamma_{e0} - 1)^{1/2} \right], \tag{12}$$

q is a factor describing the ion current relative to the electron current

$$q = (J_i/J_e)(m_i/Zm_e)^{1/2}, \tag{13}$$

and the γ_0 factors correspond to electrons and ions at the full gap potential (V)

$$\gamma_{i0} = 1 + \frac{ZeV}{m_i c^2} \tag{14}$$

$$\gamma_{e0} = 1 + \frac{eV}{m_e c^2}. \tag{15}$$

We can solve for a steady state of this system in a self-consistent manner by alternating solutions of the Fowler–Nordheim equations with those of Poisson's equation [5]. We start with an initial guess for J_e, then solve Fowler–Nordheim for E_s. This E_s is plugged into Poisson's equation to find a new value for J_e. This process is repeated until J_e converges within a chosen tolerance, such as .01%:

$$\frac{J_n - J_{n-1}}{J_n} < 10^{-4}. \tag{16}$$

2.2. Saturation in various regimes

Now that we have a mechanism for getting solutions for J_e in this system, we can explore various values of q, our ion current parameter. $q = 0$ corresponds to no ion current at all, and increasing q means increasing the ion current from the cathode. We can define a saturation value (q_s) by setting the surface electric field to zero at the cathode, and solving Eq. (11) for q, evaluating at the cathode ($\gamma_i = 1$):

$$q_s = (\gamma_{i0} + 1)^{-1/2} (\gamma_{e0} - 1)^{-1/2} \left[(\gamma_{e0}^2 - 1)^{1/2} + \frac{\epsilon_0 e E_s^2}{2m_e c J_e} \right]. \tag{17}$$

This corresponds to space-charge limited emission of ions, and should indicate a maximum steady-state value for both J_i and J_e.

By expanding Eqs. (14)–(15) into Eq. (17), we get Eq. (18), a full expression of the saturation factor q_s,

$$q_s = \left(\frac{ZeV}{m_i c^2} + 2\right)^{-1/2} \left(\frac{eV}{m_e c^2}\right)^{-1/2} \times \left[\left(\left(\frac{eV}{m_e c^2} + 1 \right)^2 - 1 \right)^{1/2} + \frac{\epsilon_0 e E_s^2}{2m_e c J_e} \right], \tag{18}$$