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Issues on beam-plasma instability - early simulations focusing on the development of a compact neutron generator

(Considerações sobre instabilidade feixe-plasma - simulações iniciais centradas no desenvolvimento de um gerador compacto de nêutrons)

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The first issue on compact neutron generator design is the definition of the plasma generation process following the analysis of the physical plasma state. The plasma features and the nuclear reactions of fusion involved in the operation of the generator, deuterium-deuterium or deuterium-tritium, as well as the system which determines the trajectories of the particles and the target, are decisive to predict the neutron yield from the generator. Hence, the plasma behavior analysis under established conditions becomes an important evidence. This analysis may be done by means of plasma simulation models. Particle simulation of plasmas, employed since 1960s, provides a picture of the general plasma characteristics. Plasma physics is determined in most cases by simple equations, *i.e.* equations of motion of electrons, ions and neutrals atoms including the effect of collisions and self-consistent electric and magnetic fields. Computer simulation of plasmas comprises two general areas based on kinetic and fluid. While fluids simulation proceeds by solving numerically the magnetohydrodynamic (MHD) equations, assuming approximate transport coefficients, kinetic simulation considers more detailed models of plasma involving particle interactions through the electromagnetic fields. This article is focused on the simulation and analysis of injected beam into a steady state and periodic plasma. The applied calculation model, for this simulation purpose, is referring to an electrostatic one dimension code, based on kinetic simulation, which simulates periodic plasmas illustrating various fundamental considerations of plasma simulation and make it useful in simulations of the beam optic system for neutron generators. The main goal of this research is explore the PIC code reviewing the computational and physics theory necessary to build the structure of the elementary principles intending to introduce concepts of plasma physics and the computational theory. Moreover, foundations of plasma analysis for neutron generators will be stated.

Keywords: plasma simulation, pic code, compact neutron generators.

A primeira consideração no projeto de um gerador compacto de nêutrons é a definição do processo de produção de plasma seguido da definição da análise do estado físico desse plasma. As características do plasma e as reações nucleares de fusão envolvidas na operação do gerador, deutério-deutério ou deutério-trítio, bem como o sistema que determina as trajetórias das partículas e o alvo, são decisivos para estimar o rendimento de nêutrons do gerador. Dessa forma, a análise do comportamento do plasma sob condições estabelecidas se torna uma evidencia importante. Essa análise pode ser feita por modelos de simulação de plasma. A simulação de partículas de plasma, empregada desde a década de 1960, fornece uma descrição das características gerais do plasma. A física de plasma é determinada, na maioria dos casos, por equações simples, isto é, equações de movimento de elétrons, íons e átomos neutros incluindo o efeito das colisões e campos elétricos e magnéticos auto-consistentes. As simulações computacionais de plasma compreendem duas áreas gerais baseadas em cinética e análise fluidodinâmica. Enquanto a simulação em dinâmica de fluidos se procede por meio da resolução numérica de equações da magnetohidrodinâmica (MHD), assumindo coeficientes de transporte; a simulação cinética considera modelos mais detalhados de plasma, envolvendo interações das partículas com os campos eletromagnéticos. Esse artigo é focado na simulação e análise de um feixe de elétrons injetado dentro de um plasma estacionário e periódico. O modelo de cálculo empregado, para este propósito de simulação, é referente a um código unidimensional, baseado em simulação cinética, que simula plasmas periódicos ilustrando várias considerações fundamentais em simulação de plasma e se torna útil em simulações do sistema da óptica de feixe para geradores de nêutrons. O objetivo principal desse estudo é explorar o código PIC revisando a teoria física e computacional necessária para construir a estrutura dos princípios elementares com intenção de introduzir conceitos da teoria física de plasma e da teoria computacional. Além disso, os fundamentos da análise de plasma para geradores de nêutrons serão declarados.

Palavras-chave: simulação de plasma, código pic, gerador de nêutrons compacto.

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1. Introduction

Plasma is the fourth state of matter, consisting of free electrons, ions and atoms or molecules. It is characterized by its collective behavior. Plasmas are many-particle ensembles; the charged particles are coupled by electric and magnetic self-generated and self-consistent fields [1]. Ionization, which produces the plasma in most devices, can be introduced by extreme heat, pressure, electrostatic and magnetostatic fields or through electromagnetic discharges as commonly designed in a modern compact neutron generator [2].

Compact neutron generators are devices that contain linear accelerators that produce neutrons based on fusion of hydrogen isotopes. Fusion reactions take place in those devices via acceleration of deuterium or tritium ions, or the mixture of the both isotopes, towards a hybrid target of metal also composed of deuterium, tritium or a mixture of two. Neutron sources that use reactions D-D (deuterium - deuterium), D-T (deuterium - tritium) offer a surprising technology, because they can supply a neutron beam of high flux from a small source, pulsed-type electronically collimated. Thus, neutron generators based on those reactions can be used as a powerful tool in several fields in which there is demand of a small beam of neutrons [3]. The reaction D + D → ^{3}He + n + 3.3 MeV was first to provide monoenergetic fast neutrons. However, the most applied fusion reaction is from deuterium-tritium. This fusion reaction is the easiest to perform and also the most used in neutron generators. Reaction T + D → ^{4}He + n + 17.6 MeV occurs with more probability because the neutron in excess on the tritium nuclide increases the size of nucleus and therefore the cross section of fusion reaction.

The basic project of a compact neutron generator includes the design of a modern and compact accelerator, including a gas-control reservoir, plasma and ion source to generate and put the ions in a beam shape, respectively; and a target constituted of material loaded of hydride and metal. A schematic design of a neutron generator based in a work of Worpole [4] is shown in Fig. 1. A subject of study on the plasma behavior for neutron generators is the optimization of the plasma generator device to produce higher charge states and a higher number of particles. The ion source produces the ions created from the plasma through an electrode system, subsequently the ions of deuterium or tritium are accelerated toward a metal target loaded with deuterium, tritium or mixture of both, where occur the neutron generation reactions. Plasma is produced inside an ion source and its proprieties and characteristics determine to a large extent the kind of ion beam that is produced [5]. In according to the design of the neutron generator tube, it is necessary to collimate the ion beam, once the ions have same charge. The system to collimate the beam is not required since the length of the transport system is very small; in this case the ion beam is sufficiently nondiverging [6].

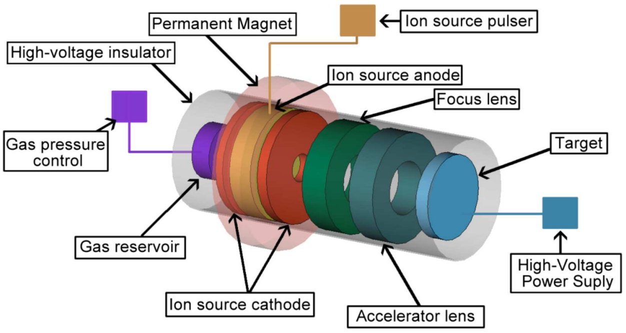

Figure 1 - Illustration of a neutron generator with a Penning ion source.

A method to produce plasma in neutron generator devices is using electrostatic and magnetostatic fields. For example, Penning ions sources [7] use electrostatic fields to separate the nuclei of deuterium or tritium of its electron. The electrons are accelerated into the plasma chamber by means of the electrostatic fields generated by a cathode and an anode to produce more ionization helping to sustain the plasma. Analysis done here give an idea of the physical quantities as product of this interaction.

A beam of electrons interacting with a plasma will be simulated with the goal of describing the PIC code used in the beam optics simulations of particle accelerators, and in this article in our plasma simulation - inside of an ion source. The idea of this code will be depicted.

Problems found in plasma physics encourage the planning of computational simulations that also contribute to the development of a plasma theory. Computer simulations of plasma became a great physical planning tool to provide prognosis of performance in the physical plasma applications such as neutron generator as well as fusion reactors and other equipments.

Based on evaluation of the plasma behavior under particular conditions defined by electron beam injected into a steady state plasma, a variety of concepts will be examined. The investigation will be done on a weak beam, generated in space and time in terms of electric field, electric potential, kinetic energy, field energy and total energy (kinetic plus energy stored in electrostatic field). In the following sections, the required concepts of the basic theory of plasma computer simulations and likewise the necessary mathematical and physical principles of the plasma physics will be discussed.

2. Preliminary concepts

Simulation of plasmas is performed by basically solving the equation of motion of the group of charged particles interacting with each other. When appropriate methods are used, relatively small systems can indeed simulate accurately the collective behavior of real plasmas.

2.1. The electrostatic model

The model predicts the behavior of charged particles motion due to forces of their own and applied fields. Physical examination is rooted in the fact that a charged particle produces a field - electric field anyway and magnetic field if it is in motion, a force is generated due to the interaction of the field(s) with other particles, this force determines the equation of motion.

The fields are calculated through Maxwell equations by knowing the positions of the particles and their velocities. The forces on the particles are found using the electric and magnetic fields in the Newton-Lorentz equation. Initially the fields are calculated from the first charge and current densities, then the particles are moved to small distances and subsequently the fields are recalculated due to new positions and velocities which the particles acquire; this process is repeated for many time steps. The one dimensional geometry model, treated here, is shown in Fig. 2.

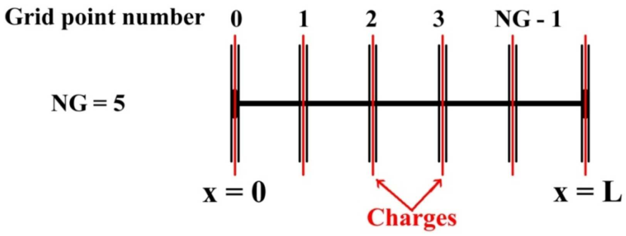

Figure 2 - Geometry of the one-dimensional simulation box consisting of a many sheet charges, with self and applied electrical field along the axis x. The first grid point is placed at $x = 0$.

2.2. Mathematical description and considerations

The model employed here is the Particle in Cell (PIC) [8], originated from the work of J.M. Dawson [9-11] in the late fifties. In this model, the plasma is represented by macroparticles, since each particle used in the simulation represents thousands of particles of a real experiment. The macroparticles are used to represent the system and thus include its kinetic behavior. PIC code is able to integrate in time the trajectories of a huge numbers of charged particles in their self-consistent electrostatic fields. The PIC system assumes that particles do not interact with each other directly, but through the fields which they produce according to the Maxwell's equations. Particles can be located anywhere in space; nevertheless, the field quantities are calculated on a fixed grid.

Computational cycle starts with the knowledge of the initial particle position x_i from which the charge density $\rho(x_n)$ is found at the grid points x_n by interpolation

$$\rho(x_n) = \Sigma_i q_i S(x_n - x_i), \tag{1}$$

in which S is the particle shape function which replaces point charges with a finite size charge cloud to reduce close range collision effects. The particle charge is q_i with center x_i [12]. Next, the electric field $E(x_n)$ is found at the grid points by solving Poisson's Equation

$$\nabla E(x_n) = -\nabla^2 \phi = \rho(x_n)/\varepsilon, \tag{2}$$

using the Fast Fourier Transform [13]. This electric field is then used to calculate the force on each particle whose trajectories are updated by integrating Newton's Law,

$$d\upsilon_i/dt = E(x_i)q_i/m_i \tag{3}$$

$$dx_i/dt = \upsilon_i \tag{4}$$

The velocity and position of each particle are advanced in time using a time centered leap-frog scheme [14]

$$\upsilon_i(t + \Delta t/2) = \upsilon_i(t - \Delta t/2) + [F_i(t)/m_i]\Delta t, \tag{5}$$

$$x_i(t + \Delta t) = x_i(t) + \upsilon_i(t - \Delta t/2)\Delta t. \tag{6}$$

This cycle then is repeated for the duration of the simulation. Diagnoses are computed along the way and all lengths are normalized to the grid spacing. These lengths are related back to physical lengths later.

PIC code applied in simulations of charged particle dynamics or beam optics of the transport system in particle accelerators is well discussed in the literature [15] and used in various software as CST Particle Studio [16].

2.3. Computational cycle: brief remarks

At each time step, the algorithms solve the field for the particles and then move it. This cycle is illustrated in Fig. 3.

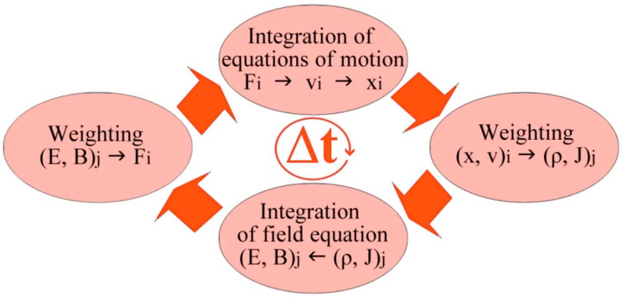

Figure 3 - Characteristic cycle in a particle simulation program for one step time. The particles indices are $i = 1, 2, \ldots$, NP; the indices of the mathematical grid, *i.e.* the discretization of space, are j. The time follows in clockwise rotation.

At $t = 0$, the cycle is initiated jointly with proper initial condition of the particle position and velocity.

Numbers of time steps are dictated, thus the computer runs printing out different diagnoses in form of snapshots at particular times, as kinetic energy *vs.* time, potential or field distributions, for example.

3. Instability analysis and considerations on the simulation

The Eq. (7) shows the relation of dispersion used by the code for this simulation

$$1 - \omega_p^2/\omega^2 - \omega_b/(\omega - k \cdot \upsilon_0)^2 = 0. \tag{7}$$

Usually the injected beam density η_b is much smaller than the plasma density η_p, such that $\omega_b^2 << \omega_p^2$, where ω_b is the beam frequency and ω_p is the plasma frequency. This hypothesis is the vital principle of the called weak-beam model [17]. The interactions in weak-beam model are of type electron-electron with a static neutralizing ion background, that is $m_i/m_e \rightarrow$ infinity, where m_i and m_e are the ion and the electron mass respectively. The plasma frequency ω_p is prevailing and the interesting wave numbers are close to $k = \omega_p/\upsilon_0$, where υ_0 is the electron beam velocity.

The instability inspected here is due to the interaction of plasma with a weak (by choosing $\omega_b^2/\omega_p^2 = 0.001$) beam, passing through it. The crucial purpose of this simulation is the understanding of general plasma behavior under the described circumstances, without interest in specific data in the graphs. Then, the more important characteristic that will be analyzed is the general behavior of the curves.

With $\omega_b^2/\omega_p^2 << 1$, particles of the plasma could be considered as a linearized fluid or assumed by a linear susceptibility. One essential observation is if the plasma frequency presents a linear response to the beam, there is freedom of choose a small value for q/m to make sure that the plasma keeps linear [18]. This permits to use a small number of plasma particles, as few as one per cell. The diagnosis studied here is obtained from XES1 one dimensional plasma simulation code [19]. Simulation results will be shown in all graphs at the same time in the end of simulation, 251494 μs, by means of the characteristics of interaction of the cold plasma and cool electron beam, which will be presented in diagnoses.

A cold plasma is classically characterized by the situation where there is a low degree of ionization. Rigorously, a cold plasma is one in which ionized electrons do not have sufficient energy to escape from the influence of its corresponding ion, and thus do not exhibit random motion [20]. A cool electron beam is drifting through cold unperturbed plasma. The low temperature of the beam avoids the non-physical cold beam instability, so the only phenomenon is the growth of the physical beam plasma instability [21]. The distribution function of the cool electrons was described by Gyergyek and Èerèek [22].

The parameters used in the simulation jointly with its values are listed in Table 1. Length of the grid is referring to stage of the computational cycle. Number of particles of the plasma refers to the particles that interact with the beam, *i.e.* electrons.

Table 1 - Parameters and Input data of simulation.

Description	Input value
Number of species	2
Time step	0.1
Total number of steps	4000
Number of grid points	1000
Length of the grid	2π
Number of particles of the beam	512
Number of particles of the plasma	1024
Velocity of the plasma electrons	0
Drift velocity of the electrons in the beam in x direction	1.0

4. Simulation results

Figure 4 shows the electric field *vs.* position at a specific time. The electric field is smoother than the density of charge, since the spatial integral of the charge density is the electric field. XES1 code uses the electric field to determine the electrostatic force on particles in the mover [23]. The electric field observed in the diagnosis is periodic, as it should be according to theoretical model proposed.

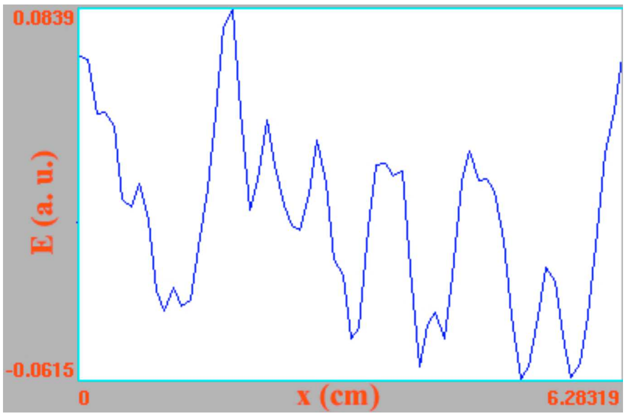

Figure 4 - Electric field E (arbitrary units) *vs.* position x (cm) along the grid. The positions are points situated on the grid.

The potential diagnosis displayed in Fig. 5 shows the value of the potential at the grid points. The potential is the double spatial integral of the density, it presents even less noise than the electric field as one can see comparing the diagnosis shown in Fig. 4. The potential is also periodic, as expected. The profiles of electric potential and electric field vary exceedingly in space and time during each cycle.

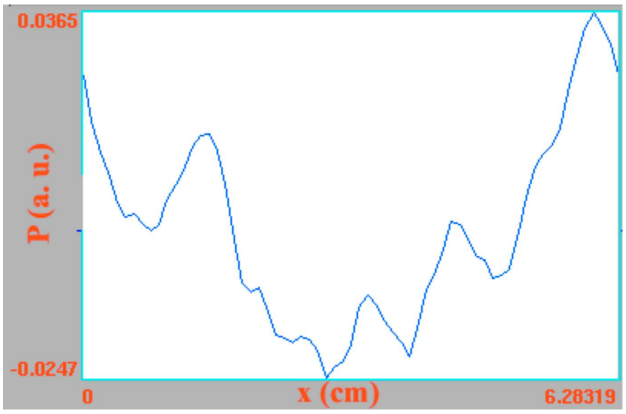

Figure 5 - Electric potential P (arbitrary units) *vs.* position x (cm) along the grid.

Figure 6 shows the time evolution of field energy (FE). One can see that the FE oscillates substantially in time, as predictable by exceeding variation observed in electric field in position (Fig. 4) and time (while the simulation is running). The mean behavior of FE does not vary appreciably.

Diagnoses of kinetic energy (KE) are displayed in Fig. 7, these analysis are made as a function of the time history of the total kinetic energy for all species.

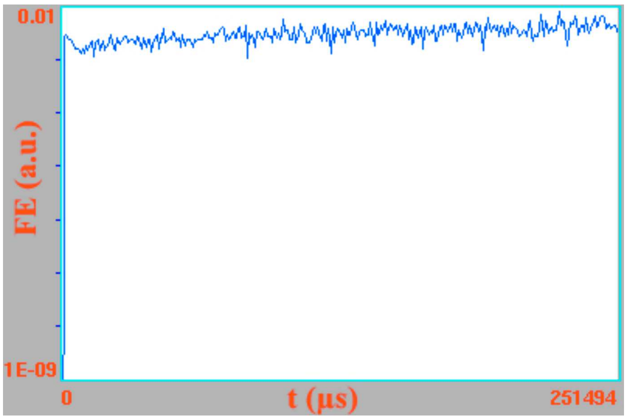

Figure 6 - Field energy FE (arbitrary units) in function of time t (μs).

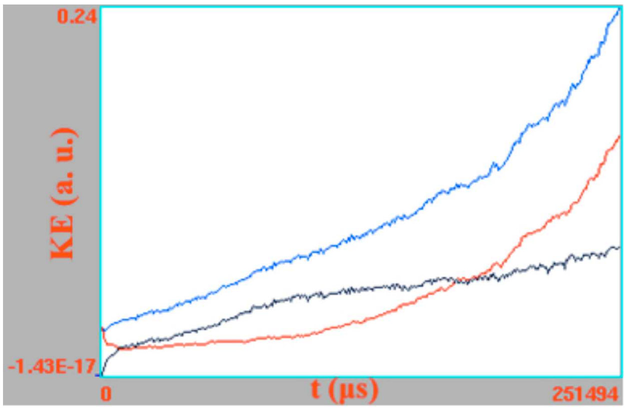

Figure 7 - Kinetic energy KE (arbitrary units) in function of time t (μs). Blue line represents the sum of electron beam kinetic energy (red line) and plasma kinetic energy (black line).

Total energy (TE) is evaluated in Fig. 8. This diagnostic displays the time history of the total energy of all species, plasma and beam; *i.e.* total energy = kinetic + field energies. This history is a semi-log plot, calculated from $\log(TEi) = \log(KEi + FEi)$. The total energy of a given simulation should be conserved. As showed in Fig. 7, the total energy is certainly an increasing function in time, since the plasma state is being continually disturbed by the beam, and the total kinetic energy is likewise an increasing function in time.

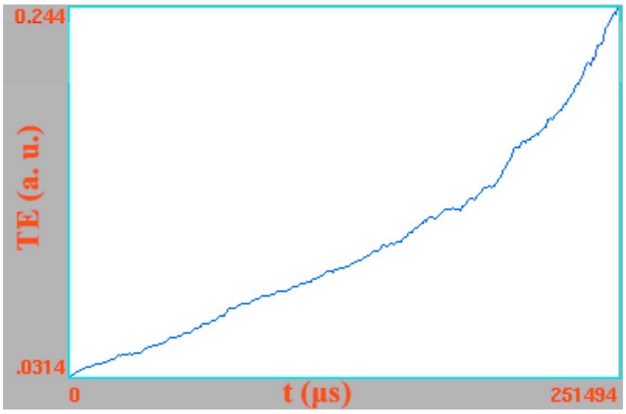

Figure 8 - Total energy TE (arbitrary units) in function of time t (μs).

An interest reader can download the code and perform by himself new simulations, experimenting with parameters. XES1 is a free software and can be downloaded in Berkeley web site indicated in Ref. [19]. A manual is available in Ref. [23].

5. Conclusion

We have studied the behavior of a plasma instabilized by an injected beam of electrons, surveying and illustrating some basic concepts of plasma physics theory and simulations. This article showed a simple one dimensional code that allows exploring some ideas of this branch of physics. The PIC code was introduced by means of simple equations of dynamics and electrodynamics, and the base of the computational design was described. Simulation results explored in the diagnosis showed an expected behavior of the analyzed physical quantities, as was reported and discussed. Analysis conducted allows a better conception of the physical parameters used for describing the essential behavior of the plasma disturbed by an electron beam. The application of the PIC in accelerator devices was stated. The review can be used for appreciating the principle of PIC code focused on the analysis of the beam optics in the transport system of a neutron generator, to have an idea of the plasma behavior submitted to beam of electrons accelerated by an electrostatic field into a plasma chamber and also for stimulating the study of the plasma physics in other types of investigations.

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