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Ion injection in electrostatic particle-in-cell simulations of the ion sheath

A. Tejero-del-Caz [a,*], J.I. Fernández Palop [b], J.M. Díaz-Cabrera [c], G.F. Regodón [b], R. Carmona-Cabezas [b], J. Ballesteros [b]

[a] Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Av Rovisco Pais, 1049-001 Lisboa, Portugal
[b] Departamento de Física, Universidad de Córdoba, E-14071 Córdoba, Spain
[c] Departamento de Ingeniería Eléctrica, Universidad de Córdoba, E-14071 Córdoba, Spain

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ABSTRACT

A particle injection algorithm has been developed for its use in electrostatic particle-in-cell (PIC) simulations of the ion sheath which takes place in the surroundings of a planar electrode immersed in a plasma when negatively biased. The algorithm takes into account the acceleration of ions along the presheath and evaluates their flux and velocity distribution when entering the simulation at the sheath edge. It has been verified by comparing the results obtained from the PIC simulation with those provided by fluid models of the ion sheath. The algorithm can be easily extended to cylindrical or spherical geometries and, in fact, it has already been successfully used to study the transition from radial to orbital behaviour of ions in the surroundings of cylindrical Langmuir probes.

1. Introduction

Nowadays, many surface treatment techniques rely on plasma technology [1] which, ultimately, depend on the sheath that takes place between a neutral plasma and the surface that is going to be treated. In many cases, in order to perform the functionalisation of the surface, it is polarised in such a way that it attracts positive ions. Also, plasma diagnosis by using electrostatic Langmuir probes, which constitutes one of the few methods that provides local measurements on plasma parameters [2–7], depends on the plasma-sheath properties. Likewise, one of the most attractive conditions to perform the diagnose with Langmuir probes, is to negatively bias them with respect to the plasma as, by doing so, the current collected by the probe and drained from the plasma is diminished and so the disturbance produced by the presence of the probe [8–10]. Because of the aforementioned reasons, the theoretical knowledge of the structure of the ion sheath that is developed between a neutral plasma and a negatively biased metallic surface, results of great importance.

There are two main approaches when it comes to obtain theoretical knowledge about the ion sheath: fluid or kinetic modelling and particle simulations [11]. On the one hand, fluid or kinetic modelling is fast and sometime allow us to obtain analytical expressions that are useful when it comes to diagnose a plasma. However, because of their lack of selfconsistency and macroscopic nature, in the case of fluid models, they are not always the most suitable approach. On the other hand, particle simulations [11–13] constitute a selfconsistent first principles approach that provides the most detailed information about the system. Nevertheless, there are some drawbacks when it comes to use particle simulations. The computational

* Corresponding author.
E-mail address: antonio.tejero@tecnico.ulisboa.pt (A. Tejero-del-Caz).

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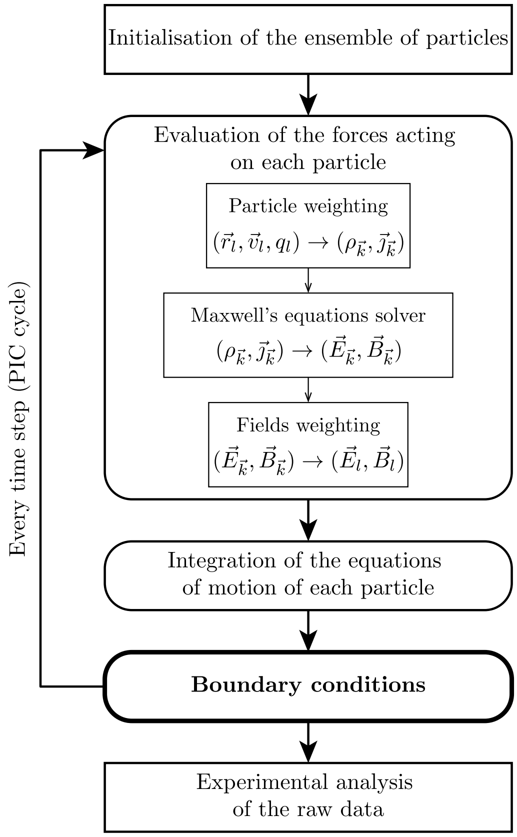

Fig. 1. General scheme of a PIC simulation. The l subindex refers to particles while the $\vec{k}$ subindex refers to grid nodes.

resources needed are huge, and one has to be careful with the different physical mechanisms and algorithms implemented in the simulation, since they can greatly affect its behaviour and the results provided by it, as we will see in this paper.

When we talk about particle simulations in plasma science, we mostly refer to the well known particle-in-cell (PIC) codes [13]. The main difference between PIC and any other particle simulation lies in the force evaluation algorithm. In PIC simulations, the simulation domain is gridded and, the forces acting on each particle are evaluated by considering a macroscopic field which is evaluated at the nodes of the grid. In Fig. 1 the general scheme of a PIC simulation can be seen. However, in this paper we will be focused on the case of electrostatic simulations, *i.e.* non magnetised plasmas.

PIC simulations are well known algorithms [11–13] and, the effects of the different numerical schemes that can be used in the various steps, that can be seen in Fig. 1, have been extensively studied [14–16]. However, there exists a common problem that appears when simulating an ion sheath, *i.e.* the contact of a plasma with a negatively biased metallic surface. When the loading of particles, or more precisely of the ions, is not performed properly a "source sheath" may appear [17–19].

Some solutions to this problem have been proposed [20], however, they depend on macroscopic coefficients such as diffusion or mobility coefficients, which are not usually easy to obtain. In this paper, we present an iterative selfconsistent algorithm that allows to avoid the appearance of this source sheath, without the need of macroscopic coefficients.

The rest of the paper is organised as follows: in 2 the statement of the problem is presented, defining what a source sheath is and explaining the reasons of its appearance. In 3 the proposed algorithm for the ion injection is introduced. Then, in 4, the results obtained when using the proposed injection algorithm are shown. Finally, in 5, the conclusions of the present research are outlined.

2. Statement of the problem

Let us start by defining what a source sheath is. A source sheath is a sheath-like potential drop that occurs at the boundary where particles are injected into the simulation, *i.e.* the source of particles. Source sheaths appear in PIC simulations of the contact of an electrode with an unperturbed plasma. They are more pronounced when the electrode that is being simulated has planar geometry, however, it has also impact when other geometries are considered. The appearance of source sheaths has been observed since long time ago [17], however they are still a common problem [18,19].