DESIGN OF A SEMI-ANALYTICAL METHOD TO DESCRIBE PLASMA-WALL INTERACTIONS

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Abstract

Electric probes are objects immersed in the plasma with sharp boundaries which collect of emit charged particles. Consequently, the nearby plasma evolves under abrupt imposed and/or naturally emerging conditions. There could be localized currents, different time scales for plasma species evolution, charge separation and absorbing-emitting walls. The traditional numerical schemes based on differences often transform these disparate boundary conditions into computational singularities. This is the case of models using advection-diffusion differential equations with source-sink terms (also called Fokker-Planck equations). These equations are used in both, fluid and kinetic descriptions, to obtain the distribution functions or the density for each plasma species close to the boundaries. We present a resolution method grounded on an integral advancing scheme by using approximate Green’s functions, also called short-time propagators. All the integrals, as a path integration process, are numerically calculated, what states a robust grid-free computational integral method, which is unconditionally stable for any time step. Hence, the sharp boundary conditions, as the current emission from a wall, can be treated during the short-time regime providing solutions that works as if they were known for each time step analytically. The form of the propagator (typically a multivariate Gaussian) is not unique and it can be adjusted during the advancing scheme to preserve the conserved quantities of the problem. The effects of the electric or magnetic fields can be incorporated into the iterative algorithm. The method allows smooth transitions of the evolving solutions even when abrupt discontinuities are present. In this work it is proposed a procedure to incorporate, for the very first time, the boundary conditions in the numerical integral scheme. This numerical scheme is applied to model the plasma bulk interaction with a charge-emitting electrode, dealing with fluid diffusion equations combined with Poisson equation self-consistently. It has been checked the stability of this computational method under any number of iterations, even for advancing in time electrons and ions having different time scales. This work establishes the basis to deal in future work with problems related to plasma thrusters or emissive probes in electromagnetic fields.
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This chapter briefly reviews the theoretical basis needed to understand the Plasma Physics used in this work and, at the same time, it is stated the notation and nomenclature that remains throughout the text.

Finally, since this work focuses its attention in the design of a computational method, some references are given to the state of art in the numerical simulation of plasmas.

1.1 Ionized gases and plasmas

A plasma is a gas where a fraction of its particles are ionized atoms or molecules, it is a mixture of ions, electrons and neutral gas atoms or molecules that interact among themselves. Plasmas can be fully ionized (when there is no neutral atoms) or a partially ionized (when not all the particles are ionized). The large amount of free charges results in high electrical conductivities and the possibility of sustaining electric currents that make the plasma very sensible to the action of electromagnetic fields[3, 8, 10, 11].

In the thermodynamical equilibrium, the atoms of a gas obey a Maxwell-Boltzmann velocity distribution determined by the temperature of the system. The average velocity of these particles is

\[ V_{\alpha,\text{Th}} = \sqrt{\frac{8k_bT}{\pi m_\alpha}}, \]

(1.1.1)

where \( \alpha \) represent neutral atoms, electrons or ions. When the temperature grows up, the kinetic energy of an increasing fraction of the neutral atoms lies over the ionization threshold \( (E_I) \) of the neutral gas and it starts the ionization process. The detailed analysis of the relation between the equilibrium temperature \( T \) and the ionization degree for a gas is not established in this text, but an important relation between them is given as a classical result called the Saha equation

\[ \frac{n_e n_i}{n_a} \simeq 2.4 \times 10^{21} T^2 \exp \left( -\frac{E_I}{k_bT} \right), \]

(1.1.2)

where \( n_e, n_i \) and \( n_a \) represent the number of electrons, ions and neutral atoms per unit volume. The ionization of an appreciable ratio of the gas require a very high temperature and the energy
is lost by different physical mechanisms as the emission of visible light, electric current and heat transport, etc. These losses are sustained by an external source of energy as external radiation, electromagnetic fields, etc.

1.1.1 Properties characterising a plasma

As said above, plasma can be defined as a mixture of charged ions, electrons and neutral particles which constitutes a macroscopic electrically neutral medium that responds to electric and magnetic fields in a collective mode\(^1\). Some properties of the plasma concerning this electromagnetic response are

- The charged particles interact through long distance electromagnetic forces and the number of positive and negative charges is equal, so that, the medium is electrically neutral, as a whole.

- The electromagnetic interaction can be considered as instantaneous in the plasma medium. We will not cope with relativistic effects, that means, the force experienced by charged particles are, driven by the electromagnetic fields, that can be approximated by the Lorentz force.

- The plasma is an electrically neutral medium in the sense that the average charge density is null over macroscopic volumes with typical sizes larger than the Debye length \(\Lambda_D\). This requires an average of equal number of positive and negative densities of charged particles inside a Debye sphere.

- The typical length of the system \(L\) is always considered larger than the Debye length, \(i.e., L \gg \Lambda_D\). Therefore, the characteristic distances \(L_{sh}\) for the Debye electric shielding, \(L_{sh} \sim \Lambda_D \ll L\), are also smaller compared to the typical longitudes \(L \gg L_{sh}\).

- The number of electrons (and ions) \(N_D\) contained within a sphere of radius \(\Lambda_D\) must be large enough to allow the Debye shielding the internal and external low amplitude electromagnetic field fluctuations.

- In accordance to the magnitude of the magnetic field, the plasmas are classified as magnetized or unmagnetized. In magnetized plasmas the Larmor radius \(R_l\) of electrons (or ions) is smaller than the characteristic distance \(L < R_l\).

1.1.2 The ideal Maxwellian plasma

In a neutral gas, composed by a single kind of atoms with mass \(m\), the equilibrium distribution can be represented by the well-known Maxwell-Boltzmann energy distribution:

\[
f(v) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp\left(-\frac{mv^2}{2k_B T}\right),
\]

where the vector \(v\) represents the particle velocity. The integral over all possible velocities reads

\[
\int_{-\infty}^{+\infty} f(v) \, dv = \int_{-\infty}^{+\infty} f(v) \, (4\pi v^2) \, dv = 1.
\]

\(^1\)The collective response to external response means the perturbations caused by electric or magnetic fields involve a large number of particles.
In the thermodynamical equilibrium, the number of particles per unit volume \((n_0)\) is uniform, therefore, it can be expressed as
\[
\int_{-\infty}^{+\infty} n_0 f(v) \, dv = n_0 \tag{1.1.5}
\]
The magnitude \(dn = n_0 f(v) \, dv\) indicates the amount of particles with velocity between \(v\) and \(v + dv\) for a differential volume.

The average kinetic energy reads
\[
e_i = \left\langle \frac{1}{2}mv^2 \right\rangle = \frac{1}{n_0} \int_{-\infty}^{+\infty} f(v) \left(\frac{1}{2}mv^2\right) \, dv = \frac{3}{2}k_B T \tag{1.1.6}
\]
and the average speed of the plasma can be expressed as
\[
\bar{v} = \left\langle |v| \right\rangle = \left\langle \sqrt{\mathbf{v} \cdot \mathbf{v}} \right\rangle = \int_{-\infty}^{+\infty} n_0 f(v) v \left(4\pi v^2\right) \, dv = \left(\frac{8k_B T}{\pi m}\right)^{\frac{1}{2}} \tag{1.1.7}
\]

The Maxwell Boltzmann distribution function can be used for the thermodynamic equilibrium state in an ideal plasma, each particle species is characterized by:

1. The energy distribution for the plasma species have a common kinetic temperature\(^3\) \((k_B T)\).
2. To preserve the plasma neutrality, the number of electrically charged species (ions and electrons) are practically the same. In consequence, the electric field is close to zero for the whole plasma.
3. The electric potential is constant almost along the plasma out equilibrium. This means that no currents or transport of particles exist in a Maxwellian plasma.

### 1.1.3 The Debye length

Let us consider a quasi neutral plasma \((n_e \simeq n_i \simeq n_a)\) which has a low amplitude plasma potential fluctuation \(\phi(r)\) produced by a small charge \(\delta \rho_{\text{ext}} = q \delta(r)\), where \(\delta(r)\) represents the Dirac delta and \(r\) is the radial coordinate in a spherical geometry. The charge produces very small variations of \(\phi(r)\) close to the equilibrium position \((r = 0)\). The local perturbed charge density is,
\[
\delta \rho = q \delta(r) + e [n_i(r) - n_e(r)] \tag{1.1.8}
\]
If we assume that the potential difference caused by the charge is small compared with the thermal energies \((\frac{e \phi(r)}{k_B T_\alpha} \ll 1\), with \(\alpha = e, i\)), the equation for the Maxwellian plasma for each species become
\[
n_\alpha(r) \simeq n_0 \left(1 \pm \frac{e \phi(r)}{k_B T_\alpha}\right) \tag{1.1.9}
\]
Now, the well-known Poisson equation reads
\[
\nabla^2 \phi = -\frac{\delta \rho}{\varepsilon_0} = -\frac{1}{\varepsilon_0} \left[q \delta(r) + \frac{e^2 n_0}{k_B T_i} \phi(r) + \frac{e^2 n_0}{k_B T_e} \phi(r)\right] \tag{1.1.10}
\]
\(^2\text{As explained above, there is no such a thing as an equilibrium state in plasma, but equilibrium can be here referred to an ideal quasi-neutral plasma state.}\)

\(^3\text{The temperature is normally measured in eV because, normally, it is very large (1eV = 11600K).}\)
and grouping terms the expression for the potential results
\[
\left( \nabla^2 - \frac{1}{\Lambda^2_D} \right) \phi (r) = - \frac{q \delta (r)}{\epsilon_0}, \text{ where } \frac{1}{\Lambda^2_D} = \frac{1}{\lambda^2_{Di}} + \frac{1}{\lambda^2_{De}} \quad (1.1.11)
\]

The parameters \( \lambda_{Di} \) and \( \lambda_{De} \) are the Debye lengths for the ions and electrons,
\[
\lambda_{Da} = \sqrt{ \frac{\epsilon_0 k_B T_\alpha}{e^2 n_0}}. \quad (1.1.12)
\]

Assuming spherical symmetry, and introducing the potential \( \phi (r) = \frac{q}{r} f (r) \), the Poisson equation (for \( r > 0, a > 0 \)) can be expressed as
\[
\frac{d^2 f}{dr^2} = \frac{1}{\Lambda^2_D} f \Rightarrow f = \exp \left( - \frac{r}{\Lambda_D} \right) \quad (1.1.13)
\]
finally, the potential is,
\[
\phi = \frac{q}{r} \exp \left( - \frac{r}{\Lambda_D} \right) \quad (1.1.14)
\]

In order to recover the potential for a point charge when \( \frac{r}{\Lambda_D} \ll 1 \), the parameter \( a \) has to be \( a = \frac{q}{4\pi \epsilon_0} \). Finally, the electric potential for \( r > 0 \) is,
\[
\phi (r) = \frac{q}{4\pi \epsilon_0} \exp \left( - \frac{r}{\Lambda_D} \right) \quad (1.1.15)
\]

The amplitude of a fluctuation of the plasma potential decays in space exponentially with a rate \( \frac{1}{\Lambda_D} \). Equivalently, the local charge perturbation \( q \) becomes shielded out by a cloud of opposite charge with a radius proportional to \( \Lambda_D \). In other words, the Debye length is the minimum distance from which the plasma can be considered quasi-neutral.

### 1.1.4 Characterization of plasmas

A very large and different kinds of plasmas exist in Nature. Each kind of plasma can be characterized by its Kinetic Temperature \( k_B T \) and its density \( n \). In Figure 1.1.1 on page 5 a graph with a classification based in the plasma density and in its temperature is displayed.

As we can see, a great dispersion in the kind of plasmas exists whose characteristic densities differ in orders of magnitude, then, the expected behavior of a low density low temperature plasma is way far different from a fusion plasma. That will have a big influence in the plasma physic, e.g. in the collisions between particles.

### 1.2 Physical models for plasma

Most of the plasmas are found in partial equilibrium, like the plasma in a glow discharge or the plasma inside a Hall thruster. In order to take into account the non-equilibrium interactions and properties, new models, besides the Maxwellian distribution function, have to be introduced.

There are two main kinds of theoretical approaches to describe the plasma which roughly speaking are related to the macroscopic and microscopic theories.
The microscopic model approaches are less dependent on experimental parameters. Here the plasma is considered as a discrete set of particles. With these models, the key is to find the distribution function \( f_\alpha (r, v, t) \). With this distribution function, all the plasma macroscopic parameters and properties can be calculated. To find the distribution function, the Boltzmann equation (1.2.1 where \( C_s (f_\alpha) \) is the collisional term) has to be solved. This equation takes into account the sinks and sources of particles, the collisions and the forces acting over the plasma.

\[
\frac{\partial f_\alpha}{\partial t} + \mathbf{v} \cdot \nabla_r f_\alpha + \frac{\mathbf{F}}{m_\alpha} \cdot \nabla_v f_\alpha = C_s (f_\alpha)
\]  

(1.2.1)

In (1.2.1), the force \( \mathbf{F} \) normally represents the gravitational force (\( \mathbf{F}_g \)) and the force due to the magnetic and electric field or self-generated fields (\( q (\mathbf{E} + \mathbf{v} \wedge \mathbf{B}) \)).

The macroscopic models consider the plasma as a continuum medium with a high number of particles per unit volume. The characteristic length of the problem \( L \) has to be much larger than the Debye length \( \Lambda_D \) to allow the application of these models. The equations for the fluid motion are directly derived from the conservation of mass, momentum and energy. Some plasma parameters (as the viscosity, the thermal conductivity, etc.) are needed to close the fluid equations and have to be supplied by external considerations or by experiments. The goal of these models are to obtain the velocity and/or the particle density distribution. The fluid equations can be derived from the Boltzmann equation using the momentum equation,

\[
M_\alpha^{(k)} (r, t) = \int_{-\infty}^{+\infty} \left( \mathbf{v} \otimes \mathbf{v} \otimes \mathbf{v} \otimes \ldots \right) f_\alpha (r, \mathbf{v}, t) \, d\mathbf{v}
\]  

(1.2.2)

Figure 1.1.1: The characteristic densities and temperatures of different plasmas in nature and in the laboratory. After L. Conde[5] with permission.
Figure 1.2.1: Physical models for an statistical ensemble of interacting particles. After L. Conde[3] with permission.
The Continuity Equation can be obtained as the first order moment of the Boltzmann equation (1.2.1),

\[ \int_{-\infty}^{+\infty} \frac{\partial f_\alpha}{\partial t} dv + \int_{-\infty}^{+\infty} v \nabla_r f_\alpha dv + \int_{-\infty}^{+\infty} \frac{F}{m_\alpha} \nabla_v f_\alpha dv = \int_{-\infty}^{+\infty} C_s (f_\alpha) \]

The Momentum Transport equation can be obtained multiplying the Boltzmann equation by \( m_\alpha v \) and integrating over the velocity space [8, 1],

\[ \int_{-\infty}^{+\infty} m_\alpha v \frac{\partial f_\alpha}{\partial t} dv + \int_{-\infty}^{+\infty} m_\alpha v \nabla_r (v f_\alpha) dv + \int_{-\infty}^{+\infty} v F \nabla_v f_\alpha dv = \int_{-\infty}^{+\infty} m_\alpha v C_s (f_\alpha) \]

(1.2.3)

\[ \int_{-\infty}^{+\infty} m_\alpha v \nabla_r (v f_\alpha) dv = \nabla_r (m_\alpha n_\alpha \langle v \otimes v \rangle) = \nabla_r \tilde{S}_\alpha (r, t) \]

where \( \tilde{S}_\alpha (r, t) \) is the stress tensor. The next equation is the Energy Transport equation, and it is calculated by multiplying (1.2.1) by \( \frac{m_\alpha v^2}{2} \) and integrating over the velocity space,

\[ \frac{\partial}{\partial t} \left( n_\alpha \left( \frac{m_\alpha v^2}{2} \right) \right) + \nabla_r \left( n_\alpha \left( \frac{m_\alpha v^2}{2} \right) v \right) dv + \int_{-\infty}^{+\infty} \frac{v^2}{2} F \nabla_v f_\alpha dv = \int_{-\infty}^{+\infty} \frac{m_\alpha v^2}{2} C_s (f_\alpha) \]

(1.2.4)

This formidable set of equations can be simplified in many practical situations.

1.3 The plasma sheath

Plasmas in Nature and in the laboratory are, normally, limited or in contact with metallic or dielectric walls which interact with the plasma modifying its behavior. In the experiments, the plasma is normally enclosed inside a vacuum tank or a glass discharge tube and the electrodes, surfaces and/or probes are boundaries that interact with the plasma. In space applications, the external metallic surfaces from vehicles also interact with the ionospheric plasma and, according to the electric polarity, a particle current may appear changing the electric potential of the vehicle with respect to its surroundings. This charging process may produce electric shocks and, at high altitude, electric discharges in orbiting spacecrafts.

This interaction between the wall and the bulk plasma is a classical unsolved problem. The potential of the metallic wall generally differs from the plasma bulk and both values have to connect in a certain length scale, denominated plasma sheath. This process is very important
for the Plasma Physics because in this small sheath the plasma current collection and another processes take place[16, 21]. Moreover, the sheath can affect the measures made with probes and the inner plasma structure in certain conditions.

To explain this process, a one dimensional fully ionized and cold unmagnetized plasma is assumed. The plasma is enclosed within a vacuum chamber of finite dimensions and the walls have a negative potential ($\varphi_w$) respect to the plasma potential ($\varphi_p$). In the non-emissive case, the electrons are normally reflected in the wall what increases the ionization. The potential function is uniform in the unperturbed plasma its the variation is restricted in one small layer close to the wall[16].

The calculation of the plasma potential from $\varphi_w$ close a wall located at $x = 0$ up to the plasma bulk plasma $\varphi_p$ requires to solve the Poisson equation for $\varphi(x)$ with appropriate boundary conditions. In general, this leads to a complex nonlinear partial differential equation that becomes reduced to a simpler problem by making the following assumptions:

- The potential of the wall is negative with respect to the plasma, $\varphi_w < \varphi_p$, so, the ions are attracted and the electrons repelled.
- In the plasma bulk (far enough from the wall) the quasi-neutrality condition is satisfied $n_e \simeq n_i \simeq n_{eo}$.
- The ions are considered cold ($k_B T_e \gg k_B T_i$) and the electrons have a Maxwell Boltzmann distribution\(^4\).
- The ionization is negligible in the considered volume; all ions entering into the plasma sheath finally reach the wall. Then, the current density of ions $\Gamma_i = n_i u_i$ is constant in the sheath $\frac{d\Gamma_i}{dx} \simeq 0$. Therefore, at each point $x$ between plasma volume and the wall we have,

\[
\Gamma_i = n_{i0} u_{i0} = n_i(x) u_i(x) \tag{1.3.1}
\]

With these conditions, the energy for an entering ion with velocity $u_{i0}$ is,

\[
\frac{1}{2} m_i u_i^2 (x) + e\varphi(x) = \frac{1}{2} m_i u_{i0}^2 \tag{1.3.2}
\]

and with what we saw in 1.3.1 the ion density reads

\[
n_i(x) = \frac{n_{i0} u_{i0}}{\sqrt{u_{i0}^2 - 2e\varphi(x)/m_i}} \tag{1.3.3}
\]

Now, the Poisson equation results

\[
\epsilon_0 \frac{d\varphi(x)}{dx} = -en_e \left\{ \exp \left( \frac{e\varphi(x)}{k_B T_e} \right) - \frac{u_{i0}}{\sqrt{u_{i0}^2 - 2e\varphi(x)/m_i}} \right\} \tag{1.3.4}
\]

This equation can be written in non-dimensional forum with the following variables:

\[
N_e = \frac{n_e}{n_{e0}}, \quad N_i = \frac{n_i}{n_{i0}}, \quad V = \frac{u}{e_i} \tag{1.3.5}
\]

\(^4\)This is possible because we are assuming a high temperature for the electrons and that allow them to thermalize faster than the ions
where \( c_{is} = \sqrt{\frac{kT_i}{m_i}} \) is the ion sound speed. This is an example of how non-linear equations appear in plasma theory although a very simple Physics is involved in the model. The solutions of this equations up to first order in \(|\varphi|\) leads to the so-called Bohm criterion for the sheath formation that can be found in many texts\([1, 3, 16]\).

### 1.4 Probes in plasma

As said above, to characterize a plasma some measurements have to be done. The most usual plasma diagnostic technique are based on electric probes. These probes are, basically, a piece of metal connected to an external electric circuit, they are able to emit or collect charges establishing a measurable electric current. Through the use of these probes, the plasma potential can be obtained, what leads in combination to some theoretical assumptions, to a potential profile and to an estimation of, for example, the plasma electron temperature.

These probes have different geometries, but the most employed are the cylindrical and the spherical ones. A lot of works have been done to try to characterize a plasma close to a probe, but this topic is still a matter of continuous research in plasma scientific community.

For a review of the elementary theory of plasma probes see, for instance, \([3, 10, 16, 18, 19, 21]\) and references therein.

### 1.5 Numerical Methods in plasma simulation

In scientific and industrial environments, a lot of numerical methods have been developed to solve the plasma equations and to simulate plasmas dynamics\([9]\). As in many other branches in Physics, the main numerical techniques used by the plasma community are classified as follows.

- **Finite Element Methods (FEM).** These methods use an approximation for the spatial derivative and a time advancing scheme to iterate the problem. Many schemes can be found in the literature, these schemes have been adapted to almost every practical domains appearing in plasma experimental devices, or in astrophysical plasmas. These methods have been improved to describe plasma systems, specially when conservative magnitudes appear, however, there are many issues related to the convergence and stability as well as to maintain physical feasible solutions.

- **Monte Carlo methods\([13]\).** The modern version was invented in the 40s by Stanislaw Ulam. They consist in a broad class of algorithms that rely on repeated random sampling to obtain numerical results. Monte Carlo methods are very useful for simulations where many coupled degrees of freedoms appear, they are used to simulate plasmas under a statistical point of view dealing with large number of particles in the simulation.

- **Full Particle-In-Cell (PIC) codes.** The key in these methods is to calculate the trajectories of each macro-particle. A macro-particle, or test particle, is a cluster of neutrals, ions and electrons. It requires a high computational effort. In plasma physics applications, the method amounts to follow the trajectories of electrically charged particles in self-consistent electromagnetic (or electrostatic) fields computed on a fixed mesh.

None of these numerical methods completely describe a plasma with a reasonable computational cost and preserving the Physics involved in the description of the system. Therefore, the search to create numerical methods is always an open topic.
1.6 Aim of this work

In this work a new method is introduced to solve the advection-diffusion equations, in particular, the plasma wall interactions. Roughly speaking, this is a semi-analytical integral method based on the exact resolution of the Fokker-Planck equation with constant coefficients for a short-time of evolution.

Furthermore, the method improves previous stages by including how to deal with boundary conditions, a subject not accomplished up to now. A comparative between Finite Difference Method and the new Propagator Integral Method is included in this work, focusing specially in analyzing the improvements of the new method with respect to the Finite Difference method. The obstacles we have found to impose the boundary conditions by using this method are also presented and explained in this work. Finally, some results and some guidelines about the future research in this field are presented.

The main goal that could be considered of this work is to have been able to improve and to give a new numerical method to calculate the plasma-wall interaction. At the same time, an important result is related to the fact that the new method is highly flexible to be applied in several theoretical frames in plasma where the advection-diffusion equations appears. The method can be also applied without the recourse of linearizations. With this method we believe that a new research line in numerical calculation has been opened that can provide a new approach to numerical simulations in problems when other methods fails.
Many laws in Physics obey diffusive differential equations. Among them the Fokker-Planck equation appears in both fluid and kinetic plasma descriptions governing the time evolution of density or distribution functions in plasma processes. These equations are usually non-linear and the resulting equations are difficult to be solved analytically. Because of this, several numerical methods have been developed to provide solutions for this kind of equations. The most used numerical methods are based on difference schemes such as: Finite Differences or Finite Elements methods. Although these methods are well established, they present many disadvantages, specially if they are applied to solve non-linear problems with complex initial and boundary conditions: they may loose their physical meaning of the original equation. This fact, for instance, appears in those schemes that are non-conservative when dealing with conservative problems. More further, the addition of non-homogeneous terms can perturb the physical solutions. In order to cover these drawbacks in the classics methods, it is necessary to design new numerical methods with another mathematical theoretical basis.

In this chapter a new method will be introduced to deal with general advection-diffusion equations such as the Fokker-Planck equation. This new method will preserve the physical origin of the equation and will solve another problems from the numerical methods that we will introduce in chapter 4.

2.1 The Fokker-Planck equation

Many systems in Physics can be described by the so-called Fokker-Planck equation, which present the general form:

\[ \frac{\partial}{\partial t} f(t, q) = -\sum_{i} \frac{\partial}{\partial q_i} \left[ a_i(t, q) f(t, q) - \sum_{j} \frac{\partial}{\partial q_j} (b_{ij}(t, q) f(t, q)) \right] = L_{FP} f(t, q) \]  

(2.1.1)

where vector \( q \) represents a generic point in a \( N \)-dimensional space with coordinates \( q_i \) \( (i = 1, N) \) and the Einstein Summation Convention has been assumed. The problem function \( f(t, q) \) is governed by the advection and diffusion coefficients \( a_i(t, x) \) and \( b_{ij}(t, x) \) also called transport coefficients as a whole. The Fokker-Planck equation appears in many branches in Mathematical
Physics, for example, it describes the time evolution of the probability density of some kind of stochastic processes. In this work the function, $f$ will play the role of the distribution function of any plasma species or another macroscopic measurable quantity obeying convection and diffusion effects.

In general, the Fokker-Planck operator adopts the form:

$$L_{FP} = -\frac{\partial}{\partial q_i} \left[ a_i(t, q) - \frac{\partial}{\partial q_j} (b_{ij}(t, q)) \right]$$  \hspace{1cm} (2.1.2)

This operator can be a non-linear one because the coefficients can also depend on the problem function $f$ itself. For these reasons, sometimes, the notation explicitly includes $f$ in the arguments of the coefficients $a_i$ and $b_i$. For an exhaustive review of these equations see, for instance, the book of Risken[17].

### 2.1.1 The Fokker-Planck equation applied to a plasma

As we introduced in section §1.2, plasma can be described by a Fokker-Planck equation governing the distribution function for the different species under the theoretical frame of Kinetic theory.

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{v} \frac{\partial f_\alpha}{\partial x_i} = -\left[ \frac{\partial}{\partial v_i} \left( D_i(t, \mathbf{x}) + \frac{F_i}{m_\alpha} \right) - \frac{\partial}{\partial v_j} D_{ij}(t, \mathbf{x}) \right] f_\alpha$$ \hspace{1cm} (2.1.3)

For the plasma Fluid models, we will study here the one dimension fluid dynamic equation (2.1.4) that also has the form of a Fokker-Planck equation[14]. The advection and the diffusion phenomena depend on the parameters $A_\alpha$ and $D_\alpha$.

$$\frac{\partial n_\alpha}{\partial t} = -\frac{\partial}{\partial x} \left[ A_\alpha(x, t) - \frac{\partial}{\partial x} D_\alpha(x, t) \right] n_\alpha$$  \hspace{1cm} (2.1.4)

In this work, we are going to study our particular method applied to (2.1.4) with the parameters $A_\alpha(x, t) = \mu_\alpha E$, where $\mu_\alpha$ is the mobility and $E$ is the electric field; and $D_\alpha(x, t) = \mu_\alpha T_\alpha(eV)$ where $T_\alpha(eV)$ is the temperature of the species $\alpha$ in electron-volts[3, 8].

Few analytical solutions can be found in practical problems. Therefore, numerical methods have been applied for decades with reasonable good results in several problems. However, the standard methods cannot work in some realistic problems and the designing of alternative numerical procedures is always an open topic of research. In the following section we present the foundations of a new integral method based on the use of Green’s functions for general Fokker-Planck equations.

### 2.2 The numerical integral method

In this section, we introduce the theoretical principles of this new numerical integral method for the Fokker-Planck equation. This method has been established and used previously[5].

To start with this task let us consider the general Cauchy problem:

$$\frac{\partial f_\alpha}{\partial t} = L_{FP} \cdot f_\alpha + q_\alpha$$  \hspace{1cm} (2.2.1)
where $\varrho_\alpha$ is a non-homogeneous term that can depend on $t, q$ and $f$.

Another way to express (2.2.1) is using the probability current $J$,

$$
\frac{\partial f_\alpha}{\partial t} = -\nabla \cdot J_\alpha + \varrho_\alpha
$$

(2.2.2)

This formulation will be very useful in the following sections when we analyze the conservation of the total amount of $f_\alpha$ and the inclusion of the boundary conditions.

Formally, we can express the relation between $f_\alpha (q, t)$ and $f_\alpha (q, 0)$ through the operator of evolution $U_{t,0}$ for $t > 0$ as,

$$
f_\alpha (q, t) = U_{t,0} f_\alpha (q, 0)
$$

(2.2.3)

In general, for a time $t > t' > 0$ the above expression can be written in terms of the evolution operator $U_{t,t'}$,

$$
f_\alpha (q, t) = U_{t,t'} f_\alpha (q, t') = \int_D f_\alpha (q', t') \Pi (q, t; q', t') \, dq'
$$

(2.2.4)

where $\Pi (q, t; q', t')$ is the integral kernel associated to $U_{t,t'}$. This kernel is also known with the name of propagator. This propagator has the property to transfer information instantaneously from $t'$ to $t$ and from $q'$ to $q$. For $t' = 0$ we recover the expression (2.2.3). Sometimes (2.2.4) is called the Boltzmann Integral or Chapman-Kolmogorov equation, which is equivalent to the differential evolution equation (2.2.1), and $\Pi$ can be interpreted in probability theory as a transition probability function. From a more general point of view, $\Pi$ can be understood as the corresponding Green’s function that solves (2.2.1) where $\varrho_\alpha = 0$ and all the boundary conditions are natural (accounted in $\Pi$).

The general properties satisfied by these propagators are

$$
limit_{t' \to t} \Pi (q, t; q', t') = \delta (q - q')
$$

(2.2.5)

and

$$
\Pi (q, t; q', t') = \int_D \Pi (q, t; t'', q'') \Pi (q'', t''; q', t') \, dq''.
$$

(2.2.6)

The first relation accounts the initial condition for $\Pi$. This is to say if $t' = t$, $\Pi$ is the Dirac delta function. The second relation represents the independence of intermediate times $t''$ to calculate the transition from $t'$ to $t$. This important property can also be expressed as $U_{t,t'} = U_{t,t''} \cdot U_{t'', t'}$ in the notation of integral operators, which is a very familiar property in the theory of Markovians processes and in stochastic processes theory. For Markovians processes\(^1\), the propagators are transition probability functions. The equation (2.2.4) for a stochastic process for the conditional probability $P(q, t; q', t')$ is the Consistency Equation.

$$
f_\alpha (q, t) = \int_D f_\alpha (q', t') P(q, t; q', t') \, dx
$$

(2.2.7)

Although the evolution of $f_\alpha$ comes from (1.2.3), the expression for $P$ is unknown in general because $P$ satisfies the differential equation (2.2.1) for an impulsive non-homogeneous term $\varrho_\alpha = \delta (q - q') \delta (t - t')$[17, 23]. However, the analytical form of $P$ could be found by,

\(^1\)A stochastic process $x(t)$ is called Markov if for every $n$ and $t_1 < t_2 < \ldots < t_n$, we have $\Pi (x, t_n; x, t_{n-1}) = \Pi (x, t_n; x, t_{n-1})$.
\[ P(q, t; q', t') = \delta (q - q') + \sum_{n=1}^{\infty} \int_t^{t'} \int_{t_n}^{t_{n-1}} dt_n \delta (q, t_n) \delta (q - q') \] (2.2.8)

which is the Dyson Series [6], a formal and non-operative relation that can be useful for a short transition time \( \tau = t - t' \), giving for a time independent \( L_{FP} \)

\[ P(q, t + \tau; q', t) = \exp (\tau L_{FP} (q)) \delta (q - q') \] (2.2.9)

For a time dependent \( L_{FP} \) up to first order in \( \tau \) the previous expression still holds, providing a first order approximation of the propagator as

\[ P(q, t + \tau; q', t) \simeq \exp (\tau L_{FP} (t, q)) \delta (q - q') \] (2.2.10)

that can be transform into a more compact and operative expression given in the following section.

The propagator for short-time \( P_{\tau} \), that we will study in the next section, has to be consistent with the original problem (2.2.1) and we will use the equation (1.2.3) to solve the problem. The problem will require (for practically all the cases) the numerical integration of (1.2.3).

In the difference based method, the complex dependence of the transports coefficients in the Fokker-Planck equation leads to a linearization to solve the problem, that can destroy the non-linear Physics of the problem. This method was develop in some previous works [4, 5, 22, 23], but here we will give it a new point of view with a new treatment of the boundary conditions and explaining all the advantages from this method over other numerical methods.

### 2.3 The short-time propagator \( P_{\tau} \)

As we have mentioned, the specific exact propagator for a given problem is as difficult to be found as to solve the original equation. For this reason, an approximate expression for this propagator in the short-time regime of evolution \( \tau \) has to be used in order to apply the integral advancing scheme

\[ f_\alpha (q, t + \tau) = \int_D f_\alpha (q', t) \cdot P(q, t + \tau; q', t) \, dq' \] (2.3.1)

where \( P(q, t + \tau; q', t) \) is the transition probability for \( f_\alpha \) from \( t \) to \( t + \tau \) with \( \tau > 0 \) and for \( \alpha \) to \( q \). For the sake of simplicity, we have considered the homogeneous problem with no \( \rho_\alpha \) term. The way to include this term will be given in the following sections. Up to first order in \( \tau \), a general expression for the short-time propagator can be derived as follows.

The property equation (2.2.5), valid for any \( P \), allows us to write:

\[ P(q, t + \tau; q', t) = (1 + \tau L_{FP} + O(\tau^2)) \delta (q - q') \] (2.3.2)

as a first order Taylor expansion in \( \tau \).

Where \( L_{FP} \) is the Fokker-Planck operator and \( O(\tau^2) \) is a second order operator assume as negligible. Thus, this expression can be rewritten as

\[ P(q, t + \tau; q', t) \simeq \exp (\tau L_{FP} (q, q', t)) \delta (q - q') \] (2.3.3)
as one of its simplest form. At this point, it is important to specify that the primed variables are usually call \textit{source variables}, while the non-primed variables are call \textit{field variables}, as it is usual in the electromagnetic theory. Observe that $L_{FP}$ is a new auxiliary operator evaluated at time $t$ in source and field variables. Source variables are dealt as constant parameters for the calculation of the short-time propagator. This formal relation can be expressed in a compact form as a function acting as the integral kernel in (2.2.4).

It is easy to prove that if

$$L_{FP}^* (q', t) \equiv L_{FP} (q, q', t) = \frac{\partial}{\partial q_i} \left[ D_i (t, q') + \frac{\partial}{\partial q_j} (D_{ij} (t, q')) \right]$$

(2.3.4)

the final form of the short-time propagator is:

$$P_{\tau} (q; q', t) = \frac{1}{\sqrt{D' \cdot 4\pi \tau}} \exp \left[ -\frac{(q_i - q_j - A_i \tau) (q_j - q_j' - A'_j \tau)}{4\pi D'_{ij}} \right]$$

(2.3.5)

$$D'_{ij} = D_{ij} (q', t); \quad A'_i = A_i (q', t); \quad i, j = 1, \ldots, N; \quad \tau > 0$$

(2.3.6)

which is a multivariate Gaussian, corresponding to the exact solution of the Fokker-Planck equation with constant coefficients in the whole $N$-dimensional space. For a detailed derivation of this expression see the works [4, 17, 24].

We can mention here that the previous propagator can be easily derived by using the well known Fourier transformation techniques, in particular it is used the Dirac delta Fourier transform as $\delta (q) = (2\pi)^{-N} \int \exp (-ik \cdot q) dk$. However, it is important to recall that the previous form of the short-time propagator is not unique, since a large variety of propagators can be found for a given advection-diusion operator, being all of them equivalent for $\tau \rightarrow 0$[17, 22]. In particular for each problem one can construct a suitable short-time Green function $P_{\tau}$ for a given problem solving an auxiliary Fokker-Planck equation.

2.3.1 Properties of $P_{\tau}$

In spite of the propagator $P_{\tau}$ is non-unique, any propagator has to satisfy a set of essential properties in order to be consistent with the original problem. This probability of transition has to satisfy the following important properties, that are also satisfy by the unknown exact propagator:

1. The norm in the domain $D \subseteq \mathbb{R}^N$ has to be equal 1.

$$\int_D P_{\tau} (q; q', t) \, dq = 1$$

(2.3.7)

this property is satisfied in the limit $\tau \rightarrow 0$, however it is important that it holds for any finite $\tau$ for numerical proposals.
2. In the limit $\tau \to 0$, the first and second order moments of the Fokker-Planck equation have to lead to the exact expression of the advection and diffusion coefficients, being zero the higher order moments, that is

$$D^{(1)} = A_i (q', t) = \lim_{\tau \to 0} \int_{D} \frac{q_i - q'_i}{\tau} P_\tau (q; q', t) \, dq$$

$$D^{(2)}_{ij} = D_{ij} (q', t) = \frac{1}{2} \lim_{\tau \to 0} \int_{D} \frac{(q_i - q'_i)(q_j - q'_j)}{\tau} P_\tau \, dq$$

3. Obviously, it has to satisfy the initial condition:

$$\lim_{\tau \to 0} P_\tau (q; q', t) = \delta (q - q')$$

Taking into account these properties and the procedures of calculation explained above, it is possible to construct a suitable propagator for different domains and variables.

### 2.3.2 Calculation of $P_\tau$

For now on, to simplify the notation we shall limit the development and presentation of the method to the one-dimensional case. To start with our discussion of how to obtain an approximate Green function $P_\tau$, let us consider the general problem. For this case, the equation to be solved for the exact propagator $P$ is:

$$\frac{\partial P}{\partial t} = L_{FP} \cdot P (x, t; x', t') + \delta (x - x') \delta (t - t')$$

where an impulsive source term $\rho = \delta (x - x') \delta (t - t')$ has been included. Alternatively, the corresponding homogeneous equation can be solved with the initial condition $P_\tau (x, t'; x', t') = \delta (x - x')$.

In addition, the boundary conditions have to be imposed under a quite a general boundary condition form as

$$a_k (t) P (x_k, t; x', t') + b_k (t) \frac{\partial P}{\partial x} \bigg|_{x=x_k} = g_k (t)$$

where the index $k$ indicates any of the boundary points of the domain $D = [x_1, x_2]$. The functions $a_k$, $b_k$ and $g_k$ are given functions. Observe that this form summarizes both Neumann and/or Dirichlet boundary conditions. This is, in most cases, as hard as solve the original problem analytically. That is why we will calculate an approximation. For an analytical and unsolvable problem an approximate short-time propagator has to be found. As we have said, an auxiliary Fokker-Planck equation can be constructed with an appropriate $L_{FP}$ operator for the short-time propagator $P_\tau$

$$\frac{\partial P_\tau}{\partial t} = L^*_{FP} \cdot P_\tau (x, t; x', t')$$
satisfying the initial condition studied

\[ P_\tau (x, t'; x', t') = \delta (x - x') \]  

(2.3.14)

and the boundary conditions suitable to account with the source variables

\[ a_k (t) P (x, t; x'_k, t'') + b_k (t) \left. \frac{\partial P}{\partial x'} \right|_{x' = x'_k} = g_k (t) \]  

(2.3.15)

where \( k \) indicates any of the boundary points of the domain.

The main feature of this procedure is related to the fact that one can take advantage of the analytical solutions, that can be found in the literature, for more simples Fokker-Planck equations. In this sense, an exhaustive collection of Green’s function are provided, for instance, in the handbook of Polyakin[15], among others.

The calculation and/or the appropriate election of \( P_\tau \) is the key to apply the integral advancing scheme. As we shall see, it is not possible to use any form of propagator to solve a given problem, because it depends on the domain of the variable, apart of the dependence on the boundary conditions. For the open space \( \mathbb{R} \) a common and suitable propagator is the Gaussian (2.3.5) specialized for the one-dimensional case. However, this Green’s function does not work properly in half space or finite domains, as we have tested in several cases[22]. Therefore, it could be convenient to have generic functions suitable to be used as short-time propagators in the domains \([0, +\infty[ \) and \([0, L]\). These intervals are considered here as references to be used in any problem. Furthermore with these generic propagators, the non-natural boundary conditions can be imposed in a more direct way, as we will see in the next chapter.

In the following subsections we present some forms of the short-time propagator that can be employed as generic propagators in the aforementioned domains.

### 2.3.2.1 The one dimensional general propagator in \((-\infty, +\infty)\)

This propagator in the whole 1-D real space can be obtained by simple particularizing (2.3.5) for the one-dimensional case, although, it can be derived from the solution of the constant coefficients Fokker-Planck equation, as auxiliary problem, providing

\[ P_\tau (x; x') = \frac{1}{\sqrt{4\pi D' \tau}} \exp \left( -\frac{(x - x' - A'^\tau)^2}{4D' \tau} \right) \]  

(2.3.16)

This expression can be used to build up the rest of the standard propagators in other domains. The main analytical properties of this propagator are:

\[ \int_{-\infty}^{+\infty} P_\tau (x, x') \, dx = 1 \]  

(2.3.17)

\[ \lim_{x \to \pm \infty} P_\tau = 0 \quad \lim_{x \to \pm \infty} \frac{\partial P_\tau}{\partial x} = 0 \]  

(2.3.18)
Generic propagator test in \((-\infty, +\infty)\). In this case, the total evolution time is 1, a time step of \(\tau = 10^{-2}\), a total length of \(L = 20\), divided in 501 points. \(A = D = 1\). For this simple test problem, numerical and analytical solution have been compared[22] and no distinguishable evolving solutions were found in this grid. This Green’s function has been also tested in several non-linear Fokker-Planck equations as it can be seen in [22].

What is important in this simple example is that the initial condition is a histogram-like function. The solution is smooth and positive for any time step, since non-numerical derivative has been used in this method, two properties that cannot be usually met with finite difference schemes.

Another important feature is that the solution tails approach zero exponentially, in both numerical and analytical cases, this means that our method can feasibility reproduce the behavior of the distribution at infinite (large values of the computational grid in the numerical problem).

2.3.2.2 Generic propagator in the half-open space

For half-space in one dimension, the domain \([0, +\infty)\), a general expression for the short-time propagator can be found by following the previous procedure of finding the solution of a Fokker-Planck equation with constant coefficients. Although, a useful technique for solve these equation is the so call method of images that can be found in many textbooks. The final result, after imposing the reflecting condition at the origin,

\[
J(P(x = 0)) = A(x = 0) P(x = 0) - \frac{\partial}{\partial x} DP \bigg|_{x=0}
\]

(2.3.19)

gives

\[
\begin{align*}
P_\tau(x; x') &= \frac{1}{\sqrt{4\pi D'\tau}} \left( \exp\left(-\frac{(x - x' - A'\tau)^2}{4D'\tau}\right) + \exp\left(-\frac{A' x'}{D'} - \frac{(x - x' - A'\tau)^2}{4D'\tau}\right) \right) \\
&\quad - \frac{A'}{2D'} \exp\left(\frac{A' x'}{D'}\right) \left( 1 - \text{erf}\left(\frac{x + x' + A'\tau}{\sqrt{4D'\tau}}\right) \right).
\end{align*}
\]

(2.3.20)

Once again, prime indicates that the coefficients have to be computed in source variables for non-constant coefficients \(A\) and \(D\). This short-time Green’s function satisfies the reflecting
boundary condition and, also, it decays to zero exponentially as $x \to +\infty$ as (2.3.16). This can be considered as a basis propagator to solve our problem to describe the plasma-wall interaction because $[0, +\infty)$ seems to be the natural interval to study this problem.

As we have said, many other $P_\tau$ can be designed for a particular problem to be used as propagators, but we will explain in the following sections (3.9) that this form (2.3.20) is the best option to simply apply our method with any boundary conditions at the origin in the specific domain.

**Simple test of the $[0, +\infty]$ general propagator**  The figure below shows the time evolution of an histogram-like initial condition with the same parameters as the previous example 2.3.2.1.

![General Propagator between $[0, +\infty)$](image)

**Figure 2.3.2**: Generic Propagator in the domain $[0, +\infty)$.

It can be seen how the propagator acts on an abrupt initial condition and which evolves smoothly from the first time step tending to zero when $x \to \infty$, exponentially.

### 2.3.2.3 The one dimensional $[0, L]$ general propagator

To end with this section providing quite standard propagators to be used in the common one-dimensional domain, we give here an expression of the Green's function valid for the finite interval $[0, L]$, again, null probability current at both boundaries and following the arguments given in the previous cases, such a propagator can be constructed from the axillary problem 2.3.13 with constant coefficients. The solution of this problem can be found in several text books[15] and it reads

$$P_\tau = \exp \left( \frac{A'(x' - x)}{2D'} - \frac{A^2 x}{4D'} \right) \sum_{n=1}^{\infty} \frac{1}{B_n} y_n(x) y_n(x') \exp \left( -D' \mu_n^2 \tau \right)$$ (2.3.21)

as an expansion of the orthogonal eigenfunctions $y_n$ given by

$$y_n(x) = \cos(\mu_n x) + \frac{-2 D' \mu_n}{2 D' \mu_n^2} + A' \sin(\mu_n x)$$ (2.3.22)

The coefficients of the Fourier expansion are given by
\[ B_n = \frac{2D' b_2}{a_2} - A' \frac{4D' \mu_n^2}{2} \left( \frac{-2D' b_1}{a_1} + A' \right)^2 + \frac{-2D' b_1}{a_1} + A' \right)^2 + \frac{l}{2} + \frac{l}{8D' \mu_n^2} \], \quad (2.3.23) \]

being the eigenvalues \( \mu_n \) the positive roots of the transcendental equation:

\[ \frac{\tan (\mu l)}{\mu} = \frac{4D' \left( \frac{-b_1}{a_1} + \frac{b_2}{a_2} \right)}{4D' \mu^2 - \left( -2D' \frac{b_1}{a_1} + A' \right) \left( 2D' \frac{b_2}{a_2} - A' \right)}. \quad (2.3.24) \]

This form of the propagator is a more cumbersome expression than the ones used in unbounded 1-D domains, but in general, the series converges quickly because of the exponential term depending of finite \( \tau \). Furthermore, some techniques to accelerate the convergence of the series could also be used if \( \tau \) is small.

The above relation can be simplified for a zero probability current at the domain edges (see (2.3.15)). In other words, this propagator is very general and this expression can be simplified in most of the problems. Finally, it is important to note that any problem in the general interval \([x_1, x_2]\) can be translated to the problem lying in the interval \([0, 1]\) by a simple linear transformation of variable \(x\) (by shifting and homothetic transformations).

**Simple test of the \([0, L]\) general propagator**  We illustrate how the propagator works with an example

![Figure 2.3.3: Generic Propagator in the domain \([0, L]\).](image)

This case was executed with a total time of 10 units, a time step \( \tau = 1 \), a length of \( L = 10 \), 501 points for the space discretization, and \( A = D = 1 \). We also have used only \( N = 10 \) iterations. In the figure, we can see how the propagator starts from an initial condition \( f(x) = 1 \) and then evolves to adjust the domain and the general boundary conditions (current 0 at the boundaries). This propagator is difficult to be evaluated since it requires hard calculation and analysis, but for time independent \( A \) and \( D \) it has to be computed at the first time step only.
2.3.3 Some guidelines to construct a new propagator

As it has been explained in section 2.3.2, the form of the propagator is non-unique. However, in order to be able to extend the numerical integral method to solve any boundary problem, a task not done up to now, we have constructed our propagators to fulfill the boundary condition \( J(P) = 0 \). Likewise, another boundary conditions can be imposed, but in a practical problem it is almost impossible to find a \( P_\tau \) that fulfills these conditions. However this inconvenient can be solved if we follow some rules concerning the Green’s function should satisfied for short-time to build up the numerical scheme. From our experience, we are in position to furnish here the main rules to be considered for the aim we have pointed out:

1. The analytical norm of the propagator has to be 1. So that, the numerical norm has to be close to unity. In section §2.4 we will remark the importance of the norm in the numeric propagator and in 3.9 we will solve the problems that can appear if a non-normalized propagator are used.

2. As said, a short-time propagator satisfying the prescribed boundary conditions cannot be usually found. To have such a Green’s function would be the ideal case (as in 3.9). But this is in practice impossible for almost all the boundaries conditions, and require a hard analytical study. A good choice is to build up the propagator with the boundary conditions seen in (2.3.19). This would simplify the numerical scheme. The Green’s function theory can be applied to solve the problem under any boundary conditions, as we shall see.

3. A third important guideline to be followed in other to have an appropriate \( P_\tau \) is that the expression chosen for this has to be defined for an axillary Fokker-Planck problem with the same domain of the original function problem.

In resume, the optimal propagator has to follow the standards of being normalized to unity in the same interval as the original problem and null probability current at the domain.

2.4 Normalization of \( P_\tau \), the importance of the numeric norm

As we explained by equation (2.3.7), it is important that the propagator has a norm equals to 1. However, this property does not hold in unbounded domains in the numerical case, not only for the accurate of the numerical computation, but also because of our numerical domain is finite and the integration has to be truncated in any finite the numerical domain. This unavoidable fact encourages us to redefine the form of the numerical short-time propagator, but taking as a basis the analytical one. Let’s say that we have a numerical problem with a mesh defined on\([-L, L]\) when \( L \) is a finite value (but large enough value)

\[
\int_{-\infty}^{+\infty} P(x, t; x', t') \, dx = 1
\]

\[
\int_{-L}^{+L} P_\tau(x, x') \, dx = N_\tau(x')
\]

where \( N_\tau(x') \) is what we will call the Numerical Norm, but here \( \int_{-L}^{+L} \) has to be understood as a numerical integration scheme. In the ideal case \( N_\tau(x') = 1 \) for any \( x' \), so, we have to perform a renormalization as

\[
\frac{P_\tau(x, x')}{N_\tau(x')} = P^*_\tau(x, x')
\]
\begin{equation}
\int_{-L}^{+L} P^*_\tau (x,x') \, dx = 1
\end{equation}

As we have said above, the norm of the propagator we want to apply to our problem can also be not equal to 1. In this case, the analytical and numerical propagator norms are

\begin{equation}
\begin{split}
\int_{-\infty}^{+\infty} P (x,t;x',t') \, dx &= N(x') \\
\int_{-L}^{+L} P_\tau (x,x') \, dx &= N_\tau (x')
\end{split}
\end{equation}

and the renormalization to be performed is similar to the previous case:

\begin{equation}
\frac{P_\tau (x,x')}{N_\tau (x')} N (x') = P^*_\tau (x,x')
\end{equation}

\begin{equation}
\int_{-L}^{+L} P^*_\tau (x,x') \, dx = N (x')
\end{equation}

With these transformations, it is achieved that the numerical norm in the numerical domain matches the corresponding for the analytical one in the original domain.

We have checked that this renormalization ensures the correct behavior of the propagator for any finite time step. Therefore, without this renormalization, the solution would be perturbed, mainly in the boundaries, and we would not be able to use a propagator that follows the guidelines and properties we gave in 2.3.1 and 2.3.3.

This renormalization is a required procedure, even if it increases the computational efforts for our integral numerical scheme.

We observe in figure 2.4.1 that the values of the solution without the renormalization deviates from the renormalized ones for small \( \tau \) and we can only obtain the same results with and without renormalization when \( \tau \sim 1 \), this is to say, the renormalization process is less important as \( \tau \) increases. However, when we apply the renormalization the solutions are non-distinguishable, thus, in order to be able to use the propagator method for arbitrary finite time step, the renormalization of the propagator is needed.

Figure 2.4.1: Solutions for time evolution \( t = 10 \) with different \( \tau \) values for the same initial distribution with and without the renormalization or the propagator.
Moreover, in 2.4.2 we note that the norm $F = \int_0^L f(x) dx$ of the test function, which has to be constant in this problem, increases if the propagator is not normalized. On the contrary, with $P^\tau_\ast$ this norm remains constant (it is a conserved quantity) in every time step for any $\tau$. At this point, we advance that this renormalization process is very important when dealing with conservative problems.

![Figure 2.4.2: Norm of the solution $f$ with and without normalization for different time steps.](image)

From now on, the renormalized propagator $P^\tau_\ast$ will be called $P_\tau$ to simplify the notation in the following sections.
CHAPTER 3

THE PROPAGATOR METHOD TO SOLVE THE PLASMA-WALL INTERACTION

This chapter illustrates the application of the integral method introduced in Chapter 2 to a physical problem. Here some of the advantages and drawbacks of the integral method are shown. We also apply the procedure to introduce in the numerical advancing scheme the boundary conditions and the non-homogeneous terms. At the same time, the resolution of the particular problem proposed here reveals a way to implement the scheme in a simplified way.

3.1 Description of the physical problem

To simplify the development and to clarify the explanation of our method, we deal here with a one-dimensional plasma system near to a wall that can emit or collect electric charges. From the mathematical point of view, this wall is a source or a sink term localized at the boundary. We analyze the time evolution of the densities of several plasma species. The problem functions are defined on $[0, +\infty)$ and plasma neutrality is considered far from the wall.

The fluid model (3.1.1) studies the densities of a uniform temperatures plasma in the diffusive approximation. The problem itself is non-linear because the coupling with the Poisson equation is considered.

In this approximation, the equations involved in the model of the 1-D plasma-wall interaction can be cast into

\[
\frac{\partial n_i (x, t)}{\partial t} = \frac{\partial}{\partial x} \left\{ A_i (x, t) - \frac{\partial}{\partial x} D_i (x, t) \right\} n_i (x, t)
\]

\[
\frac{\partial n_e (x, t)}{\partial t} = \frac{\partial}{\partial x} \left\{ A_e (x, t) - \frac{\partial}{\partial x} D_e (x, t) \right\} n_e (x, t)
\]

\[
\frac{\partial^2 \varphi (x, t)}{\partial x^2} = -\frac{1}{\epsilon_0} q (x, t)
\]  

(3.1.1)

The governing equations for the electron and ion densities ($n_e$ and $n_i$) are advection-diffusion equations where the drift and diffusion coefficients are related to the electric field $E$, through the
Figure 3.1.1: Description of physical model for the plasma wall interaction. This model simulates the behavior of a quasi-neutral plasma close to a wall.

species mobilities $\mu_e$ and $\mu_i$, kinetic temperatures $T_e$ and $T_i$ measured in electron-volts (eV) are assumed uniform and $e$ as the elementary charge\[10, 14\]

\[
\begin{align*}
A_i(x,t) &= \mu_i E(x,t) ; \\
D_i(x,t) &= \mu_i \frac{T_i}{e} \text{ (eV)} \\
A_e(x,t) &= -\mu_e E(x,t) ; \\
D_e(x,t) &= \mu_e \frac{T_e}{e} \text{ (eV)}
\end{align*}
\] (3.1.2)

To complete the model, the Poisson equation obeyed by the plasma potential $\varphi$ accounts for the spatial charge density $\varrho(x,t) = e(n_i - n_e)$.

This is a simple model and it is valid in a specific range of pressure and temperature, but it will be useful to illustrate how to carry out the integral semi-analytical method and present some examples of application related to a laboratory plasma. At the same time, a realistic physical problem is solved and related to some specific plasma phenomena, as the emission of an electrode or an emissive probe. As explained in Chapter 2, this method can be also extended to solve other drift-diffusion equations as, for instance the non-linear heat transfer equation 4.2.1 and the viscous Burgers’ equation in 4.5.1 as well as transports equations.

With the notation introduced in Chapter 2, a summary of possible boundary conditions is given in the adjoin table, where the quantities with subscript can be constant or time-depending magnitudes.
\[
\begin{array}{|c|c|c|}
\hline
x = 0 & x \to +\infty \\
\hline
n_c & a_c n_c(0, t) + b_c n_c \frac{\partial n_c}{\partial x}|_{x=0} = g_c & a_{c\infty} n_c|_{x\to\infty} + b_{c\infty} \frac{\partial n_c}{\partial x}|_{x\to\infty} = g_{c\infty} \\
\hline
n_i & a_i n_i(0, t) + b_i n_i \frac{\partial n_i}{\partial x}|_{x=0} = g_i & a_{i\infty} n_i|_{x\to\infty} + b_{i\infty} \frac{\partial n_i}{\partial x}|_{x\to\infty} = g_{i\infty} \\
\hline
\phi & \phi_w & \frac{\partial \phi}{\partial x} |_{x \to \infty} = 0 \\
\hline
\end{array}
\]

Table 3.1: General boundary conditions

3.1.1 The dimensionless problem

To ease the establishment of a general problem solution procedure, dimensionless variables are used from now to the end of this work. The new dimensionless variables we have chosen are:

\[
\hat{n}_\alpha = \frac{n_\alpha}{n_0}; \quad \hat{x} = \frac{x}{l_c}; \quad \hat{t} = \frac{t}{t_c}; \quad \hat{\phi} = \frac{\phi}{\phi_0}; \quad \mu_\alpha = \frac{\mu}{\mu_0}; \quad \hat{E} = \frac{E}{E_0}
\]  

(3.1.3)

where the reference values \(n_0, l_c, t_c, \phi_0, \mu_0\) and \(E_0\) are not all independent, obviously, and their values can be established by means of the following relations. Replacing the above set of variables in (3.1.1).

\[
\begin{align*}
n_0 \frac{\partial \hat{n}_\alpha}{\partial \hat{t}} &= -\frac{1}{l_c} \frac{\partial}{\partial \hat{x}} \left( \mu_0 E_0 \mu \hat{E} - \frac{1}{l_c} \frac{\partial}{\partial \hat{x}} \mu_0 T_0 \mu \hat{T}_\alpha \right) n_0 \hat{n}_\alpha \\
\frac{\partial \hat{n}_\alpha}{\partial \hat{t}} &= -\frac{\partial}{\partial \hat{x}} \left( \mu_0 E_0 t_c \frac{\partial}{l_c} \hat{E} - \frac{t_c \mu_0 T_0}{l_c^2} \frac{\partial}{\partial \hat{x}} \mu \hat{T}_\alpha \right) \hat{n}_\alpha \\
\frac{\phi_0}{l_c^2} \frac{\partial^2 \hat{\phi}}{\partial \hat{x}^2} &= -\frac{e}{\epsilon_0} n_0 (\hat{n}_i - \hat{n}_e) \\
\frac{\partial^2 \hat{\phi}}{\partial \hat{x}^2} &= -\frac{e l_c^2 n_0}{\epsilon_0 \phi_0} (\hat{n}_i - \hat{n}_e)
\end{align*}
\]

and setting

\[
\begin{align*}
\frac{e l_c^2 n_0}{\epsilon_0 \phi_0} &= 1 \\
\frac{t_c \mu_0 T_0}{l_c^2} &= 1 \\
\frac{\mu_0 E_0 t_c}{l_c} &= 1 \\
\frac{\phi_0}{l_c} &= E_0
\end{align*}
\]  

(3.1.5)

we can determine the parameters for the dimensionless problem as

\[
t_c = \frac{\epsilon_0}{\mu_0 e n_0}; \quad l_c = \sqrt{\frac{\epsilon_0 T_0}{e n_0}} = \lambda_D; \quad \phi_0 = \frac{e l_c^2 n_0}{\epsilon_0}; \quad E_0 = \frac{e l_c n_0}{\epsilon_0}.
\]  

(3.1.6)
Now, taking \( \mu_0 = \mu_e, T_0 = T_e, n_0 = n_e \) the problem (3.1.1) become:

\[
\frac{\partial \hat{n}_i (\hat{x}, \hat{t})}{\partial t} = - \frac{\partial}{\partial \hat{x}} \left\{ \hat{\mu}_i \hat{E} (\hat{x}, \hat{t}) - \hat{\mu}_i \hat{T}_i (\hat{x}, \hat{t}) \frac{\partial}{\partial \hat{x}} \right\} \hat{n}_i (\hat{x}, \hat{t}) \]
\[
\frac{\partial \hat{n}_e (\hat{x}, \hat{t})}{\partial t} = - \frac{\partial}{\partial \hat{x}} \left\{ -\hat{E} (\hat{x}, \hat{t}) - \frac{\partial}{\partial \hat{x}} \right\} \hat{n}_e (\hat{x}, \hat{t}) \]
\[
\frac{\partial^2 \hat{\psi} (\hat{x}, \hat{t})}{\partial \hat{x}^2} = -(\hat{n}_i - \hat{n}_e) . \tag{3.1.7}
\]

Observe that with this election the characteristic time of the problem is the electronic time scale. This is important to define the finite time step of the numerical advancing scheme. This means that \( \tau \sim 1 \) is a very small time step for the point of view of the ion time scale, since the ion mobility is very small if compared with the electron one. The same happens with the ions temperature, because usually, the ions temperature is very small compared to comparative of the electron temperature \( \frac{T_i}{T_e} \ll 1 \).

Right from now on, we will drop the hat (\( \hat{\cdot} \)) to simplify the notation.

### 3.2 Introduction of the numerical problem

Due to the fact that our method is based on a numerical integration scheme (instead of establishing differences) the infinite domain of the analytical problem has to be transposed into a finite interval for numerical purposes. Therefore, the \([0, +\infty)\) interval is represented by a finite length \( L \) where the extreme \( x = L \) is chosen in such a way that the problem smoothly reach the boundary conditions in \( L \gg 1 \). The mesh in the numerical scheme also contains enough number of points to accurately simulate the effect of the infinite. Usually, an uniform grid is employed, but our method is not restricted to this kind of uniform grid.

After this introductory remarks, it is important to mention that several different methods of numerical integration can be used, however, to present the method, the simple Rectangle Rule of integration in a refined mesh is applied. Therefore, the integral of a function \( f (x) \) reads

\[
\int_a^b f (x) \, dx = \sum_{i=0}^N f (x_i) \, h \tag{3.2.1}
\]

where \( x_i \) is the value of the variable at the \( i \)-th point, \( N \) is the maximum number of grid points and \( h \) is the distance between points, i.e. the spatial step. With this integral model the implementation of the numerical scheme is relatively simple and can be expressed in a matrix multiplicative form as many other finite numerical difference schemes[22, 23].

For the calculation of the electric potential (and the electric field) we use a finite difference scheme to solve the Poisson equation. This scheme uses a direct matrix inversion procedure and a first order derivative approximation to calculate the electric field from the plasma potential. Although this is not the most accurate procedure to solve the Poisson equation, it is good enough to solve the main equations by the numerical integral method. With the boundary conditions of Table 3.1 on page 27 where \( \varphi_w \) is the potential at the wall and the electric field is set to zero at the infinity, the potential in the \( n + 1 \) step is given by

\[
\mathbf{A} \cdot \Phi^{n+1} = \theta^n \tag{3.2.2}
\]
where the matrix $A$,

$$
A = \frac{1}{h^2} \begin{pmatrix}
2 & -1 & 0 & 0 \\
-1 & 2 & -1 & 0 \\
& & \ddots & \ddots \\
0 & 0 & -1 & 1
\end{pmatrix}^{N \times N}
$$

(3.2.3)

comes from the common discretization scheme of the derivative up to second order in $h$, and also includes the boundary conditions mentioned above. The $n+1$-it potential is finally given by

$$
\Phi^{n+1} = A^{-1} \varrho^n
$$

(3.2.4)

with

$$
\Phi^{n+1} = [\Phi_1, \Phi_2, \ldots, \Phi_N]^T ; \varrho^n = [\varrho_1, \varrho_2, \ldots, \varrho_N]
$$

(3.2.5)

where $T$ means transposed. In addition, we have to apply the boundary condition at $x = 0$:

$$
\Phi_0 = \varphi_W
$$

(3.2.6)

The electric field is given by

$$
E_0^{n+1} = -\frac{\Phi_1^{n+1} - \Phi_0^{n+1}}{h}
$$

$$
E_i^{n+1} = -\frac{\Phi_{i+1}^{n+1} - \Phi_{i-1}^{n+1}}{2h}, \; i = 1, \ldots, N - 1
$$

$$
E_N^{n+1} = -\frac{\Phi_N^{n+1} - \Phi_{N-1}^{n+1}}{h}
$$

(3.2.7)

This approaches introduce a small error because the charge density $\varrho$ is taken from the step $n$ to calculate the potential in the step $n + 1$. It is an acceptable error since it does not affect the semi-analytical method we are applying in advancing $n_\alpha$.

### 3.3 The general advancing scheme

In (2.3.5) the general formulation to advance the problem in time without non-homogeneous term or boundary conditions has been established. In order to solve the actual real physical problem, the scheme (2.3.1) has to be accomplished. To this aim, the general theory of Green’s functions can be applied for this kind of differential equations, in the same manner that it is done, for instance, with the Green’s function for problems in Electromagnetism. One of the pioneer works on this topic can be found in the paper of Wehner and Wolfer [23]. The authors established here a quite general result for any Fokker-Planck operator, by performing a derivation based on the use of $L_{FP}$ operator and its adjoin with the assumption of a known Green’s function $P$. The theoretical analytical expression for the evolution of a function $f(q,t)$ is given by

$$
f(q,t) = \int_{V} dq' P(q,t; q', t') f(q', t') + \int_{t'}^t d\tau \int_{V} dq\varrho(q', \tau) P(q,t; q', \tau)
$$

$$
- \int_{t'}^t d\tau \oint dS_0 \left[ J(q', \tau) P(q,t; q', \tau) + D(q', \tau) f(q', \tau) \frac{\partial P}{\partial x}(q,t; q', \tau) \right]
$$

(3.3.1)
where \( \rho (q', \tau) \) represents a possible non-homogeneous term in the Fokker-Planck equation and \( \tau \) is an intermediate time between \( t' \) and \( t \) to allow the time integration. The surface integrals, which is the boundary integral, accounts for the probability current \( J \), associated to \( f \) across the boundary surface. Observe that this scheme reduces to (2.3.1) without boundary prescription and \( \rho = 0 \), but the same propagator \( P \) is used as in the homogeneous problem with natural boundary conditions.

Now, we have to convert the analytical continuous formal solution (3.3.1) to a practical numerical scheme in agreement with the establishments presented in Chapter 2.

To do this, the first step is to transpose the formal scheme to a short-time evolution time \( \tau \). This can be done by simply taking \( t \rightarrow t + \tau \) and \( t' \rightarrow t \). For the one dimensional case, the surface integrals collapses to its argument values at the boundary points \( x_1 \) and \( x_2 \),

\[
S = \oint dS_0 \left[ J(q', \tau') P_\tau(q; q') + D(q', \tau') f(q', \tau') \frac{\partial P_\tau}{\partial x'} (x; q') \right] \\
= \left[ J_{x_2} (x_2, \tau') P_\tau (x; x_2) + D (x_2, \tau') f (x_2, \tau') \frac{\partial P_\tau}{\partial x'} (x_2; x_2) \right. \\
- \left. J_{x_1} (x_1, \tau') P_\tau (x; x_1) + D (x_1, \tau') f (x_1, \tau') \frac{\partial P_\tau}{\partial x'} (x_1; x_1) \right] \quad (3.3.2)
\]

With these properties, (3.3.1) becomes

\[
f(x, t + \tau) = \int_{x'}^{+\infty} dx' P_\tau(x; x') f(x', t) \quad (3.3.3) \\
+ \int_0^\tau dr' \int_0^{+\infty} dx' \rho(x', \tau') P_\tau(x; x') - \int_0^\tau Sdr'
\]

This expression provides us a more general integral advancing scheme than the one given by (2.3.1). All the integrals over the source variables \( x' \) appearing in this scheme have been performed using the rectangle rule while the integrals over intermediate times \( \tau' \) are dealt as explained in the following sections.

### 3.4 Mesh-free and large values for the spatial and time discretization

As we will see in Chapter 4, the Finite Difference methods have a great dependence on the spatial and time discretizations of the problem. However, in our semi-analytical method we are free to impose a spatial discretization, no matter the value of \( \tau \) is. For this reason, we call this method a mesh-free method[2, 12]. This important feature means that we are highly free to choose the meshing. This freedom mainly comes from the reason that this method establishes an explicit time advancing scheme without any specification on how to perform the spatial integral. From a physical point of view, this is to say that we are only interested in the transition from the information given at point \( x' \) in time \( t \) to the information points \( x \) at \( t + \tau \), again, no related to the mesh. This important property allows the method to be applied even in a non-uniform grid.

This independence on the size of \( \tau \) is a capital property in order to deal with different possible time scales in coupled equations as the actual problem of electron and ion plasma. In other words we can analyze with the same time step both species without affecting the stability of the integral.
scheme. One can use time steps corresponding to the slower species and the faster ones will evolve in a feasible mode and vice-verse. This topic will be clarified in the following sections.

We present two examples to prove this kind of independence of the spatial and the time steps.

3.4.1 Mesh-Free in the time discretization

To demonstrate the independence of $\tau$ an example with a constant spatial discretization (501 points) and different time step $\tau$ is computed. Here we have analyzed a total time $t = 1$ with different number of iterations (10, 100 and 1000) to compare the different solutions evolving in time. The parameters for this problem are $A = 0.5$ and $D = 0.5$. An initial abrupt condition (histogram-like) is used.

As expected, the numerical solutions are almost identical (Figure 3.4.1 on page 32) for the different time steps meanwhile the computational cost is reduced as the number of iterations decreases. However, the computational time is not exactly linear respect to the number of iterations. Close to the wall the solutions for any $\tau$ may be slightly different.

3.4.2 Mesh-Free in the spatial discretization

The spatial discretization is less flexible because we are using a simple scheme integration in the $x$ coordinate. In other words we are not free to choose any number of points $N$ in the grid to obtain approximated results. However, this limitation is not restricted, fortunately, by the required finite time step, its only depends on the rectangle based integration scheme. Also, after a minimum $N$ is established, the increasing of $N$ does not substantially modify the solution. This effect could be improved with a more accurate integration scheme beyond the simple rectangle scheme.

In the example in 3.4.2, a non-variable $\tau = 10^{-2}$ and $t = 1$ are used but we changed the number of points in our grid. We have chosen for $N$ the values 101, 201, 501, 1001, 2001 and 5001 to compare the solutions. The parameters for this problem are again $A = 0.5$ and $D = 0.5$ and the initial condition is a histogram-like function.

It can be seen that for $N \leq 501$ the solutions differ from each other and for $N \geq 1001$ the solutions are indistinguishable.

3.5 Boundary condition, the problem of the infinite

As said before (Section 3.1) we are interested in dealing with the problem of plasma-wall interaction by assuming that at large distance from the wall, the plasma remains unperturbed because our analysis should be applied to the research of an emissive probe. From the numerical point of view the boundary condition when $x \to \infty$ has to take into account the existence of a quasi-neutral plasma, what means $n_i = n_e = n_\infty$ (where $n_\infty = 1$ in the dimensionless problem).

To hold this condition at the numerical infinite, we have to reformulate the integral advancing scheme having in mind that our propagator asymptotically vanishes for large $x$. To amend this problem, an alternative is to calculate a new propagator to ensure that the desired condition in the infinity is satisfied. However, determinate this propagator could be very difficult and this task is out of the scope of this work, where we try to establish the standard method taking by from the literature appropriate usual expressions for the propagator.
Figure 3.4.1: Example of Mesh-Free in the time domain. To solve a problem with the same, different time steps are used and the results are indistinguishable.
Figure 3.4.2: Mesh Free in the spatial discretization.
A first approach to solve this problem at infinite is to impose an additional boundary condition in the maximum point of our grid. This treatment means that the original problem is replaced by another one in the interval \([0, L]\) instead of \([0, +\infty)\), but still using the form of the short-time Green’s function for half-space. This method fails because, from the analytically point of view, a boundary condition for \(x \rightarrow \infty\) cannot be imposed due to \(P_\tau |_{x' \rightarrow \infty}\) and \(\frac{\partial P_\tau}{\partial x'} |_{x' \rightarrow \infty}\) go to zero. Furthermore this approach would transport a physical problem in half space to another domain dealing with a plasma between walls. When we apply the boundary condition method seen above to our numerical integration at infinite, we introduce an spurious solution that will not behave as a quasi-neutral plasma.

Our definite approach to simulate quasi-neutral plasma far from the wall consists in using a simple change of variables in order to ensure a new function that naturally vanishes at infinite. Because of with the general propagators we are able to obtain \(n_\alpha = 0\) where \(x \rightarrow \infty\), the change of variable we propose to describe the plasma species is the usual shifting

\[ f_\alpha = n_\alpha - n_\infty. \]  

(3.5.1)

We have to apply this change of variable for all the \(\alpha = e, i\) species in the plasma. With these shifting of the plasma species densities, our problem is now described by

\[ \frac{\partial f_\alpha}{\partial t} = -\frac{\partial}{\partial x} \left\{ A_\alpha f_\alpha - \frac{\partial}{\partial x} D_\alpha f_\alpha \right\} - n_\infty \frac{\partial}{\partial x} \left\{ A_\alpha - \frac{\partial}{\partial x} D_\infty \right\} \]  

(3.5.2)

Observe that this transformation gives rise a non-homogeneous term \(\rho (x, t) = -n_\infty \frac{\partial}{\partial x} \{ A_\alpha - \frac{\partial}{\partial x} D_\infty \}\) for each \(\alpha\). These terms poses no problem for the integral numerical scheme. Let us assume that the parameter \(D_\alpha\) is uniform (that means constant temperature and mobility for all \(x\)) and also with \(A_e = -\mu_e E; A_i = \mu_i E\) and \(\frac{\partial E}{\partial x} = \varrho (x, t) = (n_i - n_e) = (f_i - f_e)\) the definitive problem is:

\[ \frac{\partial f_i (x, t)}{\partial t} = -\frac{\partial}{\partial x} \left\{ A_i (x, t) - \frac{\partial}{\partial x} D_i (x, t) \right\} f_i (x, t) - \mu_i n_\infty (f_i - f_e) \]  

(3.5.3)

\[ \frac{\partial f_e (x, t)}{\partial t} = -\frac{\partial}{\partial x} \left\{ A_e (x, t) - \frac{\partial}{\partial x} D_e (x, t) \right\} f_e (x, t) + \mu_e n_\infty (f_i - f_e) \]

\[ \frac{\partial^2 \varphi (x, t)}{\partial x^2} = -\varrho (x, t) \]  

and now we can use \(\rho_i (x, t) = -\mu_i n_\alpha (f_i - f_e)\) and \(\rho_e (x, t) = \mu_e n_\alpha (f_i - f_e)\) as the non-homogeneous terms to apply the advancing solution (3.3.1). This procedure slightly increase the integration time and introduce a new numerical error due to the calculation of \(\rho_i\) and \(\rho_e\) requires the use of the previous time steps values.

This method to incorporate the effects of the infinite is treated exhaustively in Section 3.8.

### 3.6 Boundary condition at the wall

Now we have to deal with a very important problem in order to calculate the plasma properties near the wall, the boundary condition for electrons and ions. These conditions will be crucial for the physical problem because they drive the physics of the plasma-wall interaction. In particular, we can simulate the effects on a plasma of both emitting and collecting probes. This is also one of the main difficulties to apply our integral method to any real problem, what constitutes a
topic that is still under research. Let us analyze the term responsible of the boundary condition in \( x = 0 \). From (3.3.1), we can replace the surface integral for our one dimensional problem as \( x_1 = 0 \) and \( x_2 \to \infty \) for a generic \( f \) as,

\[
\int dS_0 \left[ J dq P_\tau + Df \frac{\partial P_\tau}{\partial q} \right] \to \left[ -J_0 \left. P_\tau \right|_{x' = 0} + Df \left. \frac{\partial P_\tau}{\partial x'} \right|_{x' = 0} \right]
\]

(3.6.1)
a term that has to be integrated over \( \tau' \) in the interval \([0, \tau]\). This time integration could be very complex if it is done numerically and we have found that the precision of the plasma density near the wall is highly related to this expression computation.

A first approach would be the to use a propagator for which \( P_\tau \big|_{x' = 0} \) and \( \left. \frac{\partial P_\tau}{\partial x'} \right|_{x' = 0} \) are both zero, but this Green’s function would not allow us to impose any boundary condition. Another approach would be use a propagator with one of \( P_\tau \big|_{x' = 0} \) or \( \left. \frac{\partial P_\tau}{\partial x'} \right|_{x' = 0} \) are zero. This would allow us to impose the boundary condition using the current \( J_0 \) or the function value \( f \) at \( x = 0 \). In particular, we can use a \( P_\tau \) satisfying \( \left. \frac{\partial P_\tau}{\partial x'} \right|_{x' = 0} \) if the probability current applied to the propagator is zero at the wall (reflecting boundary condition for the Green’s function). For a clear review of the adjoint boundary conditions for the Fokker-Planck operator see reference[23]. So, if we use a non-standard propagator, the full term (3.6.1) has to be calculated, but with a generic propagator this term results in

\[
S^{n+1}_0 = -J^{n+1}_0 \left. P_\tau \right|_{x' = 0}
\]

(3.6.2)
When (3.6.1) is integrated over the time, it works as a source or sink near the wall, that is, this gives the effects of the boundary conditions that also affects the whole grid. To impose the boundary condition we have to calculate the current \( J_0^{n+1} \) (the flux of particles, in fact, at the \( n + 1 \)-th step) or use its fixed value imposed as a boundary condition given by the problem. In case we have to calculate the probability current to imposes the boundary condition, we need to use some information from the previous step. For example, if one of our boundary conditions impose a value \( f_0 \) for \( n_\alpha (x = 0, t) \), the numerical current has to be build by means of

\[
J^{n+1}_0 = A^n f_0 - \frac{D^n (x_1) f^n (x_1) - D^n (x_0) f_0}{h}
\]

(3.6.3)
Again, to calculate the value for the iteration \( n + 1 \) we have to use the information from the previous time step, but it is a procedure which does not introduce a significant source of errors.

If we have a more complex boundary condition, we have to found a way to construct the current \( J_0 \) by a process similar to (3.6.3).

Observe that the current parameter is the key to establish the boundary condition at \( x = 0 \), but is also important the calculation of \( \int_0^\tau \left( -J_0 \left. P_\tau \right|_{x' = 0} \right) \, dr \). As we mentioned, this integration is hard to perform numerically and another procedure should be found. If we assume that the current we impose as a boundary condition \( J_0 \) is constant over the time or evolves slowly enough to be taken as a constant, we apply the operator \( J \) over the field variable \( x = 0 \) to the integration scheme

\[
J \left( f^{n+1} \right) = f^n_0 J (P_\tau) + J_0 J \left( \int_0^\tau P_\tau \, d\tau' \right) = J_0 J \left( \int_0^\tau P_\tau \, d\tau' \right)
\]

(3.6.4)
and due to \( J \left( f^{n+1} \right) \) has to be \( J_0 \) to fulfill the boundary condition, it results that the probability current for the integral over the auxiliary time \( \tau' \) of the propagator \( J \left( \int_0^\tau P_\tau \, d\tau' \right) \) has to equals 1 for \( x = 0 \).

As we explain in the following section, this issue requires a more involved way to calculate \( \int_0^\tau P_\tau \, d\tau' \) than numerical approximations to ensure the correct addition of the boundary conditions to this problem.
3.7 The importance of the propagator probability current for the boundary conditions

In Section 3.6 the importance of the boundary integral value to include the boundary conditions was stressed. Besides this property, it is also very important to establish the norm of the propagator, which, for numerical proposes it should be equals 1 (at least analytically) as explained in 2.3.1. Let us explain what this means.

If we consider the problem with non-homogeneous term and without boundary sink/sources, the total amount of \( n_\alpha \), that is, the norm of the problem function should remain constant at each step in the numerical step in absence of additional source and/or boundary terms. The advancing scheme would be

\[
n^{n+1}_\alpha = \int_0^L n_n^\tau \rho dx'
\]

so that, the norm \( N_\alpha \) of \( n_\alpha \) in time \( t + \tau \) would read

\[
\int_0^L n_n^{n+1} dx = N^{n+1}_\alpha = \int_0^L n_n^\tau \int_0^L \rho \tau dx dx'
\]

Then, if the norm of the propagator equals one, \( N_\alpha \) is constant.

\[
N^{n+1}_\alpha = N^n_\alpha
\]

meaning that the total amount of particles is conserved in time, as expected for this case. Therefore, if we use a propagator of norm 1, the creation/destruction of particles is only caused by the boundary conditions and by the non-homogeneous terms. If we include now a boundary condition at \( x = 0 \) (the wall) with a propagator having its associated probability current zero, the term \( S_n^\alpha \) appears in the advancing scheme.

\[
S_n^\alpha = \int_\tau d\tau' J_0(0, \tau') P_{\tau \alpha}(x; 0)
\]

Integration over \( x \), with \( J_0(0, \tau') = J_0(0) \) a constant, the contribution to the norm of \( n_\alpha \) is given by

\[
\int_0^L S_n^\alpha dx = J_0 \int_\tau d\tau' \int_0^L dx P_{\tau \alpha}(x; 0) = J_0 \tau
\]

That properly accounts with the physical effects of the wall in the physical problem, as expected. Then, we can conclude that the best choice for the form of \( P_{\tau} \) is the one that corresponds to a zero associated probability current, \( J(P_{\tau}) = 0 \). We think that this is a landmark in the setting of the new goals provided by the integral numerical method.

Returning to the numerical implementation scheme we have to mention that the probability current associated with \( P_{\tau} \) is not exactly zero when computed in the first point of the numerical grid. This is a natural problem brought out by the discretization process, as at the same way the norm of \( P_{\tau} \) was not exactly 0. However, as it is usual in numerical schemes, this effect can be improved by introducing a correction in the numerical value of the propagator.
At this point, it is important to recall that we are providing a method to construct a numerical propagator from the analytical one. This problem can be solved as explained as follows, with some practical examples.

Figure 3.7.1 on page 37 shows the evolution of a function $f$ for different values of $\tau$, it can be observed that at large distances from the origin all solutions are in practical the same. Meanwhile, close to the wall, the values of $f$ are different. This happens because the propagator probability current is not exactly zero, as we have mentioned above. In this example, the imposed current for $f$ should be zero in this particular case.

In Figure 3.7.2 on page 38, the current values at different time steps are shown, we observe that this values are far from zero, especially for very small time steps. Although this is a particular case, in general, it is desirable to obtain a good approximation for the solution in the boundaries. Moreover, it could be important to obtain the exact values prescribed by the analytical formulation of the problem.

Note that this property is important to preserve the norm conservation, or to predict the value of the norm, if it can change in time because it is related with the current in the boundaries. The solution we have found is simple.

We propose a translation of the propagator value at $x = 0$ for all $x'$. This translation can be seen as a second re-normalization to adjust $J(P_\tau)$, the value of the current. Because this probability current is

$$J (P_\tau) = A(x_0) P_\tau(x_0, x') - \frac{D(x_1) P_\tau(x_1, x') - D(x_0) P_\tau(x_0, x')}{h} \quad (3.7.6)$$

and at $x = 0$ has to be zero we redefine the values of $P_\tau$ in the first channel for all $x'$ as

$$P_\tau(x_0, x') = \frac{D(x_1) P_\tau(x_1, x')}{A(x_0) h + D(x_0)} \quad (3.7.7)$$
With this redefinition of the propagator, the current of \( f \) is close to zero, within the range of numerical errors, without affecting the smoothness of the advancing scheme (see figures 3.7.3 and 3.7.4)

The previous results ensure us that, in absence of the contribution of the boundary terms of the integral scheme, no spurious fluxes through the boundaries can appear. Now, our task is to ensure that the boundary effects enter in the numerical solution only if they are prescribed in the formulation of the problem and taken into account in the boundary condition of the integral advancing scheme.

First of all let us bring up at this point what happens if we use the first order approximation

\[
\int_{\tau'} P_\tau d\tau' \simeq \tau P_\tau
\]  

(3.7.8)

for the temporal integration. With this approximation the contribution of the boundary term will be proportional to \( \tau P_\tau \) at \( x = 0 \), leading to a zero contribution to the current associated to \( f \) instead of being any given value. This is because we have taken \( J (P_\tau) = 0 \), as explained in the previous paragraph, this leads us to \( J (\tau P_\tau) = \tau J (P_\tau) = 0 \).

To fix this problem, we have found a solution that consists in using the analytical expression of the propagator integral over \( \tau' \). For the standard propagators, this integral can be easily performed giving rise to expression depending of exponential and error function, in particular, in the domain \([0, \infty)\) we have, after some tedious calculations and using the integral tables of
Figure 3.7.3: Final solution after the translation for $P_\tau$.

Figure 3.7.4: Current at $x = 0$ after applying the translation for $P_\tau$. 
\[ \int_{\tau'} P_{\tau} d\tau' = IP_{\tau} = \sqrt{\frac{\tau}{\pi D(x_0)}} \exp \left( -\frac{(x_i - A(x_0)\tau)^2}{4D(x_0)\tau} \right) \]
\[ + \frac{1}{2D(x_0)A(x_0)} \exp \left( \frac{A(x_0)x_i}{D(x_0)} \right) \left( A(x_0)x_i + D(x_0) + A(x_0)^2 \tau \right) \left( \text{erf} \left( \frac{x_i + A(x_0)\tau}{\sqrt{4D(x_0)\tau}} \right) - 1 \right) \]
\[ - \frac{1}{2A(x_0)} \left( \text{erf} \left( \frac{x_i - A(x_0)\tau}{\sqrt{4D(x_0)\tau}} \right) - 1 \right) \]

(3.7.9)

To be coherent with the translation made with the original propagator, a similar process has
to be done for \( IP_{\tau} \) in the first channel \( x_0 \) in order to ensure that the contribution of the current
from this term is exactly 1. The formula similar to (3.7.7) for \( IP_{\tau} \) results in

\[ IP_{\tau}(x_0) = \frac{h + D(x_0)IP_{\tau}(x_1)}{A(x_0)h + D(x_0)} \]  

(3.7.10)

We can see how with this redefinition, the current is exactly one, i.e. \( J(IP_{\tau}) = 1 \), and
we have the precision required to impose any boundary condition at the wall. The figure 3.7.5
displays the values of the probability current of \( IP_{\tau} \), with and without the translation explained
above for the same time steps used in the previous figure.

### 3.8 Non-Homogeneous term

If we go back to the general integration scheme (3.3.3) we observe we have to dealt with the
calculation of a generic non-homogeneous term \( \rho \). As it happened with the integral over the prop-
gagator for the boundary conditions, explained in Section 3.7, we have to perform an integration
over the time as well.

Finally, by assuming that the non-homogeneous term is constant over time, or the charac-
teristic time of variation is larger than the time step, we can express the non-homogeneous from
the integration advancing scheme as

\[ \Psi = \int_0^L dx' \rho(x') \int_0^\tau d\tau' P_{\tau}(x;x') = \int_0^L dx' \rho(x') QP_{\tau}(x;x') \]

(3.8.1)
where \( QP_\tau \) is the integral over time of the short-time propagator \( P_\tau \) which is

\[
QP_\tau (x; x') = \left( 1 - \exp \left( \frac{x-x'}{2A'} \right) \right) \cdot \text{sign} (x - x') + \sqrt{\frac{\tau}{\pi D'}} \exp \left( - \frac{A'x' - (x + x' - A'\tau)^2}{4D\tau} \right) \\
+ \exp \left( \frac{A'x}{D'} \right) \left[ \frac{\exp \left( \frac{A'x}{D'} \right) \text{erf} \left( \frac{x + A'\tau - x'}{\sqrt{4D\tau}} \right) - \text{erf} \left( \frac{x - A'\tau}{\sqrt{4D\tau}} \right)}{2A'} \right] \\
- \frac{\text{erf} \left( \frac{x - A'\tau - x'}{\sqrt{4D\tau}} \right)}{2A'} \quad (3.8.2)
\]

for \( A' \neq 0 \) and

\[
QP_\tau (x; x') = \sqrt{\frac{\tau}{\pi D'}} \left[ \exp \left( \frac{-(x - x')^2}{4D'\tau} \right) - \exp \left( \frac{-(x - +)^2}{4D'\tau} \right) \right] \\
+ \frac{(x - x') \text{erf} \left( \frac{x - x'}{\sqrt{4D\tau}} \right) - (x + x') \left( 1 - \text{erf} \left( \frac{x + x'}{\sqrt{4D\tau}} \right) \right)}{2D'} \\
- \left| \frac{x - x'}{2D'} \right| \quad (3.8.3)
\]

if \( A' = 0 \). It is easy to deduce that this expression requires considerable computational effort. Therefore, if the parameters of the Fokker-Planck equation \( A \) and \( D \) depend on time the function \( QP_\tau \) has to be recalculated at any step. Some properties of this function are

1. The norm of the integral function \( \int_0^L QP_\tau dx \) equals \( \tau \).

2. If we substitute \( x' \) by 0, we recover the expression for \( IP_\tau \).

3. The probability current operator \( J \) at the boundary applied to this function, \( J (QP_\tau) \), is 1 for \( x' = 0 \) and zero for the rest of the source variables.

Our experience tells us that there is not notable difference between the use of \( QP_\tau \) and the first order approximation of the integral \( \tau P_\tau \) and, therefore, the extra calculation effort is necessary. However, if we want a precise boundary condition value, we can use a \( QP_\tau \) function of the form

\[
QP_\tau (x; x') = \begin{cases} 
IP_\tau (x) & \text{if } x' = 0 \\
\tau P_\tau (x; x') & \text{if } x' > 0
\end{cases} \quad (3.8.4)
\]

which ensures us the correct behavior close to the wall.

To observe the impact of this term we solve a problem with \( A = 1 \), \( D = 1 \) and a non-homogeneous term \( \rho = L - x \) where \( L = 10 \) is the length of the grid. Figure 3.8.1 shows small differences in the evolution of the problem, mostly in the points close to the wall, but they are not large enough to justify the increase of computational time needed for the term \( QP_\tau \).
Figure 3.8.1: Differences for the same problem when the analytical integral term $QP$ and then a first order approximation $\tau P$ are used to advance the non-homogeneous term.
3.9 Comparative: Boundary conditions using sink/source terms or with a propagator that fulfills the boundary conditions

This section pays attention to a comparative between the results given by different propagators well posed in the interval $[0, +\infty)$, but satisfying different boundary conditions at the origin. The test problem now is to give the time evolution for $f(x, t)$ satisfying $f(x = 0) = 0$ for any $A$ and $D$ coefficients. We analyze here the difference between when use is made of the method given in the above section and the results obtained with a propagator that fulfills the boundary condition by itself. We introduce a new $P_\tau$ given by:

$$P_\tau(x, x') = \frac{1}{\sqrt{4\pi D}} \left( \exp \left( \frac{(x - x' - \tau A)^2}{4D\tau} \right) - \exp \left( -\frac{A'x' - (x + x' - \tau A)^2}{4D\tau} \right) \right) \quad (3.9.1)$$

which has the property $P_\tau(x, 0) = 0$. This Green’s function is usually called the “absorption propagator” and the integral advancing scheme $(3.3.3)$ gives the solution of this particular problem for absorbing conditions for $f(0, t) = 0$. The question that now arises is that this solution can also be obtained by using the same scheme with our generic propagator and the techniques set in the previous sections to construct the needed current $J_0$, as seen in $(3.6.3)$ that now take the form

$$J_{n+1}^0 = -\frac{D^n(x_1) f^n(x_1)}{h} \quad (3.9.2)$$

The solutions found with both propagators are displayed in Figure 3.9.1 on page 43 and they basically coincide not only with the value close to the wall, but also at any point.

In conclusion, although the reflecting Green’s function does not meet the absorbing boundary condition new boundary terms can be added to satisfy any boundary condition. In other words, our standard propagator and the method exposed in Section 3.7 can be considered as a general
Another important quality testing parameter is the norm of $f$ ($F = \int_0^L f dx$), displayed in Figure 3.9.2 on page 44, not conserved in the real problem because of the boundary condition. As expected, the decrease of the norm $F$ is the same for both propagators, and for the value of the function at $x = 0$ (figure Figure 3.9.3 on page 45) which is within range of the numerical errors.

This results are really noticeable. Since we have stated that our generic $P_\tau$ (2.3.20) can be applied for any boundary condition at the origin.

A question that naturally arises at this point is that the absorbing propagator could be applied to reproduce another boundary condition different of $f(0) = 0$. The answer to this questions, by means of our experience, is that, in general, it cannot be done because (3.9.1) is not normalized to the unity and it does not allow impose boundary conditions due to $P_\tau$ and $\frac{\partial}{\partial x}P_\tau$ are zero for $x = 0$. This question is explained in the following subsection.

3.9.1 The attempt to impose boundary conditions to a non-generic propagator

This subsection gives a more exhaustive explanation for the disposal of the abortion propagator as a generic (standard) one. The first issue is the propagator norm for (3.9.1) which reads

$$\int_0^L P_\tau dx = N_{abs} = \text{erf} \left( \frac{\tau A' + x'}{\sqrt{4D'\tau}} \right) + 1 - \exp \left( -\frac{A' x'}{D'} \right) \left( \text{erf} \left( \frac{\tau A' - x'}{\sqrt{4D'\tau}} \right) + 1 \right)$$

(3.9.3)

It can be seen that the re-normalization (3.9.3) would require more calculation (more time) that can introduce a new source of errors. Also, the discussion of 3.7 to obtain the term $S_\alpha$.
Figure 3.9.3: Value of $f$ at $x = 0$. We appreciate how the absorption propagator reach the desired value and the generic propagator has an error of order $10^{-4}$.

would not be valid for this propagator, what means that in a practical sense, different boundary conditions would not be incorporated directly. Furthermore, we cannot control what terms of the integration scheme are exactly the responsible to change the values at the boundaries as well as the norm of the problem function. In other words, we lose the control of the physical conditions imposed by the original problem, meanwhile with the standard reflecting propagator it does not occur.

In the following example two solutions are calculated, one of them with the generic propagator and the other one with the absorption propagator, both with the correct boundary terms to obtain $f = 1$ at $x = 0$. It can be clearly seen the different behaviors of $f$ at $x$ close to zero, where boundary terms for the abortion propagator completely destroy the final solution. Observe (Figure 3.9.4 on page 46) that the tails of the distributions behaves in a very similar forms with both short-time Green’s functions.

We can conclude that, to create a general method to solve a problem with any boundary condition, it is convenient to use our standard propagator and then, adding the boundary terms in order to perfectly fulfill any boundary condition. However our method allows us to use any alternative propagator which satisfies the boundary conditions in a short-time regime. But we stress that our main goal is to have been able to establish a quite general method to impose any condition, at $x = 0$, in the numerical integral method for the advection-diffusion equations.
3.10 Whole general problem

To end with this chapter we present the general solution of a plain problem introduced in Section 3.1. The boundary conditions are

\begin{align*}
n_i &= 0; \quad J_e = 1; \quad \phi = -1; \quad x = 0 \quad \text{(3.10.1)}
n_i &= n_e = 1; \quad \frac{\partial E}{\partial x} = 0; \quad x \to \infty,
\end{align*}

and the dimensionless parameters of the plasma $\mu_i = 0.1$ and $T_i = 0.025$. The initial condition is 1 for all the points distributions except at $x = 0$ where is 0 for ions and electrons. With these data, the problem is solved with $L = 20$, 1001 points in the grid and $\tau = 10^{-1}$ and 10 iterations. This is a simple problem and is it not related with any experimental data, it is only a benchmark to test how to incorporate all the topics we have seen in this chapter. We expect that the extension to a more realistic problem is only a straightforward application of the method. Here, we study the evolution of an initial neutral plasma evolving in the surroundings of an emissive wall.

The problem is solved in terms of the shifted function $f = n - n_\infty$ to fill the boundary condition at infinity (as we saw in Section 3.5). In the following figures, only the region close to the wall $x \in [0, 4]$ is represented in order to properly analyzing the effect of the wall.

It can be seen (Figure 3.10.1 on page 47) how the electrons quickly evolve to a final distribution. The value at the electrons density at the wall remains as an increasing function, because the constant injection of the boundary (a current greater than zero), meanwhile the ion population slowly tends to zero close to the wall. The plasma potential is also calculated. Figure 3.10.2 on page 48 displays both electric and potential fields, being the later, negative with respect to the plasma bulk at infinite[16, 21].
Figure 3.10.1: Distribution of ions and electrons.
Figure 3.10.2: Distribution of the electric field and the potential.
In this chapter we present a discussion about the differences between the classic Finite Difference Method and our new Integral Method. Likewise, the results obtained by the well-known Finite Difference Method are compared with the ones obtained by our approach. In addition, we justify the use of the Propagator Integral Method by means of its capability for solving some problems appearing when Finite Difference schemes are applied.

4.1 Numerical schemes, convergence and stability

For our discussion we deal with differential and integral numerical schemes, focusing our attention in the convergence and stability, in order to find the issues that can appear in the resolution processes. The first aspect that one needs to cover, when designing a numerical method, is to choose both, spatial and time, discretization schemes. These schemes are strictly defined and can be in fact a limitation in the applicability of the method and its convergence. This is to say, the specific relation between $\tau$ and $h$ has to be specified to avoid numerical instabilities. This well-known characteristic of the Finite Difference Methods is mentioned here to remark an important feature of the integral method: the use of propagators in the numerical scheme does not impose a relation between the discretization parameters. This is because it is a numerical mesh-free method. To properly understand this feature, we recall that no rule is specified or imposed to compute the numerical integrals over the spatial variables.

Another topic that has to be taken into account is the problem of the numerical consistency of the scheme. The consistency imposes that the discretized version of the derivatives, as well as for the full differential equation, has to lead to the correct original equation for infinitesimal $\tau$ and $h$. However, for the integral method, the consistency of the numerical scheme emerges naturally because we deal with the integral representation of the solution, and this integral form is recovered for $h \rightarrow 0$ and the short-time propagator is, in fact, a solution of the integral form of the equation for any small $\tau$, whatever $h$ is. This is also important because, under a practical point of view, the integral method we are developing can be carried out with a relatively large discretization parameters in most of the cases. In other words, $\tau$ is only limited by the Physics involved in the original problem, as well as $h$ is limited only by the selected integration scheme.
These, and other advantages, have been discussed in previous chapters. In the following sections we analyze this features in depth. Some reasons are also given to show the huge possibilities in the analysis of complex plasma structures and non-linear problems in general.

4.2 A Mesh-Free method

One of the most remarkable advantages of this integral method comes from the fact that it is independent of time and spatial discretizations, as said before. This characteristic means that, in practice we have a large range of values for both, $\tau$ and $h$, to be chosen without carrying out large significant error in the computation. This fact has been illustrated in previous sections (3.4) and now we explain the reasons for this property, which is mainly based on physical and mathematical arguments.

An important topic in any numerical advancing scheme, is to analyze how the information contained in a given channel of the numerical grid is transferred to the other channels at each time step. This topic is clearly limited in difference schemes and highly dependent on the numerical representation (two-points, three points approximations...). But not only the number of points of the representation of the derivatives drives the transmission of the information, but also the time integration scheme is important, because it can lead to an implicit or explicit one. For example, in an explicit differential scheme the information contained in a channel only affects a very few adjacent points, depending on the order of the derivative approximation. Such a transmission of the information from a channel can never reach the full grid, but in the integral scheme this could be possible, as it happens in the analytical solution of any Fokker-Planck equation in the short-time regime (a Gaussian packet).

From this point of view, the Propagator Integral Method is not the only one capable of transfer information to a whole grid, the Spectral Methods also exhibit a similar property. These Spectral Methods use an infinite series wave functions in order to construct the solution, without imposing a numerical limit on how far the information can travel from one channel to the others. Nevertheless, the Spectral Methods pose an essential problem to represent discontinuities in the solution since an infinite (large enough in the numerical scheme) number of modes would be required, whereas our integral method only requires a simple Gaussian function for each channel.

Perhaps, the most important advantage of our integral method is that it preserves the physical meaning of the original problem, in the sense that it takes into account the advection and diffusion processes at any time step. This property leads to a scheme that can transfer information to one point to all the grid, thanks to $P_\tau$ (which represents both drifting and diffusion processes almost exactly at any time). Even though the computational time increases, the capability of using relatively large time steps, the stability, almost unconditional, of the method and the physical meaning provide a more accurate solution.

To end with this section, we point out that the advancing integral scheme is quasi-universal for Fokker-Planck equations. That is: no specific integration scheme is needed for each equation, as could happen in a finite difference scheme.

4.2.1 An example: the Heat Equation

To illustrate the considerations made in the section above, we compare the results for the so-called Heat Equation (4.2.1) using the integral and difference methods. Here we simply compare
the results obtained by the Propagator Integral method and the simple numerical solutions based on Finite Differences for the problem

\[
\frac{\partial f}{\partial t} = \frac{c^2}{\partial x^2} f, \quad f = f(x, t) \tag{4.2.1}
\]

\[
f(x, 0) = f^0(x)
\]

\[
f(x \to \pm\infty, t) = 0
\]

This Cauchy problem, with constant diffusivity \( c > 0 \), has a very well known analytical solution

\[
f = \int_{-\infty}^{+\infty} f^0(z) \exp\left(-\frac{(x-z)^2}{4ct}\right) \frac{dz}{\sqrt{4\pi ct}} = \int_{-\infty}^{+\infty} f^0(z) P_\tau(x; z) dz \tag{4.2.2}
\]

and it is used as a test problem in the designing of numerical schemes. Although the analytical problem is extended from \(-\infty\) to \(+\infty\), a finite interval has to be used for the numerical solutions to set a uniform grid of basic length \( h \), with 1001 points for several time steps in \( N \) iterations.

To apply a finite difference numerical method, the following scheme is used:

\[
f_{i}^{n+1} = f_{i}^{n} + \frac{c}{h^2} \left(f_{i+1}^{n} - 2f_{i}^{n} + f_{i-1}^{n}\right) \tag{4.2.3}
\]

The scheme is stable if the relation \( c\frac{\tau}{h^2} = r \ll 1 \) is fulfilled. This relation imposes a restriction in the \( \tau \) and \( h \) parameters. For example, if we want to analyze the solution for large time with a refined grid, a small time step has to be used, which leads to many iterations. This problem may be reinforced for a non-linear \( c = c(f, x, t) \) that can reach high values. Meanwhile, \( \tau \) and \( h \) in the integral method are not related with the value of \( c \). Moreover, the addition of a numerical viscosity\[20\] for some numerical differences schemes can perturb the solution, what does not happen in the integral propagator method.

Let us start our discussion with the problem corresponding to a Dirac delta initial condition \( f^0 = h\delta(x) \) that gives the Kronecker delta in the numerical representation \( f^0 = 0; f^0(x = 0) = 1 \). Now if the scheme (4.2.3) is applied, it can be seen how the information from the channel \( i \) is only transferred to points \( i + 1 \) and \( i - 1 \). So that, in the first iteration, the information in the channel for \( x = 0 \) only modifies the value of \( f \) at points \( x = \pm h \) with this approximation of the derivative. But with the Propagator Integral Method in the domain \([−\infty, +\infty]\) the information \( f^0 \) contained in the first channel is transmitted to the whole grid or, in practice, to a number of points imposed by the value of \( \tau \).

\[
f^1 = \int_{-\infty}^{+\infty} dx' P_\tau(x, x') f^0(x') = P_\tau(x, 0) \tag{4.2.4}
\]

In other words, the information diffuses to the entire grid instantaneously and no restriction for \( r \) is required. This is the reason why we can use large values of \( \tau \) when we apply the integral method, without changing the grid. On the contrary, it may occur that the spurious numerical viscosity of the difference scheme leads to misleading solutions resulting in a more diffusive problem than it should be.

Another example with \( c = 1 \) and \( f^0 = \exp(-x^2) \) has been also dealt. We have found that for the finite difference scheme the increasing of \( \tau \) imposes an increase of \( h \) and, for relative large values of \( \tau \), the numerical Finite Difference solution does not match the correct one, however, for the propagator method, the solutions are similar for different values of \( \tau \). In order to obtain
a convergence in the finite difference scheme, we have to change the $h$ parameter resulting in a different grid. A resume can be seen in the table 4.1.

Table 4.1: Different spatial discretizations for the different time scales.

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>$h$</th>
<th>Number of points</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-4}$</td>
<td>0.039960</td>
<td>1001</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>0.3960</td>
<td>101</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td>3.3636</td>
<td>11</td>
</tr>
</tbody>
</table>

In the result for $\tau = 10^{-4}$ (figure 4.2.1) we observe how the solutions are very different. The problem emerges in the numerical calculation of the propagators because of a poor precision in the numerical computation of the exponential for very small $\tau$, this problem also appear with the analytical solution and has to be studied in depth. Strictly speaking, there is not a problem with the integral method, this is an intrinsic problem with the numerical representation.

In fact, for $\tau = 10^{-3}$ (figure 4.2.2) both results are practically the same. Now, the propagator solution behaves properly and match the numerical differences solution.

Finally, for $\tau = 10^{-2}$ (figure 4.2.3) we notice how the reduction in the number of points (Finite Difference Method) to make it stable leads to a non-evolving numerical solution where the integral numerical solution evolves as the correct analytical solution.

### 4.3 The meaning of the boundary conditions

In this section we discuss how the inclusion of the boundary conditions leads to a very different interpretation about how the information of the boundary effects is transferred to the grid. A similar situation that we found of the transmission of the information in time appears here in a similar way, when the information of the edge channel enters in the numerical scheme. Roughly speaking, in a finite difference method, the boundary condition has the meaning of a single point providing information to the grid, meanwhile, in the integral numerical approach, an effective source/sink term enters into the scheme and propagates the information from the boundary condition instantaneously, as it can be seen by a simple inspection of the term $IP_\tau(x)$ given in section §3.7. In other words, with the Green’s function scheme, the boundary effects introduced by the surface integral in the general $N$-dimensional problem works acting in the whole domain from the very first time step, although a surface (or a point in 1-D) includes the effects of the boundary. On the contrary, in a finite difference method the boundary conditions enter given a value to the function in one channel. This effect is expected to propagate to the rest of the grid along the time evolution.

To illustrate this intriguing and interesting topic, we give an example of the problem using the Fokker-Planck equation (2.2.1) with $f^0 = \frac{1}{2} \exp(-x^2)$, $f^0_0 = 1$ as a boundary condition and the parameters $A = 0.1$, $D = 1.0$ and $x \geq 0$. To have the same number of points (1001) and the same dimension-less time $t = 1$, we have chosen a time step of $10^{-3}$ and $10^{-2}$ with 1000 and 100 iterations for the propagator method and $10^{-4}$ with 10000 iterations for the numerical method. The results correspond to a grid of length $L = 100$ but to make a clear comparative, we only show the interval $[0, 5]$ (figure 4.3.1).
Figure 4.2.1: Solution for the heat equation with $\tau = 10^{-4}$. 
Numerical Method vs Propagator Method for $\tau = 10^{-3}$

Figure 4.2.2: Solution for the heat equation with $\tau = 10^{-3}$. 
Numerical Method vs Propagator Method for $\tau = 10^{-2}$

Figure 4.2.3: Solution for the heat equation with $\tau = 10^{-2}$. 
As we observe, the results are very different, what indicates that a problem may appear with the propagator method for small values of \( \tau \). This is a similar problem that appears in figure 4.2.1 with \( \tau = 10^{-4} \) without boundary terms. Again, this is a problem related to the numerical representation of \( IP_\tau \), it is not related to the inclusion of the boundary term.

### 4.4 How to deal with initial abrupt conditions

One of the problems of the traditional finite difference methods is that they cannot represent the derivatives of functions showing discontinuities or sharp jumps, even functions with high slopes. In many physical problems, such abrupt conditions appears naturally as, for instance, an emitting surface at the boundary or the discontinuities of some electromagnetic field components. The solution for a given Fokker-Planck equation with abrupt initial condition can be misleading if a Finite Difference Method is used, although the diffusive terms tends to smooth the solution over time. It has been shown, in several examples, that the inclusion of a histogram-like initial

---

Figure 4.3.1: Comparison between the numerical solution and the propagator solution for a boundary condition at the wall.
function evolves in time properly with the integral method for the very first time step. This is because we have to integrate (add), not to difference (subtract) the function.

To test how this abrupt initial condition evolves in time, we solve, again, the problem corresponding to figure 4.2.2, but now, for the histogram-like initial condition:

\[
f^0 = \begin{cases} 
1 & \text{if } x \in [-0.4, 0.4] \\
0 & \text{if } x \notin [-0.4, 0.4]
\end{cases}
\] (4.4.1)

This condition is very similar to the original one, and it is expected a similar evolving result. We can see in figure 4.4.1 how the solution based in finite differences is slightly different from the propagator’s one. Usually, the equation with a second order derivative does not lead to troubles with the abrupt condition after several iterations. Nevertheless, if a first order derivative (advection) is introduced this effect is enlarged remaining for large number of iterations and, some times affecting the stability of the Finite Difference solution. Moreover, we have found several cases where the numerical solution in the first few time steps becomes negative close to the limit of the initial histogram condition.

Another example solving the Fokker-Planck equation with the same initial condition and \( D = 1, A = 1 \) is performed, with \( \tau = 10^{-3}, 1000 \) iterations and 1001 points for the integral method, and 101 points for the finite difference method. It can be seen in figure 4.4.2 how both solutions differs leading to different final results. We have detected this problem is due to the explicit difference numerical scheme because a more sophisticated numerical scheme (Crank-Nicolson) gives the same results as the propagator method.

Another interesting advantage of the use of the propagator instead of Finite Difference to solve the advection-diffusion equation is related to the initialization of the iteration process having a given initial condition. It is well-known than higher order of 1 in \( \tau \) for a Finite Difference scheme needs more steps to apply the scheme. This is because a higher order of approximation in the temporal derivative involves the knowledge not only of the first initial condition (\( n = 0 \)), but also, at least, one step more at \( n = 1 \), what imposes to construct \( f^1 \) using an axillary scheme always of lower order. In other words, Finite Differences higher order schemes usually require more previous steps (\( n, n - 1, n - 2 \ldots \)) to obtain the step \( n + 1 \), but the analytical problem only provides us a unique initial condition. So, in order to use a higher order scheme, another integration scheme has to be used to calculate the steps needed. These schemes, always of lower order, can be a source of errors and lead to non-realistic solutions, specially if we want to analyze a short-time of evolution. Meanwhile, if we use our propagator advancing scheme, we only require an initial condition as established by the formal solution given in terms of the Green’s function. What it means is that with the integral method a given initial condition is enough to perform the advancing scheme for any order or approximation in \( \tau \) of the used propagator. Under a computational point of view, if we do not have to save in memory more steps we need less RAM memory to solve our problems.

### 4.5 Comparative for the problem of the emissive wall

To end with this chapter, the complete problem presented in 3.1 is solved using both methods, Finite Difference and Propagator Integral. This section also includes an analysis of another non-linear problem, called the viscous Burgers’ equation.

We consider two superimposed beams of species, electrons and ions, to avoid dealing with the quasi-neutrals condition for \( x \rightarrow \infty \) (this means no plasma at infinity). This kind of initial
Figure 4.4.1: Comparison with an initial abrupt condition for the Finite Difference and the Propagator Integral methods.
Figure 4.4.2: Solution using Finite Difference and the Propagator Method for an advection-diffusion problem.
conditions can be studied easily with the propagator method due to the ability to physically represent discontinuities. We solve an example with \( t = 1 \), using 10 steps in the propagator method and 10000 in the difference method to allow 1001 points in both numerical grids. In addition, we use \( \mu_i = 0.1 \) and \( T_i = 0.025 \) as parameters for the ions. For boundary conditions at the wall, we have \( n_i = 0 \) and \( J_e = 0 \) and \( \varphi = -1 \). We note that this case corresponds to a local analysis of the plasma.

![Figure 4.5.1: Distribution for ions and electrons for the Propagator Integral Method (PIM) and the Finite Differences Method (FDM)](image)

The distributions for ions and electrons are represented in 4.5.1 and it can be appreciated some differences among them close the wall. This small differences between the integral and difference schemes seem not to be important, however, the electric field is highly related to the charge density, so, the imprecision in the computation of \( n_\alpha \) gives rise to very different charge structures (figure 4.5.2). In this sense, the time evolution of the ions, much slower than the electrons one, is better solved by the integral method, because this has an appropriate response to the diffusion processes even for abrupt conditions, whereas the approximation of the derivative fails and the ion diffusion is not properly described.

Otherwise, a significant result is related to the values at the boundary. The electron flux at \( x = 0 \) (figure 4.5.4 on the right) does not match the boundary conditions and increases in time. Although the ions are not zero (figure 4.5.4, on the left) for the propagator method, they converge to the boundary value in a few iterations. But in the finite difference method the total number of particles (figure 4.5.3) is continuously increased in time instead of being constant for the electrons and slightly dismissing for ions (ions absorbing condition has been set).
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Figure 4.5.2: Electric field and potential for the plasma-wall iteration problem solved with the Propagator Integral Method (PIM) and the Finite Differences Method (FDM).

Figure 4.5.3: Total amount of electrons and ions during the problem solved with the Propagator Integral Method (PIM) and the Finite Differences Method (FDM).
4.5.1 Viscous Burgers’ equation

Another interesting equation to compare the results obtained with Finite Difference and the Propagator Integral method is the Viscous Burgers’ equation

\[
\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x} \left\{ -\frac{\alpha}{2} f - \nu \frac{\partial}{\partial x} f \right\}
\]

(4.5.1)

where \(-\frac{\alpha}{2} f\) represents a non-linear drift term and \(\nu\) is a viscosity coefficient, responsible of the diffusion process. This is a very interesting equation, because it presents a discontinuity if the viscosity is small enough. Such a discontinuity appears close to the points where \(f\) equals zero in the initial condition. Numerical methods based in finite differences usually fail when they are used in this case to detect the behavior of the discontinuities, because it is difficult to describe such a behavior of the discontinuities modeled with finite differences. Our integral method, as we have explained in previous sections, can feasibility deal with any kind of discontinuities.

To compare between the finite difference method and the propagator method, a case with a positive advection \((\alpha = 2)\) and viscosity \(\nu = 0.01\) has been numerically solved with both methods. The low value of the viscosity clearly allows the formation of a shock wave, as we have mentioned above. The problem is initialized with a histogram-like condition at \(t = 0\) and the evolution is studied in the open space \((-\infty, +\infty)\). For the propagator method we have used \(\tau = 10^{-1}\) and for the finite difference method \(\tau = 10^{-2}\). We observe in figure 4.5.5 how the shock-wave is formed and the solutions obtained by both methods are indistinguishable. Once again, we established a result that can be considered as general, what is to prove that relatively large time steps can be used in the integral method. Moreover, here the finite differences solutions are accurate enough because a refined grid and a very small time step has been used, but this requirements are not needed for the advancing integral scheme, also for free spatial mesh. The spatial mesh is chosen being aware of the physics involved in the original problem, but no by
Figure 4.5.5: Evolution over the time for the propagator solution (red) and the differences solution (green) of the viscous Burgers’ equation.

numerical criteria. That is, one can use an appropriate grid, just by testing in a few iterations which grid spacing accomplishes with the physical representation of the problem.
In this chapter, we present how the integral method, including boundary effects and non-homogeneous term, is applied to a physical problem, showing some interesting results we have found through the application of this method. Some of the resolved cases are directly related to typical situations in our plasma laboratory, describing several phenomena that are usually very difficult to analyze by means of conventional numerical schemes. Furthermore, in this chapter we present some extreme cases showing how our method can deal with non-trivial boundary conditions. Finally, we identify here some interesting properties of a plasma close to a wall in order to focus our attention to perform further researches to apply the method we have studied. All problems dealt here follow the model described in Section 3.1 but for some particular values of the physical parameters and with several boundary conditions that match physical context.

5.1 The case of the wall heating

In this section, we study the heating of an emissive wall in contact with an initially neutral plasma. This scenario appears in experimental devices, such as emissive electrical probes immersed in plasma. For these probes, a heating current operates until the metal filament reach a steady state of electron emission. Here we analyze the transit regime over the range of time until the emitted electron current reach an almost constant value of 1, in dimensionless units. The effect of heating is simulated by the inclusion of a time variable emitted electron flux, a current in our nomenclature, \( J_e(x=0) = 1 - \exp(-t) \) (in dimensionless form). The process is analyzed over a total time of 8 units. We recall that the time scale is related with the characteristic time of the electron plasma frequency, being the electron of about 1 ev in kinetic temperature. A grid of 1001 has been used and the ion temperature is \( T_i = 0.025 \) with mobility \( \mu_i = 0.1 \). With these settings the boundary conditions can be cast into the relations

\[
\begin{align*}
    n_i &= 0; J_e = 1 - \exp(-t); \quad \varphi = -1; \quad x = 0 \\
    n_i &= n_e = 1; \quad \frac{\partial \varphi}{\partial x} = 0; \quad x \to \infty
\end{align*}
\]

which account with fixed plasma wall potential, negative with respect to the plasma bulk, and a
quasi-neutral plasma with $E = 0$ at infinite. It has been also assumed that the heating current of the external circuit immediately gives rise to a wall current $J_e$ emission.

In this particular case, a huge current is obtained in a very short-time ($\sim 1$) what configures the charge structure in front of the wall, modifying the particle densities and the plasma potential close to the wall. The results are displayed by the set of figures 5.1.1, 5.1.2 and 5.1.3. We appreciate how the fast evolution of the plasma breaks the quasi-neutrality leading to an electric field pointed out to the plasma wall. The plasma potential distribution is smooth and tends to be stable. Although no steady state is found while the wall is emitting. However, we think that within the range of approximation of this model and in the time scale considered, the solution found after some time units can be considered as quasi stationary.
**Figure 5.1.2:** Electric field (left) and potential (right) over the time for the wall heating case.

**Figure 5.1.3:** Total amount of particles (left) and Probability current at $x = 0$ (right) for the wall heating case.
5.2 Smooth current at the wall

Sometimes the plasma probes in laboratory operates under controlled swept processes that externally modify the emission. In this section we simulate a characteristic situation in the laboratory when a probe starts its emission reaching an almost constant value that smoothly vanished until it starts again to repeat the same process. For this case, the dimensionless electron density current at the wall is assumed to follow the relation

\[
 J_e = \begin{cases} 
 1 - \exp(-t) & t \leq 8 \\
 1 - \exp(t - 16) & t > 8 
\end{cases} 
\] (5.2.1)

over a total time \( t = 16 \) units. The remaining boundary conditions are:

\[
 n_i = 0; \quad \varphi = -1; \quad x = 0 
\]

\[
 n_i = n_e = 1; \quad \frac{\partial \varphi}{\partial x} = 0; \quad x \to \infty 
\] (5.2.2)

The parameters for the ions are \( T_i = 0.025 \) and \( \mu_i = 0.1 \) again.

The numerical computation shows a similar behavior as that found in the previous case, when the current increased but now, a concentration of ions appears. This peak of ion density remains, even when the emission finishes. It seems they have no time to completely diffuse and they are accumulated because of the drift carried by the electric field. After this process, the ions have to diffuse but they are cold enough to have no time to experience such a diffusion. This scenario remains almost uniform because of the electrons evolve smoothly due to the effect of the controlled \( J_e \).

We want to emphasize that controlling the emission of the wall can drive the dynamics of the ions, what means that both electron and ions dynamics have to be analyzed simultaneously. Neglecting the evolution of the ion density for relatively large time of evolution (but short in the ions time scale) is not advisable, due to, it can lead to to a physical situation not related with the real scenario.

5.3 Abrupt current at the wall

In this case we study the effects of a sharp current induced at the emissive wall. In other words, we deal here with an electron flux \( J_e \) which does not evolve smoothly, as the one used in Section 5.2. Now the current for the electrons at \( x = 0 \) is simulated by

\[
 J_e = \begin{cases} 
 0 & \text{if } t \leq 1 \\
 1 & \text{if } 1 < t \leq 2 \\
 0 & \text{if } t > 2 
\end{cases} 
\] (5.3.1)

The rest of the parameters and boundary conditions are: 1001 points in the grid, \( T_i = 0.025 \), and \( \mu_i = 0.1 \) for the ions, and

\[
 n_i = 0; \quad \varphi = -1; \quad x = 0 
\]

\[
 n_i = n_e = 1; \quad \frac{\partial \varphi}{\partial x} = 0; \quad x \to \infty 
\] (5.3.2)
Figure 5.2.1: Ions and electrons distribution functions over the time for a smooth current at the wall.
**Figure 5.2.2:** Electric field (left) and potential (right) for a smooth current at the wall.

**Figure 5.2.3:** Total amount of particles (left) and current at the boundaries (right) for a smooth current at the wall.
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In figures 5.3.1, 5.3.2 and 5.3.3 the main results for this case are displayed. Highly notable differences with respect to the previous cases are found when the wall is emitting electrons and when it is cut off this emission. We note that the ions (red marks) have no enough time to return to the initial state, i.e. there is no electron emission at the wall. This ion accumulation and the fast change for the electrons lead to a change of sign in the electric field for a $t = 3.2$, which results in a new distribution for the plasma potential. These final results completely differ from those obtained in Section 5.2 with no electric field inversion. On the other hand, we have observed how the behavior of the plasma is highly sensitive to the effect of the emission current and leading to a very different plasma configurations of all plasma parameters. The ion density, which evolves slowly if compared to the electron density, does not instantaneously feel the electric field variations. For this reason, the leading mechanism modifying the ion density is the absorbing boundary condition imposed here ($n_i(0, t) = 0$).

From a numerical point of view, the effect of the boundary time variable current affects all the grid instantaneously what allows the use of electric currents that can drastically change in time.
Figure 5.3.2: Electric field (left) and potential (right) for an abrupt current at the wall.

Figure 5.3.3: Total amount of particles (left) and current at the boundaries (right) for an abrupt current at the wall.
5.4 Sinusoidal current

The examples presented above set a positive current for the electrons as a boundary condition, a fact that assumes emission of electrons from the wall. On the contrary, if we impose a negative current, we are simulating the effect of a collecting probe. This collecting probes are very important for measurements to characterize a plasma. This simulation also set the basis to study how a Langmuir probe can work under a variable current. For this reason it is important to test and compare the results using the Propagator method when the current in the boundary is negative.

To this purpose, this example with a current of the form $J_e = \sin(\pi t)$ at the wall will cover a regime of emission and a regime of electron collection. In figures 5.4.1 and 5.4.2 the different configurations for the plasma species density and electric and potential field when the wall is in the emissive or the collective regime.

Figure 5.4.3 displays the total amount of particles (on the left) and the current at the wall (on the right). A hysteresis appears in the norm of the electron density since the point where
the electron current equals zero $t = 1$, a small fraction of electrons remains in the problem.

5.5 Abrupt time varying current

To continue testing the method, a new function for the electron current at the wall is used. This current abruptly jumps from a positive (emission) to a negative (absorption) value of the current. This current (Figure 5.5.3 on page 77, on the right) produces plasma structures clearly different from those observed in the previous case with a smooth time varying current. The remaining parameters are $T_i = 0.025$ and $\mu_i = 0.1$ for ions, 1001 points for the grid, a total time of $t = 10$ and the boundary conditions:

\[ n_i = 0; \quad \varphi = -1; \quad x = 0 \]
\[ n_i = n_e = 1; \quad \frac{\partial \varphi}{\partial x} = 0; \quad x \rightarrow \infty \]  

where again, absorbing boundary conditions are set for the ions.

The figures 5.5.1, 5.5.2 and 5.5.3 show several distributions for the plasma density different from the ones obtained with a sinusoidal current (Section 5.4) and the plasma remains negatively charged respect to the infinite. That is caused because the particles emitted from the wall disappear at infinite, but when the wall is collecting electrons, an electron population comes from the plasma bulk, remaining close to the wall.

To end with this chapter, we note that an hysteretic behavior have been detected, which is highly sensitive to the excitation of the emitting wall and requires a very precise calculation.
Figure 5.4.3: Norm of the density (left) and current at $x = 0$ (right) for ions and electrons over the time for a sinusoidal current at the wall.
Figure 5.5.1: Evolution of ions and electrons for an abrupt time varying current at the wall.
Figure 5.5.2: Electric field (left) and potential (right) for an abrupt time varying electron flux at the wall.

Figure 5.5.3: Total amount of particles (left) and current at the boundaries (right) for an abrupt time varying current at the wall.
CHAPTER 6

CONCLUSIONS AND FUTURE WORK

This final chapter covers a discussion about the general advantages and drawbacks established during the development of this research. This issue is important in order to guide future lines of investigation that can be useful to extend the scope of application of our numerical integral method. Despite some of the most important aspects of our algorithm have been exhaustively treated throughout the text, we consider, at this stage, very important to remark them in order to clarify why we have developed the method and what we have achieved.

6.1 Advantages

Although this method has been applied in some previous works in several fields in Physics, as an extension of the so-called path-integral method, its potentiality under a computational point of view has not been stressed enough for decades. This under-estimated consideration of the numerical integral method has been essentially motivated by the practical absence of investigations on how to deal with the boundary conditions in a given problem. Under this point of view, we would like to draw attention to this fact by showing some of the advantages we consider that have to be underlined:

- Robustness and consistency. By virtue of our experience, we have checked out that the integral method is numerically stable and robust, without, in practice, no restriction of the parameters used for the discretizations. Otherwise, the numerical scheme reproduces, in the limit of very short evolution time, the integral representation of the original advection-diffusion equation, that means consistency.

- Truthful meaning under a physical perspective. This means that the method takes advantage of analytical solutions valid for the short evolution time. Therefore, the solutions evolve as they were analytical solutions, thanks to the action of the short-time propagator. The short-time propagators used in the method are constructed by taking into account the information provided by the original advection-diffusion equation, and the expression of the propagator can be taken from the literature specialized in Green’s functions, using the corresponding form of a more simple problem.
• Large range for the time step value without affecting the convergence. As said in section 3.4.1, this method can lead to the same results with time steps that can differ even in an order of magnitude for the same problem. This property allows the method to be able to analyze different time scales of the physical evolution without modifying the numerical scheme. This property not only can save time in the calculations but also, it saves time because there is no need to search for new integration schemes to match our problem: The scheme is general for any advection-diffusion equation. Likewise, with a large $\tau$ we can solve slowing evolving diffusive problems in a few iterations, a fact that reduces the computational effort.

• Mesh-Free method. Due to the integration scheme is based on a powerful theoretical basis, that is, as it is the use of Green’s functions, the way to advance in time the problem function gives no relation between the defined grid and the time step $\tau$. This means that one can freely design the mesh to represent the values of the problem function at any point and, after that, an appropriate time step can be chosen, by testing, without accomplishing any specific relation with the grid.

• Smoothing effects of diffusive equations. This advantage is related to the fact that the integral scheme can present smoothness effects of any abrupt initial condition, as it could be done by the (usually unknown) exact propagator. Furthermore, in those cases where the problem function has to be positive, the numerical solution remains positive at any time step.

• Useful for solutions with discontinuities. In several physical problems some discontinuities emerge. Such discontinuities are very difficult to be modeled by Finite Differences schemes. However, with the use of the Propagator Integral Method, this jumps or discontinuities can appear without distorting or destabilizing the solution. This means, it will reliably represent discontinuities, shock waves and similar effects, with precision and without divergences. For this reason, the integral method is an excellent choice to find solutions where discontinuities can appear.

• Able to deal with non-linear and non-homogeneous problems. The Propagator Integral Method can feasibly deal with possible non-linearities accounted in $A$ and $D$ coefficients, without affecting the convergence and stability. Besides this, non-homogeneous terms can be easily introduced to the advancing scheme, once again, using the theoretical frame that gives the formal solution in terms of the Green’s function.

• Abrupt boundary conditions. As explained in section §4.3, this method introduces the boundary conditions as source/sink terms. This means that the values imposed as boundary conditions affect to all the grid from the first instant, as in the analytical solution, not only affect some few points close to the boundaries, as it happens in the numerical difference schemes. For these reasons, abrupt and time varying boundary conditions can be safely introduced.

6.2 Drawbacks

Although this work has extended the applicability of the short-time propagators to provide numerical solutions, by allowing the method to incorporate the effects of boundary conditions, some disadvantages still exist. We consider it is convenient to be aware of the drawbacks of this method in order to amend them for further improvements.
• Computational effort. Although we have not insisted on the computational cost in time of our method during the previous sections, it is important to mention that the calculation of the propagators requires a great amount of computational time, specially because it has to be cast in a $N \times N$ matrix (where $N$ is the number of points of the grid) involving non-elementary functions as the error function, with complicated arguments and very sensitive to be evaluated. A way to reduce this calculations is a matter of future investigation.

• Current at the boundaries. Section 3.7 explained how the value of the probability current for the propagator and its integral exerts a high influence in the boundaries. To bring these values to the analytical ones, a translation was made for both $P_\tau$ and $IP_\tau$. However, this topic has to be deeper investigated in order to provide a simple method to numerically calculate the propagator fulfilling the exact boundary probability currents.

• Impreciseness for very small $\tau$. From the numerical point of view, the calculation of the propagator is not highly accurate when $\tau \ll 1$, because the numerical precision is lost since $P_\tau$ reassembles a Dirac delta function, which is very difficult to represent numerically. Even this is not a failure of the method, it is an issue that has to be improved increase the range of valid $\tau$ for low values.

6.3 Future work

Apart from trying to solve the drawbacks listed above, much work is still ahead to apply the method to the simulation of practical and physical situations. Among a great variety of tasks to be done in future researches, we enumerate here some of the points that can give a guideline for working towards this goal.

• Extension to high-dimensional problems. Throughout this work, we have dealt with a 1-D problem to explain the advancing scheme and the way to introduce the boundary conditions. To solve real physical problems, the method has to be extended to higher dimensions. For problems involving several variables, the method can be specially useful because of the information of the cross derivatives of the differential equation is transposed into the integral scheme through a multivariate Gaussian short-time propagator. The problem of representing the cross derivatives in a Finite Difference scheme is solve with the integral advancing scheme. For instance, in Plasma Physics, where the kinetic description[25] of a collisional plasma accounts of electromagnetic fields and diffusion between velocities and real spaces the integral advancing scheme will pose, not only a numerical scheme, but, also, a physical meaningful short-time solutions at each time step, also including the boundary effects.

• Propagators in generalized geometries. In many problems in Physics, the use of curvilinear coordinates is important. For instance, many devices for plasma ignition and sustaining are designed to be adapted to certain spatial geometry. Thus, to have a series of generic propagators adapted to the most usual geometries would be important. Our research group is particularly interested in analyzing the plasma surrounding spherical and cylindrical probes or cathodes, and in modeling the ionization cylindrical chamber of an ion electric thruster. The new propagators should be proposed to match this geometries of physical spaces. These geometrical topics also holds for velocity components in a kinetic plasma treatment.
• Application to other fields. As it is well known, the advection-diffusion equations appear in many fields in Physics and Applied Mathematics. So that, we think that this method can be applied to other fields such as: fluid mechanics, thermodynamics, quantum mechanics, etc.

• Effects of a confining magnetic field. In order to properly analyze a plasma, the presence of the magnetic field has to be taking into account. The magnetic field can affect all charged plasma species in both kinetic and fluid descriptions increasing the non-linearity of the problem. Again, the extension of the method to a multidimensional problem is needed.


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