DEVELOPMENT OF IMPLICIT KINETIC SIMULATION METHODS, AND THEIR APPLICATION TO ION BEAM PROPAGATION IN CURRENT AND FUTURE NEUTRALIZED DRIFT COMPRESSION EXPERIMENTS

BY

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DISserTATION

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Ion beams can be accelerated and focused to hit a target thus releasing high density power to achieve nuclear fusion. They can also be used to study phase transition from the solid to the Warm Dense Matter state. The Neutralized Drift Compression Experiment (NDCX) at the Lawrence Berkeley National Laboratory is being used to investigate the possibility of developing drivers for the heavy ion fusion reactors, and for Warm Dense Matter experiments. Because ion beams are positively charged, repulsive forces act on the beam ions. These electrostatic forces defocus the beam, increasing the beam size and degrading the applied compression and focus. Electrons are introduced via a preformed plasma to eliminate the electrostatic forces that defocus the beam in the NDCX. The spread of the background plasma electrons inside the beam, and the adjustment of their velocity to the beam propagation velocity is called neutralization process. Because collisions occur on time scales much larger than the time scales for the neutralization process, the plasma can be considered collision-less. Thus, the neutralization process is dominated by plasma-wave interactions instead of collisions, and the kinetic approach is required to model this phenomenon.

In this dissertation, the neutralization process in the NDCX configuration is studied. The collision-less kinetic equations of plasma are solved numerically using two implicit Particle-in-Cell methods. The implicit nature of the time-differenced governing equations leads to unconditional numerical stability. The primary numerical scheme is based on an implicit moment Particle-in-Cell approach. It has been developed for the electromagnetic case and implemented in a 3D, parallel code to study the neutralization process. In addition, a fully implicit Particle-in-Cell method to
solve the particle and field equations has been also developed and implemented for a simple one dimensional, electrostatic configuration. The goal of the fully implicit scheme was to demonstrate that a fully implicit scheme can indeed converge as it has been a challenge. It has been demonstrated that fully implicit schemes (at least 1D, electrostatic configuration) can in fact converge. The schemes developed and implemented are used extensively to study the neutralization dynamics.

The aim of this study is to analyze the dynamics that governs the neutralization process in the NDCX configuration. It has been found that the neutralization is a transient phenomenon, typically occurring on time scales of tens of plasma periods. During this transient, the ion beam undergoes through large electron oscillations. The oscillations are damped by a sheath. This sheath regulates the electron flux into and out of the beam, and because it opposes the electron oscillations, it also oscillates. The forward moving and oscillating sheath persists after the transient, and forms an oscillating shock at the front of the ion beam. The shock is in the form of a moving and oscillating discontinuity in the electric field, the charge density, and the electron average velocity.

It has been found that the background plasma and beam densities influence the neutralization process, changing the properties of the sheath at the beam-plasma interface. The damping of the oscillations is important when the background plasma and beam densities are close in value, while it is weaker when the background plasma density is higher than the beam density. Moreover, the magnetic field does not have a significant effect on the ion beam neutralization process in the current and future NDCX configurations, and the simulations can be carried out in the electrostatic limit, achieving the same results as those obtained using electromagnetic simulations.

A comparison of the implicit Particle-in-Cell methods with the explicitly time differenced Particle-in-Cell method shows that the implicit moment and the fully implicit Particle-in-Cell methods are on average 4 to 40 times computationally more
expensive if the same simulation time step is used. Because the ion beam neutral-
ization process in the NDCX occurs on the plasma period time scales and on the
Debye length spatial scales, these scales need to be resolved to correctly describe the
neutralization phenomenon. Because of these constraints on the time step and the
grid spacing, the implicit Particle-in-Cell methods are here used on space and time
scales where the explicit Particle-in-Cell method is numerically stable, hence denying
the advantage that implicit methods have over explicit schemes. However, it is clear
that implicit schemes are more efficient for problems that allow large time steps.
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## Acronyms

- **CIC** ................................................................. Cloud-in-Cell
- **CG** ................................................................. Conjugate Gradient
- **CN** ................................................................. Crank-Nicholson
- **FCAPS** ......................................................... Ferro Cathodic Arc Plasma Source
- **FEPS** ............................................................. Ferro Electric Plasma Source
- **FLOPS** .......................................................... Floating Point Operations
- **GMRes** ........................................................ Generalized Minimal Residual
- **ICF** ................................................................. Inertial Confinement Fusion
- **LBNL** ............................................................. Lawrence Berkeley National Laboratory
- **MD** ................................................................. Molecular Dynamics
- **MHD** ............................................................... Magneto Hydro Dynamics
- **NDCX** ......................................................... Neutralized Drift Compression eXperiment
- **NIF** ................................................................. National Ignition Facility
- **NK** ................................................................. Newton Krylov
- **ODE** ............................................................... Ordinary Differential Equation
- **OOP** ............................................................... Object Oriented Programming
- **PDE** ............................................................... Partial Differential Equation
- **PIC** ................................................................. Particle-In-Cell
- **WDM** ............................................................... Warm Dense Matter
Notation

\( B \) ................................................................. magnetic field
\( B_p \) ............................................................... magnetic field acting on the particle \( p \)
\( B_0 \) ......................................................... normalization value of the magnetic field
\( E \) ................................................................. electric field
\( E_p \) ............................................................... electric field acting on the particle \( p \)
\( E' \) ........................................................ corrected electric field to ensure the charge conservation
\( F \) ................................................................. residual function
\( F_E \) ............................................................ force due to the electric field
\( F_B \) ............................................................ force due to the magnetic field
\( I \) ................................................................. current
\( J \) ................................................................. Jacobian
\( J_e \) .......................................................... electron current density
\( K_B \) ......................................................... Boltzmann constant
\( L \) ............................................................. length normalization value
\( L_x \) ........................................................ simulation box length
\( N_g \) ....................................................... number of grid points
\( N_{PC} \) .................................................. number of particles per cell
\( N_s \) .................................................... number of particles for the species \( s \)
\( Q/M \) ................................................ normalization value of the charge to mass ratio
\( R \) ............................................................. rotation transformation
\( S \) ............................................................. shape function
\( T \) ............................................................. temperature
\( V \) .......................................................... computational domain
\( VEL \) .................................................. velocity normalization value
\( W \) ........................................................ interpolation function
\( X \) ................................................... vector containing the unknowns for the GMRes solver

\( b_l \) ................................................................. b-spline function
\( c \) ........................................................ speed of light in vacuum
\( e \) ........................................................ electron index
\( f \) ........................................................ distribution function
\( g \) ........................................................ grid point index
\( it \) ........................................................ iteration index
\( it2 \) .................................................... iteration index
\( k \) ........................................................ wave number
\( m_e \) ......................................................... electron mass
\( m_{Ba} \) .......................................................... Barium mass
\( m_{K} \) ............................................................... Potassium mass
\( m_s \) .............................................................. mass of particle of species \( s \)
\( n \) ................................................................. time level
\( n_{beam} \) ......................................................... beam density
\( n_{plasma} \) ...................................................... background plasma density
\( n_s \) .............................................................. number of species
\( p \) ............................................................... particle index
\( q \) .............................................................. electron charge
\( q_s \) ............................................................ charge of particle of species \( s \)
\( r \) ............................................................... residual
\( r_{beam} \) ........................................................ beam radius
\( s \) .............................................................. particle species index
\( t \) .............................................................. time
\( \bar{v} \) .......................................................... particle average velocity
\( v_{beam} \) ......................................................... beam propagation velocity
\( < v_e > \) ...................................................... average electron velocity
\( v_g \) .......................................................... group velocity
\( v_p \) .......................................................... particle velocity
\( v_{the} \) ........................................................ electron thermal velocity
\( x_g \) .......................................................... grid point position
\( x_p \) .......................................................... particle position
\( x'_p \) .......................................................... perturbed particle position

\( \beta \) .................................................. scalar chosen to minimize the residual function
\( \gamma \) ................................................ growth/damping rate
\( \Delta t \) ................................................ simulation time step
\( \Delta x \) ................................................ simulation grid spacing
\( \delta \Phi \) .................................................... electrostatic potential to correct the electric field
\( \epsilon_{EX} \) ................................................ dielectric for the explicit Particle-in-Cell method
\( \epsilon_{I} \) ................................................ dielectric for the implicit Particle-in-Cell method
\( \epsilon_{NK} \) ........ small value to calculate the directional derivative in the GMRes solver
\( \eta \) .................................. ratio of the electron thermal velocity and beam drift velocity
\( \theta \) .................................................. decentering parameter
\( \theta_s \) .................................................. bow angle
\( \Lambda_D \) ................................................. Debye length
\( \Pi \) .................................................. pressure tensor
\( \rho \) ..................................................... charge density
\( \rho_e \) .................................................. electron charge density
\( \rho_L \) .................................................. Larmor radius
\( \rho_0 \) .................................................. normalization value of the charge density
\( \Phi \) .................................................. electrostatic potential
\( \chi \) .................................................. electric susceptibility
\( \chi_N \) ........................................ numerical susceptibility
\( \omega_c \) ................................................................. cyclotron frequency
\( \omega_{cs} \) .......................................................... cyclotron frequency for a particle of species \( s \)
\( \omega_n \) ................................................................. neutralization frequency
\( \omega_{pe} \) ............................................................. plasma frequency
\( \omega_{pi} \) ............................................................. ion plasma frequency
\( \omega_{ps} \) ............................................................. plasma frequency for species \( s \)
Chapter 1

Introduction to Computer Simulation of Heavy Ion Beam-Plasma Interaction

Many technological applications of ion beams rely on the fact that ion beams can be easily transported over large distances, concentrated in very small spot size, and compressed in a short time period. Energy is transmitted to the beam by accelerators, and the beam size and shape are controlled by using magnetic and electric fields. Compressed small-spot-sized beams are capable of releasing a large amount of energy on very small surface, during a very short time interval. This capability of transporting high power densities makes the use of ion beam amenable for applications that require large deposition of energy on a small region over a very short time.

Although ion beams can effectively carry high power densities, their disadvantage is that repulsive forces among the beam particles, called space-charge forces, defocus the beam, resulting in an increase of the beam spot size and beam length, and in a degradation of the energy deposition on the target. In order to eliminate these defocusing forces, electrons can be introduced via a preformed plasma during the beam transport. Electrons are accelerated into the beam by the space-charge field
and the positive beam charge is reduced to zero: the electric fields, and the consequent repulsive forces, are eliminated. Thus, the ion beam neutralization process suppresses the expansion of the beam due to the repulsive forces. Often, the term *plasma focusing* is used to describe the effect of this neutralization process, but no net focusing happens in reality, instead only a reduction of the beam defocusing occurs. The effect of the beam neutralization is very important, and results in a considerable increase of beam current that can be transported in an accelerator. The beam would blow up if the neutralizing electrons are not present, and the beam propagation stops when the potential energy of the ion in the beam becomes comparable to the kinetic energy at the injection [1].

In experiments involving the transport of ion beams, the neutralization electrons are typically provided by means of a plasma reservoir along the beam transport line. The beam crosses a preformed plasma, and the electrons are trapped by the beam potential, and dragged by the propagating beam. Intuitively, the ion beam always captures the necessary number of electrons, if the background plasma has enough electrons. Any local charge imbalance in the beam would result in an electrostatic field, that would spread electrons in the beam to restore the beam neutrality. However, it has been found that the neutralization process is fairly complicated. Because of the electron inertia, more electrons than necessary for the beam neutralization, enter the beam, which may lead to continuous electron oscillations into and out of the beam, and to the neutralization being achieved only in the mean. On the other hand, there is experimental evidence [2] that complete neutralization is indeed achieved after the ion beam has drifted through the plasma, because the beam divergence does not increase during the beam propagation in the plasma. Computer simulations of the ion beam neutralization also [3] showed a complete beam neutralization. Thus, in a collision-less plasma some physical mechanism, other than collisions, should be present to terminate the oscillations, and enable the beam to neutralize completely.
Previous computer simulations were primarily focused on the proof of principle of the beam neutralization, rather than dedicated to the physical processes that accompany the neutralization process [3; 4]. On the contrary, this dissertation focuses primarily on the detailed study of the physical processes that lead to the beam neutralization. The neutralization dynamics has been analyzed in a simulation set-up, that mimics the NDCX configuration, varying the background plasma parameters and estimating the eventual magnetic field effect.

The chapter is organized as follows. Sections 1.1 and 1.2 present the use of ion beams for heavy ion fusion drivers, and for Warm Dense Matter experiments. The NDCX configuration, the properties of the plasma, and the time scale of the neutralization process in the NDCX are described in Section 1.3. The governing equations and their numerical solution are introduced in Sections 1.4 and 1.5. Section 1.6 concludes the chapter, presenting the scope of this thesis.

1.1 Heavy Ion Fusion

In 1975 Al Maschke from Brookhaven National Laboratory, proposed the use of heavy ion beams to produce nuclear fusion energy in the Inertial Confinement Fusion (ICF) configuration [5]. In this approach, a millimeter sized capsule, containing a Deuterium Tritium mixture, is hit and heated by a high energy, high current, ion beam. The resulting surface ablation of the capsule drives an internal compression of the Deuterium and Tritium, that triggers the nuclear fusion [5; 6].

Although the main ICF experiments in United States, such as the National Ignition Facility (NIF) experiment, use lasers, there are reasons to prefer ion beams instead of lasers [7]. First, heavy ion beams can provide a larger number (say, up to ten) of pulses per second, compared to a laser facility. In addition, ion beam drivers can currently guarantee an efficiency of 25-35%, while the efficiency for laser systems
A scheme of a nuclear power plant, using heavy ion beam, is shown in Figure 1.1. The future heavy ion fusion reactor will accelerate from 100 to 200 beams in parallel through a common set of induction cores. Beams will accelerate from an energy of 2 MeV to few GeV, over few kilometers of the accelerator [7]. At the end of the accelerator, the beam will be compressed longitudinally, shortening the pulse to 10 nano seconds. The beams would then proceed through a final focusing system, and transported to the target.

1.2 Warm Dense Matter Experiments

In addition to fusion, by heating a metallic foil heavy ion beams can also be used to study the phase transition from the solid to the plasma state. The metastable state of matter between plasma and solid is called Warm Dense Matter (WDM), and it is characterized by density typically of a solid, and temperature in the order of ten thousand Kelvins [8]. WDM comprises all those systems that are solid initially and upon heating become plasma. This state of matter is supposed to exist in the core of large planets, such as Jupiter, and it occurs in the first stages of inertial confinement
fusion and nuclear bomb explosions.

Because WDM is so rarely observed in nature, many thermodynamical properties, such as the phase diagrams and the critical points, are still not well known and need further investigations. WDM experiments require lower energy deposition on the target than those for the ICF fusion. The energy required in the WDM experiments is typically of the order of MeVs. Current experimental facilities using ion beams, such as the NDCX machine, can reach these energies, and hence they can host WDM experiments [8].

1.3 The Neutralized Drift Compression Experiment at Lawrence Berkeley Laboratory

The Neutralized Drift Compression Experiment (NDCX) at the Lawrence Berkeley Laboratory is a scaled reproduction of the future heavy fusion driver [7]. Although the experiment parameters are still far from the parameters needed to achieve nuclear fusion, the NDCX experiment comprises all the basic parts of the future heavy ion fusion driver, and it allows to study its basic working principles. In addition, the NDCX is currently being used for WDM experiments and to investigate the behavior of solid materials when hit by energetic ion beams.

The NDCX is a single beam experiment that accelerates, focuses, and neutralizes a beam of Potassium ions before hitting a target [2]. The current experimental set-up consists of four main parts: an injector, a focusing section composed of 4 solenoids, a compression drift section, and a final target chamber. Figure 1.2 shows the schematic diagram of the NDCX machine. The injector is composed of a Potassium ion source, and a diode that accelerates the beam to the energy of 300 keV, with a current of 5 mA. After the injector, four solenoids focus the beam radially. In the drift section, the beam is first compressed longitudinally to 10 nano seconds, by accelerating the
tail of the beam faster than the head, and then left to propagate in a 2.23 meters tube, filled with plasma, generated by the Ferroelectric Plasma Source (FEPS). The beam would disrupt in approximately ten centimeters [9], if it is not neutralized by the FEPS electrons. In the target chamber, the beam is focused again by a Final Focusing Solenoid (FFS), and neutralized a second time by a plasma, produced by the Filtered Cathodic-Arc Plasma Source (FCAPS).

### 1.3.1 Neutralization Plasma in the NDCX

The neutralization plasma is injected at two different stages of the NDCX: it is first injected after the longitudinal compression along a tube filled with plasma, and a second time by the FCAPS in the target chamber. This dissertation focuses on the simulation of the interaction of the ion beam with the FEPS plasma. The FEPS consists of a 2.23 meters long, and 8 cm diameter tube, filled with plasma. A Barium plasma is created from the inner surface of the tube by a pulsed electrode discharge. A ferroelectric material, Barium Titanate $BaTiO_3$, is placed between a back electrode,
Figure 1.3: a) A ferroelectric plasma source is 2.23 meters long, and it is composed of 5 sections, divided by diagnostic ports. b) An electrode with mesh structure, placed in the ferroelectric plasma source device. The two figures are from Reference [10].
and a front wire electrode, as shown in Figure 1.3 b). A bias of 5 kV is pulsed into the back electrode, operating at pressures near $10^{-5}$ Torr, producing a very large electric field in the gap between the two electrodes, where the $BaTiO_3$ is placed [10]. Because of the high electric field imposed, the $BaTiO_3$ ionizes between the two electrodes and the surface plasma is expelled from the wall to the center of the drift tube. A plasma density with values of $10^{10} - 10^{12}$ cm$^{-3}$ can be achieved using the FEPS. The life time of the FEPS plasma is 50 micro seconds. FEPS plasma is uniformly distributed inside the drift tube, and its thermal energies vary from 3 to 20 electron Volt [3; 10]. The main advantage of using FEPS, instead of other plasma sources, is that FEPS does not use a magnetic guide field for the injection of the plasma, like the FCAPS. The magnetic field generated by the plasma sources not only could influence the beam trajectory, but it would affect the neutralization process, changing the electron trajectories.

1.3.2 Time Scales in the NDCX Neutralization Process

The simulation of the beam neutralization process encompasses a large range of time scales. Because the electron to ion mass ratio of Barium and Potassium is approximately 1 to 250,000 an 1 to 72,000, the time scales of the particles species are largely separate. Figure 1.4 summarizes the multiple time scales, present in a typical plasma beam configuration in the NDCX experiment [2]. The fastest time scale is the electron plasma period ($2\pi/\omega_{pe}$): the plasma period is 60 pico seconds in the present configuration of the FEPS. The Barium background plasma frequency is 50 nano seconds, while the Potassium beam frequency is around half micro second. Although Potassium is a lighter element than Barium, its plasma period is shorter because the Barium plasma density is much higher than the Potassium beam density. The ion beam, because it is positively charged, creates a potential well, where the electrons would eventually oscillate. This electron trapping period depends on the beam den-
Figure 1.4: Time Scales in the NDCX experiment, calculated using the following parameters: background Barium plasma with density equal to $5 \cdot 10^{10} \text{ cm}^{-3}$, and 3 eV energy, 5 mA 300 keV $K^+$ beam.
sity only and it is around 3 nanosecond in the NDCX experiments. The time spent by
the beam in the FEPS plasma is few micro seconds, and the life time of the plasma in
the drift tube is 50 microseconds. The particle collision time scale is 8 microseconds:
collisions events are too rare to have an influence on the neutralization process, and
therefore the plasma can be considered collision-less. It has been found that the beam
neutralization occurs on the fast scale of the electron background plasma period and
of the beam potential trapping period. During this time interval, the neutralization
is influenced only by the electron dynamics, while the ions do not play a role, apart
from the drift movement that creates the field with which the electrons interact.

1.4 Governing Equations

There are primarily two approaches used to model the beam plasma interaction: the
fluid and the kinetic. The fluid approach describes the plasma in terms of the fluid
macroscopic properties such as the density, the current, and the pressure. The evo-
lation of these macroscopic properties is determined by solving the Magneto Hydro
Dynamics (MHD) equations. The MHD equations are the traditional fluid equations
with the electromagnetic forces described by the Maxwell’s equations. Although the
MHD approach has been very successful in modeling laboratory experiments [11; 12],
the description of an ion beam propagating in a plasma and in particular the neu-
tralization process, requires a more detailed description of the plasma. The kinetic
theory provides this more fundamental approach. The main difference between the
MHD and the kinetic approach in the context of NDCX is that the kinetic model
describes correctly the effects of the resonant interaction between a wave, and the
particles with velocities close to the wave phase velocity. These particle-wave reso-
nance interactions are very important in the neutralization process and they can not
be neglected in the modeling. In fact, the electrons non only have to spread out in
the beam during the neutralization process, but they also have to adjust their velocity to the average velocity of the beam. In the absence of collisions, such as in the NDCX configuration, this adjustment of the electrons velocity can occur only by wave particle interaction. For this reason, the neutralization process can be modeled correctly only by the kinetic methods.

The kinetic approach introduces a distribution function for the species \( s \), \( f_s(x, v, t) \), where the \( f_s dx dv \) can be interpreted as the probability of finding a particle of species \( s \) in the region of the phase space \( dx dv \) about the point \((x, v)\) at time \( t \). In a plasma, where the collisions can be neglected, the function \( f_s \) satisfies the Vlasov equation [13] (here and thereafter in CGS units):

\[
\frac{\partial f_s}{\partial t} + v \cdot \frac{\partial f_s}{\partial x} + q_s/m_s(E + \frac{v \times B}{c}) \cdot \frac{\partial f_s}{\partial v} = 0, \tag{1.1}
\]

where \( q_s \) and \( m_s \) are respectively the charge and the mass of the particles of the species \( s \), and \( c \) is the speed of light in vacuum. The electric field \( (E) \), and the magnetic field \( (B) \), can be determined by solving the Maxwell’s equations:

\[
\begin{cases}
\nabla \cdot E = 4\pi \rho \\
\nabla \cdot B = 0 \\
\n\nabla \times E = -\frac{1}{c} \frac{\partial B}{\partial t} \\
\n\nabla \times B = \frac{1}{c} \frac{\partial E}{\partial t} + 4\pi J,
\end{cases} \tag{1.2}
\]

where \( \rho \) and \( J \) are the charge and current densities, given by the moments of the distribution functions \( f_s \):

\[
\rho = \sum_s n_s q_s \int f_s dv \tag{1.3}
\]

\[
J = \sum_s n_s q_s \int v f_s dv. \tag{1.4}
\]
1.5 Numerical Solution of the Governing Equations

In this dissertation, the governing Equations 1.1, 1.2, 1.3, and 1.4 are solved numerically using the Particle-in-Cell (PIC) method. In the Particle-in-Cell method, Equation 1.1 is solved by introducing computational particles to represent the distribution function. The initial distribution function is randomly sampled by a large number of computational particles. The evolution of the distribution function is then determined by solving numerically the Newton’s equation of motion for the sampled computational particles:

\[
\begin{align*}
\frac{dx_p}{dt} &= v_p \\
\frac{dv_p}{dt} &= \frac{q_e}{m_e}(E + \frac{v_p}{c} \times B),
\end{align*}
\]

(1.5)

where \(x_p\) and \(v_p\) are respectively the particle position and velocity. The equivalence between Equation 1.1 and Equations 1.5 is derived heuristically in two textbooks [14; 15] and in a review paper [16], and mathematically by Chandrasekhar in [17] and Lapenta in [18]. At each time step, the Maxwell’s Equations 1.2 are solved on the grid points of a mesh, where the value of \(J\) and \(\rho\) have been calculated by interpolation from the particles positions and velocities.

In summary, the numerical solution of the governing equations consists of the solution of a system of two ordinary differential equations (ODE) for each computational particle, and of a set of partial differential equations (PDE) for the solution of the Maxwell’s equations on a grid. These set of ODEs and the PDEs can be differenced explicitly in time: the new values of \(x_p\), and \(v_p\), are determined using the old value of \(B\), and \(E\), and the new values of \(B\), and \(E\) are calculated using the old values of \(x_p\), and \(v_p\). However, results obtained using the explicit time differenced Particle-in-Cell scheme are numerically unstable for time steps approximately equal to the electron plasma period [14; 15]. For instance, a time step shorter than 60 pico seconds must
be used in modeling the NDCX with the explicit time differenced Particle-in-Cell scheme. A solution to the problem of short simulation time steps is to use an implicit time differenced Particle-in-Cell method. In this case, the new values of $x_p$ and $v_p$ are determined, using the new value of $B$ and $E$. The new values of $B$ and $E$ are calculated using the new values of $x_p$ and $v_p$. A direct solution of such a scheme, called fully implicit Particle-in-Cell method, has always been thought impossible because of the prohibitive computational cost and due to the belief that the numerical scheme would not be convergent [19]. Instead, approximate implicit time-differenced Particle-in-Cell methods were developed during the eighties [20; 21]. One of these approximate implicit Particle-in-Cell methods is the implicit moment Particle-in-Cell method. This technique is based on the extrapolation in time of the moments $\rho$ and $J$. The new values of the moments, are calculated by extrapolation, and plugged into the Maxwell’s equation to calculate the new value of $B$ and $E$. Once the new value of $B$ and $E$ are known, they can be used to calculate the new value of $x_p$ and $v_p$. This implicit moment Particle-in-Cell method is unconditionally stable, and it enables simulation with time steps, typically 10 to 20 times larger than the time step of the explicit Particle-in-Cell method [21].

In this dissertation, the implicit moment Particle-in-Cell method has been used to simulate the neutralization process in the NDCX configuration. Furthermore preliminary work toward the development and implementation of the fully implicit Particle-in-Cell method has been carried out.

1.6 Scope of this Thesis

The scope of this thesis is the computer simulation of the beam-plasma interaction in the NDCX configuration. An implicit moment Particle-in-cell method has been developed and implemented for this purpose. The implicit moment Particle-in-Cell
code is three dimensional and includes the capability to simulate both electric and magnetic fields. This code has been first verified by comparing the simulation results against analytical results of a series of benchmark tests, and then applied to the study of ion beam plasma interaction in the NDCX configuration. The focus of these simulations was to understand the dynamics of the neutralization process in detail. The effects of different plasma background densities, and of the magnetic field have been studied. In addition, preliminary work has been carried out to develop a fully implicit Particle-in-Cell method. This effort has resulted in the development of a simple one dimensional electrostatic code. This code is also verified and results presented. Finally the advantages and the computational cost of the implicit Particle-in-Cell methods to study NDCX have been evaluated.

In summary, the main questions that this dissertation addresses, are:

1. What is the dynamics of the neutralization process? Is it a transient phenomenon? Does it reach a steady state?

2. What are the effects of different background plasma densities?

3. What is the effect of the magnetic field? Does it have an effect on the neutralization dynamics?

4. Is it possible to develop a fully implicit Particle-in-Cell method? Does it converge? If so, what is its computational cost?

5. Is it feasible to use the implicit Particle-in-Cell methods to study the neutralization process in the NDCX configuration?

This dissertation is organized as follows. Chapter 2 presents a review of the computational methods used for the beam plasma interaction simulations, and a survey of the previous simulations of the beam neutralization. In addition, Chapter 2 introduces the Particle-in-Cell method and its numerical stability analysis.
numerical algorithms and the software implementation of the implicit Particle-in-Cell methods (implicit moment and fully implicit Particle-in-Cell) are discussed in Chapter 3. A series of tests to verify different components of the code, and the computational performance of the implicit moment Particle-in-Cell follow in Chapter 4. The simulation set-up to mimic the NDCX, the beam and plasma configuration and the simulation diagnostics, are shown in Chapter 5. Chapters 6 presents the results of two and three dimensional simulations. These results are discussed in Chapter 7. The focus of this chapter is to investigate the neutralization dynamics, and to evaluate the effects of different background plasma configurations, and of the magnetic field. The development of a one dimensional electrostatic fully implicit Particle-in-Cell method, its verification against two test problems, and its computational performances are presented in Chapter 8. Finally, Chapter 9 concludes this dissertation by discussing the advantages of the implicit Particle-in-Cell methods, applied to the simulation of beam neutralization in the NDCX configuration.
Chapter 2

Literature Survey and Theoretical Background

The goal of this chapter is to give an overview of the computational methods for the ion beam neutralization model, and to present the previous studies on modeling the ion beam propagation in a background plasma. Moreover, this chapter introduces the Particle-in-Cell method, and its numerical stability analysis using the numerical dispersion relations.

Section 2.1 reviews different computational techniques are used for modeling plasma beam interaction, and the previous studies on simulation of the ion beam neutralization. The Particle-in-Cell method, and its implicit formulation are presented in Sections 2.2 and 2.3. The numerical dispersion relations of the explicit and implicit Particle-in-Cell methods are presented in order to study the stability of the numerical methods.
2.1 Computer Simulations of the Ion Beam Neutralization

Various numerical techniques have been developed to solve the governing equations, introduced in Chapter 1. They fall in two broad categories: the direct solution of Vlasov equation approach, and the Particle-in-Cell methods [22]. The direct solution of the Vlasov equation approach includes, the Fourier-Fourier method, the Fourier-Hermite transform method [23], and the finite difference method [24]. In the Fourier-Fourier method, the Vlasov equation is first decomposed in Fourier components in \( x \); then the equation is Fourier transformed in the velocity space, and solved by the method of characteristics [23]. The Fourier-Hermite method consists of representing the distribution function \( f_s \) as a Fourier series in \( x \), and then as a Gram-Charlier series in the velocity [23]. A set of ordinary differential equations can be obtained, when the series representation of the distribution function is substituted in the Vlasov equation. This set of ordinary differential equation can be solved numerically. The finite difference solution of the Vlasov equation is the most straightforward method. It consists of using a difference scheme with rectangular mesh in the phase space \((x, v)\). In general, the direct numerical solutions of the Vlasov equation, are limited to one and two dimensional problems because of the high computational cost. In fact, a three dimensional problem would require a six dimensional grid in the phase space, and it consequently has very high computational and memory cost.

The Particle-in-Cell method can be used to simulate the evolution of the distribution function in many problems that the direct methods can not solve. The Particle-in-Cell scheme uses computational particles to sample the initial distribution function, and moves the particle by the Newton’s equation of motion to follow the evolution of the distribution function [14; 15]. Because the number of the computational particles is in practice just a small fraction of the number of the real particles in the
system, the reconstruction of the distribution function is statistically noisy. A number of numerical techniques have been studied to address this problem. For instance in the Particle-in-Cell method developed for this dissertation, the computational particles have different statistical weights to provide a good statistical description of the tails of the distribution function [16]. Other variance reduction techniques to reduce the statistical noise of the Particle-in-Cell method, include the δ-f PIC [25], and the semi-Lagrangian method [26].

The implicit Particle-in-Cell method is the simulation tool used in this dissertation for the simulation of the neutralization process. However, the implicit Particle-in-Cell techniques are not the only methods that allow large simulation time steps. For instance, it is possible to solve the reduced Darwin model, removing the light waves from the system [22; 27]. Another approach, called a hybrid because it models the electrons as a fluid, thus eliminating the electron oscillations, and the ions as kinetic particles [22]. It must be emphasized that both the Darwin and hybrid methods are reduced methods, because they completely remove part of the physics from the model being simulated. The implicit moment Particle-in-Cell method instead retains all the physics, and thus it is called a fully kinetic model [22].

Implicit methods were first introduced in the solution of the field equations of the Particle-in-Cell simulation by Nielson and Lindman in 1974 [28]. However it was only later that both the particle and field equations were implicitly solved together. Two techniques were developed for the solution of the implicit Particle-in-Cell method: the implicit direct, and the implicit moment Particle-in-Cell methods. The implicit direct method, developed by Friedman and colleagues in 1981 [29], extrapolates the future particle positions along the unperturbed orbits to estimate the future values of the field sources. The implicit moment method, developed by Mason in 1981 [30], used the fluid equations instead. The fluid equations, used in the first formulation of the implicit moment method, were then replaced by extrapolation equations to avoid
the use of equation of state to close the fluid equations [21], leading to a numerical scheme very similar to the implicit direct Particle-in-Cell method. In fact, as stated by Langdon and Barnes in reference [14]: *as moment and direct codes are borrowing features from each other, the distinction becomes more one of viewpoint in deriving algorithms and less in the resulting codes themselves.*

The first Particle-in-Cell simulations of the ion beam neutralization were completed in the mid-sixties [31–33]. The goal of these simulations was to prove the neutralization of Xenon beams to be used for the space propulsion. It was found that the electron oscillations due to the neutralization process are present in the initial stages of the transient, and that the full beam neutralization is achieved. It was suggested that self-excited fields at the electron plasma frequency would eventually dampen these oscillations. After the Heavy Ion Fusion concept was proposed in 1975 [5], the first Particle-in-Cell simulations of the beam neutralization in heavy ion fusion drivers were completed by Humphries et al. [4], and Sudan [34]. Recently, Particle-in-Cell simulations have also been carried out for the NDCX configuration [3]. The paper by Sefkow et al. presents neutralization of the ion beam by both FEPS and FCAPS plasma with realistic parameters [3]. The goal of these studies, was to show that full beam neutralization can be achieved in the NDCX, without studying in detail the physics of the neutralization process.

### 2.2 The Particle-in-Cell Method

The Particle-in-Cell approach is becoming the most commonly used numerical method for the solution of the governing equations, presented in Chapter 1. This is so, because of its capacity to deal with three dimensional configuration and its implementation simplicity [14; 15]. In the Particle-in-Cell method, the distribution function of each plasma species $s$ of Equation 1.1, is described as a collection of $N_s$ computational
particles with label \( p \). The computational particles represent small elements of the phase space with a finite size and a localized velocity. Each computational particle is characterized by a fixed shape function \( S \), and by two parameters: the computational particle position \( x_p \) and velocity \( v_p \). Thus the distribution function \( f_s \) can be written as:

\[
f_s(x, v, t) = \sum_{p=1}^{N_s} S(x - x_p)S(y - y_p)S(z - z_p)\delta(v - v_p),
\]

where \( \delta \) is the Dirac’s delta. The shape function \( S \) is symmetric, and has a unitary integral by definition. It is typically chosen as a b-spline function of order \( \ell \) in each direction [35]. If \( \Delta x \) is the grid spacing in the \( x \) direction, the shape function is defined as \( S(x - x_p) = b_\ell((x - x_p)/\Delta x) \), and similarly in the other directions. The choice of the first order b-splines as shape functions, leads to the so-called Cloud-in-Cell (CIC) Particle-in-Cell scheme [15]. Because of the linearity of Equation 2.1, the evolution of each superparticle \( p \) is described by the Vlasov equation also. Substituting Equation 2.1 in the Vlasov Equation 1.1, the equations for the evolution of the computational particles positions and velocities, \( x_p \) and \( v_p \), are derived:

\[
\begin{align*}
\frac{dx_p}{dt} &= v_p \\
\frac{dv_p}{dt} &= \frac{q_s}{m_s} \left( E_p + \frac{v_p \times B_p}{c} \right)
\end{align*}
\]

These equations of motion are simple ODEs. There are many algorithms to solve such equations in literature [36; 37]. These equations of motion can be solved using explicit or implicit methods. An explicit particle mover expresses directly the new position and velocity using values known from the previous time step, without requiring any iteration for the solution. A commonly used ODE solver is the leap-frog algorithm, known in the Molecular Dynamics (MD) community as the Verlet algorithm [37].

The average electric and magnetic fields acting on a computational particle, \( E_p \) and \( B_p \) in Equation 2.2, are defined as the integral of the the shape function, and of
the electromagnetic field over the computational domain \( V \),

\[
E_p = \int_V E(x) S(x - x_p) \, dx \quad B_p = \int_V B(x) S(x - x_p) \, dx.
\] (2.3)

Another important characteristic of the Particle-in-Cell algorithm is the use of a grid to solve the Maxwell’s equations. The Maxwell’s equations are solved on a grid. The interpolation functions \( W(x_g - x_p) \) are introduced to carry the information between the particles and the grid:

\[
W(x - x_p) = \int_{-\infty}^{\infty} S(x - x_p) b_0 \left( \frac{x - x_p}{\Delta x} \right) \, dx = b_1(x - x_p)/\Delta x,
\] (2.4)

where the general property of the b-splines \( b_{l+1}(\xi) = \int b_l(\xi')b_0(\xi - \xi')d\xi' \) is used [35]. The electric and magnetic fields acting on the particles of Equation 2.3, can be expressed more conveniently with the use of the interpolation functions, as:

\[
E_p = \sum_g E_g W(x - x_p) \quad B_p = \sum_g B_g W(x - x_p),
\] (2.5)

where the cells are labelled with a single index \( g \), and the field values in each cell are \( E_g \) and \( B_g \). In addition, the moments of the distribution function, \( \rho^n_g, J^n_g \) and \( \Pi^n_g \) (the pressure tensor), can be obtained easily by iterating over the \( N_s \) particles of the \( n_s \) species:

\[
\{ \rho^n, J^n, \Pi^n \}_g = \sum_s \sum_p N_s q_s \{ 1, v^n_p, v^n_p v^n_p \} W(x - x^n_p)
\] (2.6)

Once the field sources are known by interpolation, the Maxwell’s equations can be solved:

\[
\begin{aligned}
\nabla \times E &= -\frac{1}{c} \frac{\partial B}{\partial t} \\
\nabla \times B &= \frac{1}{c} \frac{\partial E}{\partial t} + \frac{4\pi}{c} J.
\end{aligned}
\] (2.7)

Many numerical techniques have been developed to discretize and solve Equations 2.7 on the grid. They include the Predictor-Corrector methods (Upwind method, Leapfrog scheme, Lax-Wendroff scheme), the implicit method, and the operator splitting method [22].
In addition to Equations 2.7, there are other two Maxwell’s equations that must be satisfied as well:

\[
\begin{aligned}
\nabla \cdot E &= 4\pi \rho \\
\nabla \cdot B &= 0.
\end{aligned}
\] (2.8)

It is easy to show that, if the divergence of \( E \) and \( B \) are initialized correctly at the beginning of the simulation, then they remain correct over time [14]. In fact, for the \( \nabla \cdot B \):

\[
\frac{\partial (\nabla \cdot B)}{\partial t} = \nabla \cdot (\frac{\partial B}{\partial t}) = -c \nabla \cdot \nabla \times E = 0.
\] (2.9)

For the \( \nabla \cdot E \):

\[
\frac{\partial (\nabla \cdot E - 4\pi \rho)}{\partial t} = -4\pi(\frac{\partial \rho}{\partial t} + \nabla \cdot J) = 0.
\] (2.10)

Thus, if \( \rho \) and \( J \) satisfy the continuity equation for the charge density \( \frac{\partial \rho}{\partial t} + \nabla \cdot J = 0 \), then the Gauss’ law will be satisfied, if it is initially. However, there are microscopic inconsistencies between \( \rho \) and \( J \), and the continuity equation is not exactly satisfied in the Particle-in-Cell methods, because of the use of the interpolation function and of the grid [14]. A remedy to this problem have been developed by Boris in 1970 [38], and it is widely in use in the majority of the Particle-in-Cell methods [14]. In this approach, the electric field \( E \) is first calculated using the Equation 2.7 with the uncorrected \( J \), and then corrected by \( \nabla \delta \Phi \):

\[
E' = E - \nabla \delta \Phi,
\] (2.11)

such that

\[
\nabla \cdot E' = 4\pi \rho.
\] (2.12)

This requires:

\[
\nabla \cdot (E - \nabla \delta \Phi) = 4\pi \rho,
\] (2.13)

and a Poisson solution for \( \delta \Phi \):

\[
\nabla^2 \delta \Phi = \nabla \cdot E - 4\pi \rho.
\] (2.14)
In summary, Figure 2.1 represents the four steps to solve numerically the Vlasov-Maxwell system. The equations of motion, Equations 2.2, are solved to advance the computational particles positions and velocities. The moments are then calculated by interpolation from the new computational particles position and velocity, using Equation 2.6. The Maxwell’s equations 2.7 are solved on the grid and then the electric field is corrected by Equation 2.11. Finally the electromagnetic fields acting on the particle are obtained from Equation 2.5 by interpolation.

2.2.1 Numerical Dispersion Relation of the Explicit Particle-in-Cell Method

The linear numerical stability analysis of the Particle-in-Cell method is carried by studying the numerical dispersion relation of the plasma [19; 39]. In many applications, the plasma can be treated as a conducting medium, characterized by an electric susceptibility and by a dielectric permittivity. It is possible to calculate the susceptibility $\chi$ of this plasma using the Vlasov theory in the case of a one dimen-
sional un-magnetized plasma with fixed background ions, and equilibrium distribution function $f_0(v)$ \[11\]:

$$\chi = \left(\frac{\omega_{pe}}{k}\right)^2 \int_{-\infty}^{+\infty} \mathbf{k} \cdot \frac{\partial f_0(v)}{\partial v} \frac{1}{\omega - \mathbf{k} \cdot v} dv,$$ \hspace{1cm} (2.15)

and the dielectric permittivity $\epsilon$ of the plasma given by

$$\epsilon(k,\omega) = 1 + \chi = 1 + \left(\frac{\omega_{pe}}{k}\right)^2 \int_{-\infty}^{+\infty} \mathbf{k} \cdot \frac{\partial f_0(v)}{\partial v} \frac{1}{\omega - \mathbf{k} \cdot v} dv. \hspace{1cm} (2.16)$$

The susceptibility $\chi$ measures the ability of the plasma to shield external charges. The equation for the zeros of the dielectric permittivity is called the dispersion relation, and it gives the frequency $\omega$ of a plasma wave as a function of the wave number $k$ and vice versa. The dispersion relation determines the rate at which different Fourier components of the wave disperse due to the variation of the phase velocity with the wave number.

The numerical discretization of the governing equations causes non physical dispersion of the waves present in the system. For instance, the numerical discretization can lead to nonphysical results, such as broadening of pulsed waveforms, spurious scattered waves and pseudo-refraction [40]. Moreover the numerical dispersion relation can reveal the presence of spurious modes that can grow uncontrolled, leading to numerical instability.

The numerical dispersion relation of the explicit Particle-in-Cell method is calculated from the particle equation, using the approach suggested by Langdon [19]. The particle equation of motion is linearized, and the electric field is assumed to have a $\exp(i\omega t)$ dependence. The linearized equation of motion is Fourier transformed in $x$, and the perturbed charge density is calculated. From the definition of charge density, the dispersion relation can be calculated as:

$$\epsilon_E(k,\omega) = 1 - \left(\frac{\omega_{pe}\Delta t}{2}\right)^2 \int_{-\infty}^{+\infty} \frac{f_0(v)}{\sin^2((\omega - \mathbf{k} \cdot v)\frac{\Delta t}{2})} dv. \hspace{1cm} (2.17)$$
It is obtained by integration by parts, with \( f_0(\pm \infty) = 0 \):

\[
\int_{-\infty}^{+\infty} \frac{\partial f_0(v)}{\partial v} \cot((\omega - k \cdot v)\frac{\Delta t}{2})dv = -\int_{-\infty}^{+\infty} k \frac{f_0(v)\frac{\Delta t}{2}}{\sin^2((\omega - k \cdot v)\frac{\Delta t}{2})}dv.
\]

(2.18)

If Equation 2.18 is substituted in Equation 2.17:

\[
\epsilon_E(k, \omega) = 1 + \left(\frac{\omega_{pe}}{k}\right)^2 \int_{-\infty}^{+\infty} k \cdot \frac{\partial f_0(v)}{\partial v} \frac{\Delta t}{2} \cot((\omega - k \cdot v)\frac{\Delta t}{2})dv.
\]

(2.19)

Although at first glance Equation 2.16 and Equation 2.19 have little resemblance, the two equations are identical in the limit as \( \Delta t \) approaches zero (for \( \Delta t \to 0 \), \( \cot(z) \approx 1/z \)).

In the case of a cold plasma with distribution \( f_0(v) = \delta(v) \), the dispersion relation reduces to:

\[
\sin^2\left(\frac{\omega\Delta t}{2}\right) = \left(\frac{\omega_{pe}\Delta t}{2}\right)^2.
\]

(2.20)

If \( \omega_{pe}\Delta t < 2 \), the roots are real and the equation is numerically stable. The roots are complex when \( \omega_{pe}\Delta t > 2 \), and the equation is unstable. If the \( f_0(v) \) is a Maxwellian distribution, a similar analysis can be carried out, leading to the instability condition, \( \omega_{pe}\Delta t > 1.62 \) [19].

### 2.3 The Implicit Particle-in-Cell Methods

As stated in Chapter 1, the implicit Particle-in-Cell method has been introduced to eliminate the numerical stability constraints of the explicit Particle-in-Cell method. The numerical solution of the equations of the implicit Particle-in-Cell method is not an easy task. The difficulty arises because the new electric and magnetic fields depend on the new values of the particle position and velocities, and vice-versa the computational particles position and the velocity depend on the new electromagnetic field through the particle equations of motion. The fully implicit method requires iterations over these equations (particles equations of motions and Maxwell’s equation).
The considerable computational cost and the large memory requirements, pushed toward the development of the approximate implicit Particle-in-Cell methods.

Approximate implicit Particle-in-Cell methods are based on decoupling the particle and field equations of the fully implicit approach. Here, the field equations are solved first to estimate the field sources at the future time level. Once the new (next time step) values of the electromagnetic fields are known, the particles are advanced, using the new values of the electromagnetic field in the mover as follows:

\[
\frac{x_{p}^{n+1} - x_{p}^{n}}{\Delta t} = \bar{v}
\]

\[
\frac{v_{p}^{n+1} - v_{p}^{n}}{\Delta t} = \frac{q_{s}}{m_{s}}(E_{p}^{n+\theta}(\bar{x}) + \bar{v} \times B_{p}^{n}(\bar{x})/c)
\]

where \(\bar{v}\) is the particle average velocity, defined as \((v_{p}^{n} + v_{p}^{n+1})/2\), \(\theta\) is the de-centering parameter (it is chosen between zero and one), and \(E_{p}^{n+\theta}\) is an intermediate value of the electric field given by the interpolation: \(E_{p}^{\theta} = \theta E_{p}^{n+1} + (1 - \theta)E_{p}^{n}\). Both \(E_{p}^{n+\theta}\) and \(B_{p}^{n}\) are evaluated at \(\bar{x} = (x_{p}^{n} + x_{p}^{n+1})/2\).

Approximate formulations of the implicit Particle-in-Cell scheme, such as the implicit moment Particle-in-Cell method, rely primarily on the fact that it is possible to estimate the field source values, at the future time level using either the fluid equations or the linearization of the particle equation of motion. The estimated values of the sources are first calculated and then plugged in the implicit Maxwell solver. This step leads to additional terms in the set of field equations. In the current formulation of the implicit moment method, the future values of the charge and current densities are calculated by extrapolation: the charge and current density values are extrapolated using a Taylor expansion of the interpolation function \(W(x - x_{p}^{n+1})\) [41; 42]. The Taylor expansion is carried out around the particle position at the previous time.
step \( x_p^n \), and truncated at the second order in \( \Delta t \):

\[
W(x - x_p^{n+1}) \approx W(x - x_p^n) + (x_p^n - x_p^{n+1}) \cdot \nabla W(x - x_p^n) + \frac{1}{2}(x_p^n - x_p^{n+1})(x_p^n - x_p^{n+1}) \cdot \nabla \nabla W(x - x_p^n) + \ldots \tag{2.23}
\]

\[
= W(x - x_p^n) - \bar{v} \nabla W(x - x_p^n) \Delta t + \frac{1}{2} \bar{v} \cdot \bar{v} : \nabla \nabla W(x - x_p^n) (\Delta t)^2 + \ldots, \tag{2.24}
\]

where the common tensor notation is used. Different expressions can be used for \( \bar{v} \), and lead to slight variation in the final numerical scheme. The expression for \( \bar{v} \) depends typically on the numerical scheme and on the phenomenon over which the dynamics is intended to be averaged. In general, the value of \( \bar{v} \) will depend on the value of \( E_p^{n+\theta} \). Thus \( \bar{v} \) will be expressed in function of \( E_p^{n+\theta} \) and plugged into the Maxwell solver, thus changing the structure of the equation. Details are given in Chapter 3.

### 2.3.1 Numerical Dispersion Relation of the Implicit Particle-in-Cell Method

The same calculations, used to evaluate the dispersion relation of the explicit Particle-in-Cell method, can be applied to the implicit Particle-in-Cell method. Brackbill and Forslund derived the dispersion relation for the implicit Particle-in-Cell methods [21]:

\[
\epsilon_f(k, \omega) = 1 - e^{i(\theta - 1/2) \Delta t} \left( \frac{\omega_{pe} \Delta t}{2} \right)^2 \int_{-\infty}^{+\infty} f_0(v) \frac{\cos((\omega - k \cdot v) \frac{\Delta t}{2})}{\sin^2((\omega - k \cdot v) \frac{\Delta t}{2})} dv. \tag{2.27}
\]

Equations 2.27 and 2.17 are similar, but for the exponential factor before the integral. This factor leads to increased stability of the implicit Particle-in-Cell schemes. In the case of cold plasma with \( f_0(v) = \delta(v) \) and \( \theta = 0.5 \), the dispersion relation reduces to:

\[
\tan\left( \frac{\omega \Delta t}{2} \right) \sin\left( \frac{\omega \Delta t}{2} \right) = \left( \frac{\omega_{pe} \Delta t}{2} \right)^2. \tag{2.28}
\]

The roots of the Equations 2.28 and 2.20 are the same for small time steps \( \Delta t \). However, the roots of the dispersion relation are always real and they lay in the
interval $0 < \omega \Delta t < \pi$ when the time step is large. When $\theta$ is different from 0.5, the solutions of the dispersion relations are complex: when $\theta < 0.5$ the imaginary part corresponds to a growing exponential, and the scheme is always unstable. The solution corresponds to a decaying exponential, when $\theta > 0.5$. Thus, the implicit Particle-in-Cell method is unconditionally linearly stable for $0.5 \leq \theta \leq 1.0$.

### 2.3.2 Convergence Condition of the Implicit Particle-in-Cell Method

It has been shown that the implicit Particle-in-Cell numerical scheme is linearly unconditionally stable for $0.5 \leq \theta \leq 1.0$. However, a convergence condition for the implicit Particle-in-Cell methods arises from the convergence condition of the Taylor expansion of Equation 2.23. The implicit method gives an accurate estimate of the future sources when the series of Equation 2.23 converges, that is when the electron thermal displacement per time step is smaller than the grid spacing. This results in a modified Courant-Friedrichs-Lewy condition for the implicit Particle-in-Cell method[21]:

$$v_{the} \frac{\Delta t}{\Delta x} = \Lambda_D \omega_{pe} \frac{\Delta t}{\Delta x} < 1.$$  \hspace{2cm} (2.29)

It is important to note that this inequality can be satisfied with large time steps even when the grid spacing is large compared to the Debye length $\Lambda_D$. 

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Chapter 3

Methodology and Development of Implicit Particle-in-Cell Methods

This chapter is divided into two main parts. The first part of the chapter describes the implicit moment Particle-in-Cell method in detail, in Section 3.1. Here, the expression for the particle average velocity, the implicit differenced equations for the Maxwell’s solver, and the implicit mover, are derived. Moreover, the details of the temporal and spatial differentiation, the linear solvers used, and the code implementation are provided. Section 3.2 presents the development of the fully implicit method for the one dimensional electrostatic configuration. The reduced governing equations of the problem, the differentiation scheme, and the implementation using the Newton-Krylov Jacobian-Free Matrix-Free GMRes method are presented.

Two simulation codes have been developed. First is a three dimensional electromagnetic implicit moment Particle-in-Cell code. Second is a fully implicit Particle-in-Cell code in a electrostatic, one dimensional skeleton version. The implicit moment code, with full simulation capabilities, has been used to study the ion beam neutralization dynamics in realistic NDCX configurations. The fully implicit Particle-in-Cell code has been developed for simple one dimensional configurations, to prove that the fully implicit Particle-in-Cell method can be implemented, and that the numerical
scheme converges, and to study its performance.

### 3.1 The Implicit Moment Particle-in-Cell Method

As introduced in Chapter 2, the implicit moment Particle-in-Cell method is based on the estimate of the future value of the field sources. These estimates are calculated by a Taylor expansion of the interpolation functions, $W$, around the particle position at the previous time step. The Taylor expansion requires a value for $\bar{v}$, the particle average velocity. Different implicit moment Particle-in-Cell formulations differ based on the method of calculating $\bar{v}$. The formulation used in this dissertation is based on the derivation of $\bar{v}$ from the time differenced equation of motion (other approaches are possible: for instance, Brackbill and Forslund derive different expression of $\bar{v}$ for configurations with strong magnetic field and with collisions [21]).

#### 3.1.1 Particle Average Velocity

The particle average velocity, $\bar{v}$, is defined as:

$$ \bar{v} = \frac{v_{p}^{n+1} + v_{p}^{n}}{2} \quad (3.1) $$

Using the equations of motion:

$$ x_{p}^{n+1} = x_{p}^{n} + \bar{v} \Delta t \quad (3.2) $$

$$ v_{p}^{n+1} = v_{p}^{n} + \frac{q_{s} \Delta t}{m_{s}} (E_{p}^{n+\theta} + \frac{\bar{v} \times B_{p}^{n}}{c}) \quad (3.3) $$

$\bar{v}$ can be expressed:

$$ \bar{v} = v_{p}^{n} + \frac{q_{s} \Delta t}{2m_{s}} (E_{p}^{n+\theta} + \frac{\bar{v} \times B_{p}^{n}}{c}), \quad (3.4) $$
\[ \vec{v} \times \mathbf{B}_p^n = \mathbf{v}_p^n \times \mathbf{B}_p^n + \frac{q_s \Delta t}{2m_s} (\mathbf{E}_p^{n+\theta} \times \mathbf{B}_p^n + (\frac{\vec{v} \times \mathbf{B}_p^n}{c}) \times \mathbf{B}_p^n) \]
\[ = \mathbf{v}_p^n \times \mathbf{B}_p^n + \frac{q_s \Delta t}{2m_s} (\mathbf{E}_p^{n+\theta} \times \mathbf{B}_p^n + (\frac{\vec{v} \cdot \mathbf{B}_p^n}{c}) \mathbf{B}_p^n - \frac{\mathbf{B}_p^n}{c}) \]
\[ = \mathbf{v}_p^n \times \mathbf{B}_p^n + \frac{q_s \Delta t}{2m_s} (\mathbf{E}_p^{n+\theta} \times \mathbf{B}_p^n + (\frac{\mathbf{v} \cdot \mathbf{B}_p^n}{c}) \mathbf{B}_p^n + \frac{q_s \Delta t}{2m_s} (\mathbf{E}_p^{n+\theta} \cdot \mathbf{B}_p^n) \mathbf{B}_p^n - \frac{\mathbf{B}_p^n}{c}), \]

(3.5)

where

\[ \vec{v} \cdot \mathbf{B}_p^n = \mathbf{v}_p^n \cdot \mathbf{B}_p^n + \frac{q_s \Delta t}{2m_s} \mathbf{E}_p^{n+\theta} \cdot \mathbf{B}_p^n. \]

(3.6)

Inserting Equation 3.5 in Equation 3.6, it is obtained:

\[ \vec{v} = \mathbf{v}_p^n + \frac{q_s \Delta t}{2m_s} \mathbf{E}_p E_{n+\theta} + \frac{q_s \Delta t}{2m_s} \mathbf{B}_p + \frac{q_s \Delta t}{2m_s} (\mathbf{E}_p \cdot \mathbf{B}_p) \mathbf{B}_p^n - \frac{\mathbf{B}_p^n}{c}), \]

(3.7)

that can be rearranged as

\[ \vec{v} = \mathbf{v}_p^n + \frac{q_s \Delta t}{2m_s} \mathbf{E}_p E_{n+\theta} \]

(3.8)

\[ \vec{v} = \frac{\vec{v} + q_s \Delta t}{2m_s} \mathbf{B}_p + \frac{q_s \Delta t}{2m_s} (\vec{v} \cdot \mathbf{B}_p) \mathbf{B}_p^n - \frac{\mathbf{B}_p^n}{c}), \]

(3.9)

Equation 3.9 provides the value of the particle average velocity for the implicit moment Particle-in-Cell method, used in this dissertation.

### 3.1.2 Time Differentiation of the Maxwell Solver

A second order differentiation of the Maxwell’s equations has been used in this work. In fact, the first order Maxwell’s system can be decomposed into two decoupled second order equations, one involving \( \mathbf{E} \), and one involving \( \mathbf{B} \), by using the div-curl method [43]. The Maxwell’s equation for the electric field in the second order formulation is written as:

\[ \nabla^2 \mathbf{E} - \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = \frac{4\pi}{c^2} \frac{\partial \mathbf{J}}{\partial t} + 4\pi \nabla \rho. \]

(3.10)
A similar second order equation can be derived for $B$, but once the electric field is known, the magnetic field $B$ can be derived simply from the Faraday’s law of induction:

$$\frac{\partial B}{\partial t} = -c\nabla \times E.$$  \hfill (3.11)

The two second order Maxwell’s equations provide a solution that also satisfies the two divergence equations of the first order formulation ($\nabla \cdot E = -4\pi \rho$, $\nabla \cdot B = 0$) at all times, if appropriate initial and boundary conditions are used [43]. Equation 3.10 is time differenced as follows:

$$E^{n+\theta} - (c\Delta t)^2 \nabla^2 E^{n+\theta} = E^n + c\Delta t(\nabla \times B^n - \frac{4\pi}{c} J^{n+1/2}) - (c\Delta t)^2 \nabla 4\pi \rho^{n+1}. \hfill (3.12)$$

The Maxwell’s equation source terms $\rho$ and $J$ are evaluated at the future time level: $\rho$ is evaluated at time level $n + 1$, while $J$ is calculated at time level $n + 1/2$ to consistently satisfy the Ampere’s law [21]. The value of $E^{n+\theta}$ is calculated by solving Equation 3.12, and then the electric field $E^{n+1}$ is evaluated by using the extrapolation:

$$E^{n+1} = \frac{1}{\theta} E^{n+\theta} - \frac{1 - \theta}{\theta} E^n. \hfill (3.13)$$

Once $E^{n+1}$ is known, the magnetic field is advanced in time by differencing in time the Faraday’s law (Equation 3.11):

$$B^{n+1} = B^n - c\Delta t \nabla \times E^{n+1}. \hfill (3.14)$$

The method of evaluating the implicit quantities, $\rho^{n+1}$ and $J^{n+1/2}$ for Equation 3.12, constitutes the key of the implicit moment method. The charge and current density values are extrapolated using a Taylor expansion and expressed in terms of the present and (unknown) future electromagnetic fields. The values of $\rho^{n+1}$ and $J^{n+1/2}$ are calculated using Equation 2.23 truncated at the second order in $\Delta t$, and the value of $\bar{v}$ calculated in Equation 3.9:

$$\rho^{n+1} \approx \sum_s \sum_p q_s(W(x-x_p^n) - \bar{v} \nabla W(x-x_p^n) \Delta t + \frac{1}{2} \bar{v} \bar{v} : \nabla \nabla W(x-x_p^n)(\Delta t)^2). \hfill (3.15)$$
This results in:

\[ \rho^{n+1} \approx \rho^{n} - \Delta t \nabla \cdot \mathbf{J}^{n+1/2}. \] (3.16)

\( \mathbf{J}^{n+1/2} \) is obtained in the same way:

\[ \mathbf{J}^{n+1/2} \approx \frac{1}{2} \mathbf{J}^{n} + \frac{1}{2} \sum_{s} \sum_{p} q_s \tilde{\mathbf{v}}(\mathbf{W}(\mathbf{x} - \mathbf{x}_p^{n}) - \tilde{\mathbf{v}} \Delta t \nabla \mathbf{W}(\mathbf{x} - \mathbf{x}_p^{n}) + ...), \] (3.17)

\[ \mathbf{J}^{n+1/2} \approx \hat{\mathbf{J}} - \frac{1}{4\pi} \mathbf{E}^{n+\theta} - \frac{\Delta t}{2} \nabla \cdot \hat{\mathbf{N}}, \] (3.18)

where \( \hat{\mathbf{J}} \) and \( \hat{\mathbf{N}} \) use \( \tilde{\mathbf{v}} \) from Equation 3.8, and are defined as:

\[ \hat{\mathbf{J}} = \sum_{s} \sum_{p} q_s \tilde{\mathbf{v}} \mathbf{W}(\mathbf{x} - \mathbf{x}_p^{n}) \quad \hat{\mathbf{N}} = \sum_{s} \sum_{p} q_s \tilde{\mathbf{v}} \tilde{\mathbf{W}}(\mathbf{x} - \mathbf{x}_p^{n}). \] (3.19)

\( \chi_N \) is expressed as:

\[ \chi_N = \sum_{n_s} \chi_{N_s} \equiv \frac{1}{2} (\omega_{ps} \Delta t)^2 R(\omega_{cs} \frac{\Delta t}{2}), \] (3.20)

where \( R(\omega_{cs} \frac{\Delta t}{2}) \), is a rotation transformation, defined as:

\[ \begin{pmatrix}
1 + (\omega_{cs} \frac{\Delta t}{2})^2 & \omega_{cs} \frac{\Delta t}{2} + \omega_{csy} \omega_{csz} \frac{\Delta t}{2}^2 & -\omega_{csy} \frac{\Delta t}{2} + \omega_{csz} \omega_{csz} \frac{\Delta t}{2}^2 \\
-\omega_{csz} \frac{\Delta t}{2} + \omega_{csy} \omega_{csz} \frac{\Delta t}{2}^2 & 1 + (\omega_{csy} \frac{\Delta t}{2})^2 & \omega_{cs} \frac{\Delta t}{2} + \omega_{csy} \omega_{csx} \frac{\Delta t}{2}^2 \\
\omega_{csy} \frac{\Delta t}{2} + \omega_{csz} \omega_{csx} \frac{\Delta t}{2}^2 & -\omega_{csz} \frac{\Delta t}{2} + \omega_{csx} \omega_{csz} \frac{\Delta t}{2}^2 & 1 + (\omega_{cs} \frac{\Delta t}{2})^2
\end{pmatrix}. \]

and \( \omega_{cs} = \frac{q_s B^n}{m_s c} \), and \( \omega_{ps} = \sqrt{(4\pi \rho_s q_s)/m_s} \) are respectively the cyclotron frequency vector and the plasma frequency for species \( s \). An equation for \( \mathbf{E}^{n+\theta} \) is obtained after Equations 3.16 and 3.18 are plugged into Equation 3.12:

\[ (\mathbf{I} + \chi_N) \cdot \mathbf{E}^{n+\theta} - (c\theta \Delta t)^2 (\nabla^2 \mathbf{E}^{n+\theta} + \nabla \nabla \cdot (\chi_N \cdot \mathbf{E}^{n+\theta})) = \mathbf{E}^{n} + c\theta \Delta t (\nabla \times \mathbf{B}^{n} - \frac{4\pi}{c} \mathbf{J}^{n}) - (c\theta \Delta t)^2 4\pi \rho^n, \] (3.21)

where \( \mathbf{I} \) is the identity matrix and \( \chi_N \) is called numerical susceptibility (due to similarity of Equation 3.21 to the field equation in a dielectric media). For convenience, the \( \tilde{\rho}^n \) is introduced as modified source term for the Maxwell’s equations:

\[ \tilde{\rho}^n = \rho^n - (\Delta t\theta) \nabla \cdot (\hat{\mathbf{J}} - \frac{\Delta t}{2} \hat{\mathbf{N}}). \] (3.22)
The introduction of the implicit susceptibility $\chi_N$ is the main characteristic of the implicit Maxwell’s solver. Equation 3.20 defines the implicit susceptibility as a combination of a scaling and a rotation transformation on the future value of the electric field. The effect of scaling by the factor of $1/2(\omega_{ps}\Delta t)^2$ is to reduce the electric field component due to the fast electrons oscillations that can not be resolved by the large time step. The rotation transformation $R(\omega_s \Delta t)$ includes the effect of the particle Larmor rotation induced by the magnetic field. After the field equation is solved, the electric field must be corrected to ensure that the charge density continuity equation is satisfied [14; 38]:

$$ E' = E^{n+1} - \nabla \delta \Phi, \quad \nabla^2 \delta \Phi = \nabla \cdot E^{n+1} - 4\pi \rho^n. \tag{3.23} $$

### 3.1.3 Spatial Differentiation of the Maxwell Solver

The Maxwell’s equations have been differenced in space on a uniform cartesian grid. The electric field $E_{n,n}^{n+\theta,n+1}$, the current densities $J^n, \hat{J}^n$, and the numerical susceptibility $\chi_N$ are evaluated at the vertices of the grid, while the magnetic field $B_{n,n+1}$ and charge densities $\rho^n, \hat{\rho}^n$ are calculated at the centers of the cells. The simple box scheme is used for the spatial differentiation of spatial operators in the field equations (Equations 3.21, 3.23) [40]. If $u_{i,j,k}$ is provided at vertices, the derivative $\partial u/\partial x$ at the cell centers with indices $i + 1/2, j + 1/2, k + 1/2$ is calculated as:

$$ \frac{\partial u}{\partial x} \bigg|_{i+1/2,j+1/2,k+1/2} \approx \frac{u_{i+1,j+1/2,k+1/2} - u_{i,j+1/2,k+1/2}}{\Delta x}. \tag{3.24} $$

The value $u$ at the centers of the cells are computed by averaging the neighboring vertex values:

$$ u_{i,j+1/2,k+1/2} = \frac{1}{4} (u_{i,j,k} + u_{i,j+1,k+1} + u_{i,j+1,k} + u_{i,j,k+1}). \tag{3.25} $$

Derivatives at the cell centers are approximated in a similar way. The Laplacian operator is obtained by combining the divergence and gradient operators.
spatial derivatives are approximated in this way, Equation 3.21 results in a non-symmetric matrix with variable coefficients.

### 3.1.4 Linear Solvers

The discretized equations of Maxwell’s Equations 3.21 and their boundary conditions form a non-symmetric linear system that is solved using the Generalized Minimal Residual (GMRes) method [44–46]. The Conjugate Gradient (CG) method [44], is used to solve Equation 3.23, since the discretized equation leads to a symmetric matrix. A discussion about the condition number of the matrix represented by Equation 3.21, is reported in references [43; 47]. The performance of the GMRes solver without a preconditioner, obtained by scaling the number of grid points and using different time steps, are presented in reference [42; 47]. In summary, the number of iterations to reduce the norm of initial error by three orders of magnitude is fairly low (from 4 to 10 iterations) and it is insensitive to the number of grid points in the domain. The use of a preconditioner would be surely beneficial, but the GMRes solver performance are still adequate even without it.

### 3.1.5 Implicit Particle Mover

Traditionally, the implicit direct Particle-in-Cell method used implicit generalizations of the leap-frog algorithm (the so-called $C$ and $D$ schemes) [48; 49], and the implicit moment Particle-in-Cell method has focused on the Crank-Nicholson (CN) scheme [21; 42]. The CN scheme for the particle mover is:

\[
\frac{x_p^{n+1} - x_p^n}{\Delta t} = \bar{v} \quad (3.26)
\]

\[
\frac{v_p^{n+1} - v_p^n}{\Delta t} = \frac{q_s}{m_s} (E_p^{n+\theta}(\bar{x}) + \bar{v} \times B_p^n(\bar{x})/c). \quad (3.27)
\]

The bar quantities are calculated as the average of the values at different time levels. In the implicit moment particle mover scheme the average velocity $\bar{v}$ is first deter-
mined from Equation 3.9, and then the particle position is calculated from Equation 3.26. Because $\bar{v}$, $E_n^{p+\theta}$, and $B^n_p(\bar{x})$ depend on the intermediate particle position $\bar{x}$, a predictor-corrector method is used to find $\bar{v}$. Equation 3.9 is solved by a predictor-corrector procedure [50; 51]. A typical run normally requires three iterations. Studies of the convergence and energy conservation of the mover are reported in reference [42].

3.1.6 Code Implementation

The implicit moment Particle-in-Cell code has been written in C++. An Object-Oriented (OO) design has been followed, using the so-called lite OO approach presented in a previous work by Markidis et al. [52], to achieve high computational performance. The variables related to particles, are organized as arrays in Particle objects, and divided depending on the species (electrons, Potassium, and Barium particles,...). The electromagnetic field constitutes a whole object, that comprises the electromagnetic field and field sources variables, such as $\rho$ and $J$. The OO paradigms, such as class inheritance, and the polymorphism are used to make it easy for developers to add new components, without overwriting the existing code.

The implicit moment Particle-in-Cell code is parallel and runs on supercomputers. The domain decomposition technique is used to divide the computational work-load among processors on multiprocessor architectures [53]. For implicit Particle-in-Cell code where the cost to move particles and for the field solve are of the same order (unlike explicit Particle-in-Cell code where most of the cost is in moving particles), it is crucial that both, field solver and particle mover be parallelized efficiently. An important aspect of efficiency is the need to retain the particles and cells belonging to a subdomain on the same processor. Large amounts of information is exchanged between grid and particles residing in the same physical domain and therefore it is important to avoid that this information exchange results in inter processor communication [53]. The simulation box is divided among processors using a generic Cartesian
virtual topology [54]. Particles are divided among processors also depending on their location, and communicated to adjacent processors if exiting from the processor domain. The parallelization of the code is based on MPI libraries and blocking parallel communication has been chosen for the communication among processors [54].

If the explicit Particle-in-Cell codes require very large memory to store the information of all the particles and fields, the implicit Particle-in-Cell code requires even more memory to store additional intermediate variables, such as variables for $\hat{\rho}^n$, $\hat{\mathbf{J}}^n$. Parallel computer memory is needed in order to run simulations with large number of particles and grid nodes. The choice of shared memory machines is therefore currently not feasible and distributed memory machine (clusters) have to be used to simulate large scale problems.

### 3.2 Fully Implicit Particle-in-Cell Method

An electrostatic, one dimensional model of plasma is considered for the development of the fully implicit Particle-in-Cell method. In this configuration, the particle equation of motion are time differenced using the CN scheme:

\[
\frac{x_p^{n+1} - x_p^n}{\Delta t} = \bar{v} \tag{3.28}
\]

\[
\frac{v_p^{n+1} - v_p^n}{\Delta t} = \frac{q_s}{m_s}(\theta E_p^{n+1} + (1 - \theta)E_p^n) = \frac{q_s}{m_s}(\theta \nabla \Phi_p^{n+1} + (1 - \theta) \nabla \Phi_p^n), \tag{3.29}
\]

where $\Phi = \nabla E$ is the electrostatic potential, and $\theta$ is the *decentering parameter* that controls the *implicitness* of the Particle-in-Cell method. As in the implicit moment Particle-in-Cell method, the key point in the fully implicit method is the evaluation of the particle average velocity, $\bar{v}$. In the case of un-magnetized plasma, $\bar{v}$ is simply:

\[
\bar{v} = \frac{v_p^n + v_p^{n+1}}{2} = v_p^n + \frac{q_s}{2m_s}(\theta E_p^{n+1} + (1 - \theta)E_p^n). \tag{3.30}
\]

In the electrostatic limit, the potential $\Phi$ satisfies the Poisson equation:

\[
\nabla^2 \Phi_g^{n+1} = 4\pi \rho_g^{n+1} \tag{3.31}
\]
The Poisson equation is space-differenced as follows:

\[ \frac{\Phi_{g-1}^{n+1} - 2\Phi_{g}^{n+1} + \Phi_{g+1}^{n+1}}{\Delta x} = 4\pi \rho_{g}^{n+1}. \]  

(3.32)

The potential values on the grid \( \Phi_{g} \), and the potential of the force acting on the particle \( \Phi_{p} \) are related by:

\[ \Phi_{p}^{n+1} = \sum_{g} N_{g} \Phi_{g}^{n+1} W(x_{g} - x_{p}^{n+1}). \]  

(3.33)

The charge density in Equation 3.32 is calculated by interpolation from the particle positions:

\[ \rho_{g}^{n+1} = \sum_{s} n_{s} \sum_{p} q_{s} W(x_{g} - x_{p}^{n}). \]  

(3.34)

As pointed out by Langdon in [19]: in the fully implicit method, the equation for each particle, together with the field equations, represents a very large system of nonlinear coupled equations. An iterative solution must be carried quite close to convergence if stability is to be retained. If linearized, the Jacobian matrix is large and neither sparse nor diagonally dominant. Its eigenvalues are related to the modes of oscillation of a cold plasma with particles at the same spatial locations and tend to be distributed over a wide range of values. Thus the iteration may be expensive computationally [19]. In general, the challenges of developing a fully implicit method are:

1. The non linear system composed of \( (N_{g} + n_{s} \cdot N_{s}) \) equations, needs to be solved, where \( N_{g} \) is the number of grid points, \( n_{s} \) is the number of species, and \( N_{s} \) is the number of particles for the species \( s \). The non linearity arises through the coupling of particles and grid, due to the interpolation function of Equations 3.33 and 3.34.

2. The matrix of the non linear system is very large. For instance a one dimensional simulation with 100,000 particles of one species (only moving electrons and fixed ions), and 512 grid points, corresponds to a \( 100,512 \times 100,512 \) matrix, where
100,000 equations are for the particle average velocity (Equation 3.30) and 512 equations are for the Poisson equation (3.33). Thus the computer memory storage requirement of such a matrix would be prohibitive even on present day computers with large memory.

3. Convergence of the solver is slow because the Jacobian matrix is neither sparse nor diagonally dominant.

Thus, the development of the fully implicit method requires the use of a non linear solver. Moreover it should avoid the storage of the matrix in the computer memory, following the so-called matrix-free approach. The Newton-Krylov Jacobian-Free Matrix-Free GMRes has been chosen for the solution of the non linear system. The main advantage of the method is that it does not require the memory storage of the matrix and of its Jacobian.

3.2.1 Newton-Krylov Jacobian-Free Matrix-Free GMRes

The Newton-Krylov iterative method has been used to solve the non linear system composed of Equations 3.30 and 3.32. If the system of non linear equations is written in the concise form $F(X) = 0$, where $F$ is the residual function and $X$ is a vector containing the unknowns of the problem, the Newton iteration is derived from a Taylor expansion of $F(X)$, truncated at the first order, about a point $X^{it}$

$$F(X^{it+1}) = F(X^{it}) + J(X^{it})(X^{it+1} - X^{it}),$$

(3.35)

where $J = F'$ is the Jacobian associated with $F$. The Newton method is easily derived from Equation 3.35, leading to the solution of a sequence of linear systems

$$J(X^{it})\delta X^{it} = -F(X^{it})$$

(3.36)

$$X^{it+1} = X^{it} + \delta X^{it}.$$  

(3.37)
Once the linear system given by Equations 3.36 is solved, a new approximate solution \( X^{it+1} \) of the system \( F(X) = 0 \) can be calculated using Equation 3.37. In this dissertation, the Generalized Minimal RESidual (GMRes) \([46; 55]\) approach is used to solve the linear system given by Equation 3.36. Given an initial residual \( r^0 \), calculated from an initial guess \( \delta X^0 \) as

\[
r^0 = -F(X) - J\delta X^0.
\]  

(3.38)

The \( \delta X^{it2} \) is drawn from the subspace spanned by the Krylov vectors \( \{r^0, Jr^0, J^2r^0, ..., J^{it2-1}r^0\} \) and is calculated as

\[
\delta X^{it2} = \delta X^0 + \sum_{i=0}^{it2-1} \beta_i J^i r^0,
\]  

(3.39)

where \( \beta_i \) are scalars chosen to minimize the residual using a least-square technique. It is clear from Equation 3.39 that to implement the GMRes approach, one only requires to calculate the Jacobian-vector product, that can be approximated with a directional derivative as

\[
Jv \approx (F(X + \epsilon_{NK}v) - F(X))/\epsilon_{NK},
\]  

(3.40)

where \( \epsilon_{NK} \) is a small perturbation chosen conveniently \([55]\). This approximation of the Jacobian-vector product allows a Newton iteration to be performed without forming and storing the Jacobian. Furthermore, since GMRes requires only matrix-vector products to complete the iterations, and not the individual elements of \( F \), the matrix elements to represent Equations 3.30 and 3.32 are not formed or stored.

### 3.2.2 Code Implementation

A fully implicit Particle-in-Cell code has been written in Octave/Matlab programming language. The programming language Octave/Matlab provides a software platform for fast development of numerical algorithms. In particular, it provides built-in numerical linear solvers. In addition, solvers for non linear problems are also available on
the Internet, provided by the large community of Octave/Matlab users. The Newton-Krylov (NK) Jacobian-Free Matrix-Free GMRes used for the development of the fully implicit Particle-in-Cell method has been implemented and made available by Kelley [45]. The residual equations solved by the NK GMRes, expressed in the concise form \( F(X) \) as in the previous section has the form:

\[
F(X) = \bar{v} - v^n_p + 1/2 \frac{q_s}{m_s} (\theta E^{n+1}_p + (1 - \theta) E^n_p)
\]  

(3.41)

for the particle equations, while for the field equations at each grid point:

\[
F(X) = \Phi^{n+1}_{g-1} - 2\Phi^{n+1}_g + \Phi^{n+1}_{g+1} \frac{\Delta x}{\Delta x} - 4\pi \rho^n_{g+1}.
\]  

(3.42)
Chapter 4

Verification and Performance of the Implicit Moment Particle-in-Cell Code

The implicit moment Particle-in-Cell method, described in Chapter 3, has been implemented in a computer code, that can model three dimensional domains and includes both electric and magnetic fields. The tests carried out to verify the components of the implicit Particle-in-Cell code are presented in this chapter. The implicit moment Particle-in-Cell code is composed of two main components: the particle mover component, that numerically solves the particle equation of motion; and the field solver component, that solves the Maxwell’s equations. The field solver component can be used in the problems of electrostatic nature, where the magnetic field can be neglected, as well as to solve complete electromagnetic problems.

The goal of this chapter is to present the tests carried out to verify the mover component using the Larmor gyration problem and the \( \mathbf{E} \times \mathbf{B} \) drift problem, and the field solver component using problems of electrostatic nature such as electron beam instability and Landau damping, and problems of electromagnetic nature, such as instability of a bi-Maxwellian plasma. Moreover, the problem of magnetic recon-
nection in the Earth magneto-tail is presented to show the efficiency of the implicit moment Particle-in-Cell method. The computational performance of the implicit moment Particle-in-Cell method has been studied: the number of floating-point operations, and the execution time for simulations with different number of grid points, number of particles, and different time steps, have been recorded to investigate how the computational performance depends on the simulation parameters. Finally, the computational performance of the moment implicit method is compared to the performance of the explicit Particle-in-Cell method.

The chapter is divided in two parts. The first part comprises of Sections 4.1 to 4.5, and it presents the verification tests of the implicit moment Particle-in-Cell code. The second part, Section 4.6, investigates the computational performance of the implicit moment Particle-in-Cell method. Section 4.1 presents a series of tests for the particle mover component only, i.e, the electric and magnetic fields are pre-assigned and not calculated self-consistently. The particle mover has been tested first for a configuration with constant magnetic field, and then for a configuration with a magnetic field and an orthogonal electric field that results in a drift velocity governed by \( \mathbf{E} \times \mathbf{B} \). The field solver software component is tested in Sections 4.2, 4.3, and 4.4. Two electrostatic problems, the electron beam instability and the Landau Damping, are presented in Sections 4.2 and 4.3, and a pure electromagnetic problem, the bi-Maxwellian plasma instability, in Section 4.4. The magnetic reconnection test, carried out to demonstrate the efficiency of the implicit moment Particle-in-Cell method, is reported in Section 4.5. Finally, Section 4.6 closes the chapter by comparing the computational performance of the implicit moment Particle-in-Cell method with an explicit Particle-in-Cell code performance.
4.1 Particle Motion

In this section, the tests for the verification of the particle mover component are presented. The values of the electric and magnetic field are assigned, and not calculated self-consistently using the field solver.

4.1.1 Larmor Gyration

In this simple test, a constant and uniform magnetic field $B_z$ equal to 1.0 is imposed in the $z$ direction. An electron with mass ratio $q_e/m_e$ equal to 1.0 is placed on the plane $z = 0$, at the location $(x,y) = (0.5,0.5)$, with a velocity component in the direction $y$ equal to 0.1. The light speed $c$ in the simulation is set to 1. The electron is expected to rotate with cyclotron frequency $\omega_c = \frac{q_e}{c m_e} B_z$ equal to 1.0 and Larmor radius $\rho_L = v_y/\omega_c$ equal to 0.1. Figure 4.1 shows the simulated electron trajectory. The simulated Larmor radius is correctly predicted to be equal to 0.1. Figure 4.2 shows the oscillation in time of the $y$ coordinate of the gyrating electron. The oscillation period is $T_c = 2\pi/\omega_c = 2\pi$, and it is in perfect agreement with the theoretical prediction.

4.1.2 $E \times B$ Drift Velocity

The implicit moment Particle-in-Cell code is tested against the theoretical prediction of the drift velocity of an electron in an electromagnetic field. A constant and uniform electric field in $x$ direction, $E_x = 0.05$, and a constant and uniform magnetic field in the $z$ direction, $B_z = 1.0$, are assigned. An electron with mass ratio $q_e/m_e$ equal to 1.0 is initially placed on the plane $z = 0$, at the location $(x,y) = (0.5,50.0)$ with zero velocity. The light speed $c$ in the simulation is set to 1. Figure 4.3 shows the simulated trajectory of the electron under the specified $E$ and $B$ fields. In Figure 4.3, the electric field accelerates the electron initially in the $-x$ direction, and the
Figure 4.1: The electron gyrates with the correct gyro-radius in a constant uniform magnetic field.

Figure 4.2: The electron gyrates with the correct gyro-frequency in a constant uniform magnetic field.
magnetic field makes the electron to gyrate. During half of the gyration, the electron has a velocity component parallel to the electric field, while during the other half of the gyration the velocity component is against the electric field. The electron is therefore accelerated and decelerated in a gyration cycle. During the acceleration the gyro-radius increases, while the gyro-radius decreases during the deceleration phase. This continuous change of the electron gyro-radius results in the so-called $E \times B$ drift.

The theoretically predicted drift velocity [11]:

$$v_{E \times B} = \frac{E \times B}{cB^2}$$

(4.1)

The $E \times B$ drift with the used parameters, will result only in a component in the $y$ direction with value $(E \times B)_y = -E_yB_z = -0.05$. Figure 4.4 shows that the moving average velocity in the $y$ direction, $<v_y>$, converges to the right value of -0.05, predicted by the theory.
Figure 4.4: Plot of the moving average velocity in the \( y \) direction, \( \langle v_y \rangle \), of an electron in perpendicular electric and magnetic fields. The velocity drift converges to the drift velocity (in blue) asymptotically.

4.2 Electron Beam Instability Simulation

The electron beam instability, or two stream instability, is one of the most common instability in plasma physics. It occurs for example when two electron beams move in opposite directions. The electron beam instability is due to an initial charge bunching, and to the wave particle interaction. A perturbation of the charge density is applied to a moving beam, as in Figure 4.5. If the electrons are streaming with velocity close to the phase velocity of the perturbation, then there is a resonant interaction between the perturbation and electrons. Figure 4.5 shows the wave particle interaction. Electrons are accelerated from point 2 to point 4, while they are decelerated from point 4 to point 5. The wave particle interaction leads the electrons to spend most of their time in region with an excess of negative charge. In this way the electron bunching is reinforced, and leads to instability that grows exponentially in time.

The electron beam instability has been simulated with the implicit moment Particle-in-Cell code in a one dimensional geometrical configuration. For \( t > 0 \), the two electron beams, composed of 100,000 electrons in each, flow in opposite directions with
Figure 4.5: The beam is subject to a sinusoidal charge perturbation. If the electron streaming velocity is close to the perturbation phase velocity, the perturbation and the electrons interact. The electrons are accelerated from point 2 to point 4, and decelerated from point 4 to point 5. Therefore, the electrons spend most of their time in the negatively charged region, reinforcing the electron charge bunching and leading to the instability.

propagation velocities $+0.1c$ and $-0.1c$, and thermal velocity of $0.01c$. The light speed $c$ in the simulation is set to 1. A background of ions neutralizes the system with $\omega_{pe}$ equal to 1. The simulation box $L_x$ is equal to $2\pi c/\omega_{pe}$. A perturbation of the electron beam densities is applied at $t = 0$, perturbing the electron positions $x_p$ as follows:

$$x'_p = x_p + 0.01 \times \frac{\cos(kx_p)}{k}$$

(4.2)

where $k$ is the wave number of the perturbation. The wave number of the perturbation has been chosen as $k = 1$ in the $\omega_{pe}/c$ units. The time step, $\Delta t = 0.1 \omega_{pe}^{-1}$.

Figure 4.6 shows the phase space evolution of the two stream instability. In the phase space, each electron represents a point whose coordinates are the particle position and velocity. The instability can be seen developing at $t = 20 \omega_{pe}^{-1}$. The two beams are completely mixed in the phase space at $t = 30 \omega_{pe}^{-1}$.

The same beam instability occurs when an ion beam propagates through a plasma.
Figure 4.6: Phase space evolution of the electron beam instability. The red and blue beams flow in opposite directions. A perturbation, applied at the beginning of the simulation, grows exponentially, mixing the two beams.
For this reason, this beam instability has been of major concern for the NDCX [57], and for other nuclear fusion devices, whenever the device requires the injection of a beam in a plasma. The linear theory, the simulations and the experiments are necessary to understand this instability, so that it can be avoided in the NDCX configuration [56; 57].

4.2.1 Comparison with Linear Theory

The linear theory of the electron beam instability predicts that the growth rate $\gamma$ for the most unstable wave number $k = \frac{3}{\sqrt{8}} \frac{\omega_{pe}}{v_{beam}}$ is [11; 14]:

$$\gamma = \frac{\omega_{pe}}{\sqrt{8}}$$

(4.3)

Substituting the simulation parameters in Equation 4.3, it is found that the most unstable wave number $k$, equal to 10 (in units of $\omega_{pe}/c$, has a growth rate $\gamma$ equal to 0.11. Figure 4.7 shows the growth rate of the electric field associated with the wave number $k$ equal to 10 $\omega_{pe}/c$, simulated with the implicit moment Particle-in-Cell method. The results of the implicit moment Particle-in-Cell method and the linear theory are in excellent agreement in the linear regime. They differ only when the instability is fully developed, and the electric field saturates.

4.3 Landau Damping Simulation

The Landau damping is characteristic feature of the collision-less plasmas: plasma perturbations are damped even without collisions [11; 58; 59]. The Landau damping of the perturbation occurs because of the energy exchange between the perturbation and the particles in the plasma with velocity approximately equal to the phase velocity of the perturbation. In fact, the particles with thermal velocities slightly less than the phase velocity of the perturbation are accelerated by the wave electric field; while the particles with velocities slightly higher than phase velocity are decelerated by the
Figure 4.7: Plot of the spectral component for $k = 10 \omega_{pe}/c$ for the electric field from the simulation in the blue color, and the growth of the instability predicted by the linear theory in the red color.
wave electric field, losing energy to the wave. Landau damping is due to a resonance effect between the wave and the particles. More specifically, if the perturbation in a Maxwellian plasma has positive phase velocity, the slope of the Maxwellian distribution function is negative at the perturbation phase velocity. This means that the number of particles with velocities slightly less than the propagation phase velocity is higher, than the number of particles with velocities slightly higher. Thus, more particles gain energy from the perturbation than losing to the wave. This leads to the damping of the plasma perturbation.

In this test, a uniform Maxwellian plasma is initialized with electron plasma frequency \( \omega_{pe} = 1 \), and electron thermal velocity equal to 0.5 \( c \). The light speed \( c \) in the simulation is set to 1. The simulation box \( L_x \) is long \( 2\pi c / \omega_{pe} \). A perturbation with wave number \( k = 1 \) (in the \( \omega_{pe}/c \) units) is excited in the system perturbing the electron positions:

\[
x'_{p} = x_{p} + 0.01 \times \frac{\cos(kx_{p})}{k}
\]

(4.4)

The simulation time step \( \Delta t \) is equal to 0.05.

### 4.3.1 Comparison with the Linear Theory

The decay rate \( \gamma \) of a wave with wave number \( k \) in a Maxwellian plasma, is predicted by the linear theory [58; 59]:

\[
\gamma = -\sqrt{\frac{\pi}{8}} \omega_{pe} \left( \frac{\omega_{pe}}{k v_{the}} \right)^3 \exp\left( \frac{-\omega^2}{2k^2 v_{the}^2} \right)
\]

(4.5)

where

\[
\omega^2 = \omega_{pe}^2 + 3k^2 v_{the}^2
\]

(4.6)

Substituting the simulation parameters in Equation 4.5, the decay rate for the Landau damping is calculated as,

\[
\gamma = -0.62665 \cdot 1.9827 \exp(-0.78912) = -0.126
\]

(4.7)
Figure 4.8: Simulation of the Landau damping with the implicit moment Particle-in-Cell and comparison with the linear theory. Plots of the spectral component $k = 1$ for the electric field are shown for the simulation in the blue color, for the linear decay in the red color, and for the best fit of the simulation results in the green color.

Figure 4.8 shows a comparison between the linear theory and the simulation. In addition, a best fit of the simulation results in a $\gamma = -0.221$. The Landau damping rate estimated from the simulation results higher than the result predicted by the linear theory. This is probably due in part to the additional numerical damping, introduced by the implicit moment Particle-in-Cell numerical scheme, and in part to the non linear nature of the problem.
4.4 Electromagnetic Instability of a Bi-Maxwellian Plasma

A bi-Maxwellian plasma is an anisotropic plasma, characterized by considerable difference between the thermal velocities in one direction, and in the directions perpendicular to it. The bi-Maxwellian distribution is the product of two Maxwellian distributions, that takes into account these different thermal speeds. If a plasma has temperature $T_x$ in the $x$ direction, and temperature $T$ in the plane $(y,z)$ perpendicular to the $x$ direction, the bi-Maxwellian distribution is written as [12]:

$$f = \left( \frac{m_s}{2\pi k_B T_x} \right)^{1/2} \exp\left( -\frac{m_s}{2k_B T_x} v_x^2 - \frac{m_s}{2k_B T} (v_y^2 + v_z^2) \right)$$

(4.8)

Because the magnetic field introduces anisotropy in one direction, privileging the direction along the magnetic field, the bi-Maxwellian distribution function is rather common in space and laboratory plasmas. For instance, plasma is bi-Maxwellian in the mirror machines, and in plasma sources that inject across a magnetic field, such as the FCAPS of the NDCX [12; 60]. The bi-Maxwellian distribution is stable to the electrostatic perturbations, but unstable to electromagnetic waves. The electromagnetic component of the Particle-in-Cell code is verified in this test, since the previous coupled particle mover and field problems were electrostatic in nature.

4.4.1 Comparison with the Linear Theory

The bi-Maxwellian plasma is linearly unstable to wave with wave-number $k$, characterized by the relation [12]:

$$\left( \frac{T}{T_x} - 1 \right) > \frac{k_x^2 c^2}{\omega_p^2}$$

(4.9)

The growth rate of the instability can be calculated by substituing Equation 4.8 in the dispersion relation, and calculating the zeros of it. In the limit of strong anisotropy in the temperatures, $T/T_x >> 1$, the growth rate for the most unstable
wave, \( k = \frac{\omega_{pe}}{c} \sqrt{1/3(T/T_x - 1)} \) is [12]:

\[
\gamma = \omega_{pe} \left( \frac{T}{T_x} \right)^{1/2} \left( \frac{K_B T_x}{m_s c^2} \right)^{1/2}.
\] (4.10)

The instability makes the bi-Maxwellian distribution function to relax to an isotropic Maxwellian. The electric and magnetic fields growth exponentially in time, at the expense of the disparity of energy in the perpendicular directions.

The implicit moment Particle-in-Cell code has been tested by simulating the electromagnetic instability of a bi-Maxwellian plasma. The simulation has been initialized with a plasma with \( \omega_{pe} = 1 \), with a strong anisotropy in the thermal velocity \( T/T_x = 4.0 \). Electron thermal velocity in the \( x \) direction \( v_x = 0.1c \) and speed of light in vacuum \( c = 1 \). The simulation box is long, \( L_x = 2\pi \). An initial perturbation is imposed, displacing the electron positions \( x_p \) by:

\[
x'_p = x_p + 0.01 \times \frac{\cos(k x_p)}{k}
\] (4.11)

where the \( k \) is the wave number of the perturbation, chosen as \( k = 1.0 \) in the \( \omega_{pe}/c \) units. The simulation time step is equal to \( 0.15 \omega_{pe}^{-1} \). The growth rate of the instability calculated with the linear theory (Equation 4.10) is:

\[
\gamma = 0.504
\] (4.12)

Figure 4.9 shows a comparison of the growth of the magnetic field energy, with the growth rate predicted by the linear theory. The instability very closely follows the linear growth of Equation 4.10 in the linear regime of the instability.

### 4.5 Magnetic Reconnection Simulations

The simulation of the magnetic reconnection in the Earth magnetotail is presented in this section to demonstrate the efficiency of the implicit Particle-in-Cell methods. The results are obtained by using the implicit moment Particle-in-Cell code [61; 62]. The
Figure 4.9: Semi-logarithmic plot of the evolution of the spectral component $k = 0.58$ for $B^2$ from the simulation in the blue color, and growth rate of the instability predicted by the linear theory in the red color.
Figure 4.10: Initial configuration of the electron current sheet in the magnetic reconnection. The color represents the electron current intensity.

system is initially in the magneto-tail equilibrium, the so called \textit{Harris equilibrium} \cite{Harris1962}, described in reference \cite{Cowley1978}. The physics of magnetic reconnection predicts, first the growth and saturation of the lower hybrid drift instability, followed by the onset of reconnection and the current flapping leading to the macroscopic reorganization of the magneto-tail. The process is described in detail by Lapenta and Brackbill in \cite{LapentaBrackbill1990}. Figures 4.10 through 4.14 show the evolution of the electron current sheet during the magnetic reconnection in the magneto-tail, simulated with the implicit moment Particle-in-Cell code.

This problem has been chosen to demonstrate the efficiency of the implicit moment Particle-in-Cell approach. In the explicit Particle-in-cell method, the time step must be selected according to the stability constraint presented in Chapter 2. The electron plasma frequency in the Earth magneto-tail is typically of the order of $\omega_{pe} \approx 5 \cdot 10^4 \text{s}^{-1}$, while the ion plasma frequency is of the order of $\omega_{pi} \approx 10^3 \text{s}^{-1}$ \cite{Cowley1978,Halekas2000}. The frequency scale of interest of the system is the lower-hybrid instability range $\omega_{LH} \approx 10^{-2}$ \cite{Halekas2000}, which is much smaller than the frequency scale of both the electron
Figure 4.11: Current sheet at time $1.95 \omega_{pi}^{-1}$ in the magnetic reconnection problem. The color represents the electron current intensity.

Figure 4.12: Current sheet at time $5.85 \omega_{pi}^{-1}$ in the magnetic reconnection problem. The color represents the electron current intensity.
Figure 4.13: Current sheet at time $9.75 \omega_{pi}^{-1}$ in the magnetic reconnection problem. The color represents the electron current intensity.

Figure 4.14: Current sheet at time $15.60 \omega_{pi}^{-1}$ in the magnetic reconnection problem. The color represents the electron current intensity.
and ion plasma frequencies. The time step of the implicit Particle-in-Cell simulation can be chosen equal to the inverse of ion plasma frequency. In this case, the time step still resolves accurately the lower hybrid instability range, and it saves two orders of computational cycles, when compared with the explicit case. A similar computational saving is achieved for to the calculations related to the grid. The grid spacing in the explicit Particle-in-Cell must be smaller than the Debye length to avoid the numerical instability. The Debye length in the magneto-tail is typically of the order of one hundred meters. The spatial scale of interest for the magnetic reconnection problem is between the electron and ion skin depths; respectively 10 and 100 km. The grid spacing in the implicit Particle-in-Cell method can be chosen to be 10 kilometers, saving two orders of magnitude in each spatial direction but still resolving the important scales. Thus the use of implicit Particle-in-Cell method leads to save two orders of magnitude in each direction and in time, for a total of eight orders of magnitude. This means that if a problem, simulated with an implicit Particle-in-Cell method, takes one day, it would take 800,000 years if the explicit Particle-in-Cell code is used [42].

4.6 Computational Performance of the Implicit Moment Method

In this section, the computational performance of the implicit moment Particle-in-Cell method is evaluated. An implicit moment and an explicit Particle-in-Cell codes have been developed for a one dimensional electrostatic version to allow comparison of their performance. The codes have been implemented in the Matlab/Octave programming language. The Matlab/Octave programming environment is can keep track of the floating-point operations (FLOPS) of a particular algorithm. The number of FLOPS does not depend on the architecture of the computer, the tests have been run on, and
Table 4.1: Number of FLOPS and execution time for 200 computational cycles for the implicit moment Particle-in-cell code for different number of particles $N_p$, number of grid points $N_g$, and $\theta$ equal to 0.5 and 1.0. The time step is 0.1.

<table>
<thead>
<tr>
<th>$N_p$</th>
<th>$N_g$</th>
<th>$\theta$</th>
<th>FLOPS</th>
<th>EXECUTION TIME (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5000</td>
<td>64</td>
<td>0.5</td>
<td>9.975e7</td>
<td>8.65</td>
</tr>
<tr>
<td>10000</td>
<td>64</td>
<td>0.5</td>
<td>1.375e8</td>
<td>14.08</td>
</tr>
<tr>
<td>20000</td>
<td>64</td>
<td>0.5</td>
<td>2.233e8</td>
<td>25.64</td>
</tr>
<tr>
<td>10000</td>
<td>128</td>
<td>0.5</td>
<td>1.737e8</td>
<td>17.54</td>
</tr>
<tr>
<td>10000</td>
<td>256</td>
<td>0.5</td>
<td>2.252e8</td>
<td>22.50</td>
</tr>
<tr>
<td>5000</td>
<td>64</td>
<td>1.0</td>
<td>8.959e7</td>
<td>8.47</td>
</tr>
<tr>
<td>10000</td>
<td>64</td>
<td>1.0</td>
<td>1.388e8</td>
<td>15.04</td>
</tr>
<tr>
<td>20000</td>
<td>64</td>
<td>1.0</td>
<td>2.044e8</td>
<td>25.24</td>
</tr>
<tr>
<td>10000</td>
<td>128</td>
<td>1.0</td>
<td>1.556e8</td>
<td>16.70</td>
</tr>
<tr>
<td>10000</td>
<td>256</td>
<td>1.0</td>
<td>1.994e8</td>
<td>20.71</td>
</tr>
</tbody>
</table>

It provides a good indication of the computational cost of the algorithm. The electron beam instability problem, presented in Section 4.3 of this chapter, has been chosen as the test problem. Although the computational performance depends critically on the problem chosen, and on the simulation set-up, the simple test of the electron beam instability provides an estimate of the computational cost. The performance of the implicit Particle-in-Cell code has been evaluated by counting the number of FLOPS for the beam instability test problem. A 2 GHz Intel Pentium 4 processor with 256 Mega Byte of RAM memory, and the Matlab (version 5.3) have been used for these tests.

The number of FLOPS, and the execution time for different number of particles, $N_p$, and grid points $N_g$ are tabulated in Table 4.1. Not surprisingly, the number of FLOPS and the executing time increase with the number of particles and with the number of grid points. There is no appreciable difference in the performance when $\theta$
Table 4.2: Number of FLOPS and execution time for 50 computational cycles of the implicit moment Particle-in-Cell method for different time steps $\Delta t$.

<table>
<thead>
<tr>
<th>$\Delta t$</th>
<th>$\theta$</th>
<th>FLOPS</th>
<th>EXECUTION TIME (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.5</td>
<td>2.7222e6</td>
<td>3.1350</td>
</tr>
<tr>
<td>0.2</td>
<td>0.5</td>
<td>2.7330e6</td>
<td>3.1450</td>
</tr>
<tr>
<td>0.6</td>
<td>0.5</td>
<td>3.115e6</td>
<td>3.16</td>
</tr>
<tr>
<td>1.0</td>
<td>0.5</td>
<td>3.701e6</td>
<td>3.54</td>
</tr>
<tr>
<td>1.5</td>
<td>0.5</td>
<td>3.300e6</td>
<td>3.56</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>3.010e6</td>
<td>3.51</td>
</tr>
</tbody>
</table>

is varied between 0.5 and 1. Results reported in Table 4.1 are for 200 cycles, where the cycle is composed of the solution of the particles and field equations. The time step is 0.1.

Table 4.2 shows the performance of the implicit moment Particle-in-Cell method for different time steps. These execution times are for running 50 computational cycles, 10000 particles, and with 64 grid points. The time step does not have a significant effect on the computational performance. An increase of the time step leads to a slightly increased number of FLOPS and execution time, because the field solver requires a slightly higher number of iterations to converge with larger time step.

4.6.1 Comparison of the Performance with the Explicit Particle-in-Cell Code

The computational performance of the implicit moment Particle-in-Cell method has been compared with the performance of an explicit Particle-in-Cell code in this section. The comparison of the FLOPS, running 200 computational cycles, with $\Delta t = 0.1$, with 10,000 particles and with 64 grid points, for the electron beam instability problem, is tabulated in Table 4.3. Not surprisingly, the explicit Particle-in-Cell
Table 4.3: Comparison of the number of FLOPS for the explicit and the implicit moment Particle-in-Cell methods.

<table>
<thead>
<tr>
<th>$N_p$</th>
<th>$N_g$</th>
<th>EX. PIC FLOPS</th>
<th>IMP. MOM. PIC FLOPS</th>
<th>RATIO IMP./EX.</th>
</tr>
</thead>
<tbody>
<tr>
<td>5000</td>
<td>64</td>
<td>2.147e7</td>
<td>9.975e7</td>
<td>4.659</td>
</tr>
<tr>
<td>10000</td>
<td>64</td>
<td>4.2612e7</td>
<td>1.375e8</td>
<td>3.226</td>
</tr>
<tr>
<td>20000</td>
<td>64</td>
<td>8.4883e7</td>
<td>2.233e8</td>
<td>2.631</td>
</tr>
<tr>
<td>10000</td>
<td>128</td>
<td>4.2946e7</td>
<td>1.737e8</td>
<td>4.045</td>
</tr>
<tr>
<td>10000</td>
<td>256</td>
<td>4.3631e7</td>
<td>2.252e8</td>
<td>5.161</td>
</tr>
</tbody>
</table>

code is faster than the implicit moment Particle-in-Cell code in all the tests if the same simulation time step is used. The ratio of the performances between the two methods depends critically on the number of grid points and number of particles. In particular, the implicit moment method is 2.6 times slower when a low number of grid points and high number of particles are used. The performance of the implicit moment Particle-in-Cell code is 5.2 times slower when a high number of grid points is used. This is due to the fact that the field solver in the implicit moment Particle-in-Cell code is the computationally intensive part of the algorithm and it accounts for typically 60% of all the calculations. This is evident from Figure 4.15, that reports the time spent in the field solver (in blue color), in the mover (in red color) and in the interpolation (in yellow) in a simulation using an implicit moment Particle-in-Cell code on 4 processors. The red color, representing the time spent in the field solver, covers approximately 60% of all the computational cost. On the other hand, the field solver in the explicit Particle-in-Cell code is only 5% of all the computational time and the particle mover consumes the remaining 95% [67]. Because the field solver computational time depends on the number of grid points, a large number of grid points results in a worse performance for the implicit moment Particle-in-Cell code.
Figure 4.15: Time spent at different stages of the implicit moment Particle-in-Cell. The four lines represent four processors. The blue color is the time spent in the field solver, the red color is the time spent in the particle mover, and yellow color is time spent for the interpolation of the particle to the grid. The field solver in red, comprises a large part of the computations.
Chapter 5

Simulation of the NDCX Configuration: Set-up and Parameters

This chapter reports the physical, geometric and numerical parameters to simulate the NDCX set-up. The geometrical configuration and the physical quantities of interest for the neutralization process are identified. As expected, an accurate description of the physics of the neutralization process as well as a good numerical scheme and parameters are needed to resolve particular time and spatial scales, which impose constraints on the choice of the simulation time step, grid spacing, and number of particles. The process of selection of these parameters is discussed in this chapter.

The chapter is organized as follows: the beam-plasma model, the dimensionless units, and the beam and plasma parameters are respectively presented in Sections 5.1, 5.2, 5.3 and 5.4. Section 5.5 presents the simulation diagnostics, used to characterize the neutralization process. Section 5.6 discusses the geometrical configuration and the boundary conditions. Sections 5.7, 5.8, and 5.9 describe how the simulation time step, the grid spacing, and the number of particles have been chosen, depending on the numerical and physics constraints.
5.1 The Beam-Plasma Model

The implicit moment Particle-in-Cell method, developed for here, is a three dimensional, electromagnetic model of the beam-plasma system. An electromagnetic two dimensional model has also been used to study the transversal neutralization process in a simplified configuration. This configuration allowed faster computation, and easier analysis of the results.

The beam-plasma model used in this dissertation, includes the following simplifications:

1. Neutral particles are not modeled in the simulation.

2. Plasma formation by ionization of the neutrals is not modeled.

3. Scattering phenomena are not modeled.

4. Charge exchange phenomena are not modeled.

Although all these phenomena are present in the system in some measure, they are currently not well diagnosed in the NDCX [3]. However, their effects have been estimated to be negligible, and hence not modeled in the previous simulations of the FEPS plasma [2; 3].

5.2 Dimensionless Units

It is a common practice in computational physics to use dimensionless units. To take full advantage of computers memory architecture, the variables being evaluated should remain close to order one. The use of dimensionless variables avoids the risk of using values that lay outside the range of numbers that can be represented in the computer architecture, and of incurring rounding errors.
During the normalization procedure, the simulation quantities $x_p$ (position), $v_p$ (velocity), $t$ (time), $B$ (magnetic field), $E$ (electric field), $\rho$ (charge density), and $q_s/m_s$ (particle mass ratio) are redefined as:

\begin{align*}
x_p &= x_p' L \\
v_p &= v_p'(VEL) \\
t &= t' \frac{L}{VEL} \\
B &= B' B_0 \\
E &= E' B_0 \\
\rho &= \rho' \rho_0 \\
\left(\frac{q_s}{m_s}\right) &= \left(\frac{q_s}{m_s}\right)' \left(\frac{Q}{M}\right).
\end{align*}

The quantities represented by capital letters in Equations 5.1 trough 5.7 are the normalization values; the primed quantities are the quantities expressed in the dimensionless units. The choice of dimensionless variables and parameters is dictated by the governing equations and the geometry. Consider the particle equation of motion and the divergence equation from Maxwell’s equations:

\[ \frac{d\mathbf{v}_p}{dt} = \frac{q_s}{m_s} \left( \mathbf{E} + \frac{\mathbf{v}_p}{c} \times \mathbf{B} \right) \]
\[ \nabla \cdot \mathbf{E} = 4\pi \rho. \]

These equations when written in dimensionless form lead to:

\[ \frac{d\mathbf{v}_p'}{dt'} = \left( \frac{QB_0 L}{M(VEL)^2} \right) \left( \frac{q_s}{m_s} \right)' \left( \mathbf{E}' + \frac{\mathbf{v}_p'}{c'} \times \mathbf{B}' \right) \]
\[ \nabla' \cdot \mathbf{E}' = \left( \frac{L\rho_0}{B_0} \right) 4\pi \rho', \]

suggesting the two dimensionless parameters of the system, $\frac{QB_0 L}{M(VEL)^2}$ and $\left( \frac{L\rho_0}{B_0} \right)$. If two different physical systems $S_1$ and $S_2$ are considered, the first denoted by its typical quantites $L_1, (VEL)_1, B_1, \rho_1$, and the second by $L_2, (VEL)_2, B_2, \rho_2$, then the plasma
will behave in the same manner in the two systems, if:

\[
\frac{Q_2 B_2 L_2}{M_2 (VEL)^2_2} = \frac{Q_1 B_1 L_1}{M_1 (VEL)^2_1}
\] (5.10)

\[
\frac{L_2 \rho_2}{B_2} = \frac{L_1 \rho_1}{B_1}.
\] (5.11)

Thus the governing equations can be written in terms of the dimensionless variables, with:

\[
\frac{Q B_0 L}{M (VEL)^2} = 1
\] (5.12)

\[
\frac{L \rho_0}{B_0} = 1.
\] (5.13)

Many dimensionless variables and units can be used depending on the space-time scales of interest. Because the neutralization process is dominated by the electron dynamics, as shown in Chapter 1, the choice to take the electron scales as reference, is a good choice for the neutralization problem. The charge to mass ratio, \(Q/M\), is therefore chosen equal to one for the electrons. If \(Q/M\) is the real electron charge-mass ratio, then \((\frac{q_e}{m_e})' = 1\), \((\frac{q_K}{m_K})' = -\frac{m_e}{m_K}\) and \((\frac{q_{Ba}}{m_{Ba}})' = -\frac{m_e}{m_{Ba}}\) for the Potassium and Barium mass ratio. Two parameters among \(B_0, L, VEL\) and \(\rho_0\) can be chosen freely, while the remaining two will be dictated by the previous relations. The speed of light \(c\) in the simulation has been chosen as reference velocity \(VEL\), and the background plasma density \(\rho_0\) as reference density. Thus the simulation time is normalized to the inverse of the electron plasma frequency \(\omega_{pe}^{-1}\), and the length scale is normalized to electron skin depth \(c/\omega_{pe}\). The electric field and magnetic field are normalized to \(\rho_0 c/\omega_{pe}\). All the quantities reported in the results and discussion sections of this dissertation are expressed in these normalized units, if not differently stated.

### 5.3 Beam Parameters

The necessary parameters for the simulations are the beam composition, the charge on each ion, the beam radius \(r_{beam}\), the beam velocity \(v_{beam}\), and the current \(I\). The
Table 5.1: NDCX representative beam parameters, used in the simulations.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
<th>Dimensionless Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>beam element</td>
<td>Potassium</td>
<td>-</td>
</tr>
<tr>
<td>charge status</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>beam radius</td>
<td>3 cm</td>
<td>0.84</td>
</tr>
<tr>
<td>beam length</td>
<td>6 cm</td>
<td>1.68</td>
</tr>
<tr>
<td>propagation velocity</td>
<td>300 keV</td>
<td>0.004</td>
</tr>
<tr>
<td>beam current</td>
<td>5 mA</td>
<td>-</td>
</tr>
<tr>
<td>beam thermal velocity</td>
<td>0.1 eV</td>
<td>7.98e-05</td>
</tr>
<tr>
<td>beam density</td>
<td>1.27e+08 cm⁻³</td>
<td>0.00254</td>
</tr>
<tr>
<td>electric field</td>
<td>2.8e-14 V·m</td>
<td>1.0</td>
</tr>
<tr>
<td>magnetic field</td>
<td>2.8e-08 G</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Beam velocity $v_{beam}$ is typically expressed as a temperature $T$ in units of electronvolt. The beam velocity $v_{beam}$ is calculated from the temperature [66]:

$$v_{beam} = \left(\frac{K_B T}{m_K}\right)^{1/2}, \quad (5.14)$$

where $K_B$ is the Boltzmann constant, and $m_K$ is the Potassium mass. The current $I$ is defined as [1]:

$$I = q \cdot n_{beam} \cdot v_{beam} \cdot \pi r_{beam}^2. \quad (5.15)$$

Given the beam propagation velocity from Equation 5.14, and the radius of the beam, it is possible to calculate the density of the beam from Equation 5.15.

Table 5.1 presents the parameters of a representative beam for the NDCX configuration. These values are used in the simulations carried out here. These parameters are in part from the reference [2] and [3] and in part provided by the scientists conducting experiments at LBNL [9].
Table 5.2: Background plasma parameters, used for the simulations.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
<th>Dimensionless units</th>
</tr>
</thead>
<tbody>
<tr>
<td>plasma density</td>
<td>$1 \times 2 \times 4 \times 8 \times 16 \times (1.27 \times 10^8)$</td>
<td>1.0</td>
</tr>
<tr>
<td>electron thermal velocity</td>
<td>3eV</td>
<td>0.003</td>
</tr>
<tr>
<td>Barium thermal velocity</td>
<td>3eV</td>
<td>6.81e-6</td>
</tr>
</tbody>
</table>

5.4 Background Plasma Parameters

The FEPS plasma parameters in the NDCX have been presented in Chapter 1. The parameters used in this dissertation are summarized in Table 5.2. The background plasma density has been chosen to be equal to the beam density. In addition, the background plasma density has been varied by an order of magnitude to study the effect of the background plasma density on the plasma neutralization.

5.5 Geometric Configurations

The simulations in this dissertation have been carried out in a Cartesian geometry with uniformly spaced grids. The simulation box is fixed (i.e. it does not move with the beam). The size of the simulation box is 12 times the radius of the beam in all the simulations. The beam is initialized at the center of the simulation box at the beginning of the simulation. The beam neutralization process has been investigated in two geometrical configurations: a two dimensional geometry to study the neutralization on a plane perpendicular to the beam propagation, and a three dimensional geometry to simulate the entire system. The beam is circular in the case of the two dimensional simulation, and it is an ellipsoid (long axis in the beam direction) in the case of the three dimensional simulation. The two dimensional configuration provides a simplified version of the whole system, still retaining its main characteristics. More importantly, it requires less computer memory and computational time, and
the analysis of the simulation results is considerably easier because of the reduced amount of data. Typically, the particle data is of the order of a MB per cycle for a two dimensional simulation, while it is 100 MB per cycle for the three dimensional simulations. For this reason, simulations of the phase space configuration, the velocity distribution and particle trajectories, have been carried out only in the two dimensional configuration. Figure 5.1 shows the geometrical configurations for the 2D and 3D simulations. In the three dimensional set-up, the beam moves in the $z$ direction, and an $x - y$ coordinate system is placed on the moving beam in the three dimensional configuration for diagnostic purpose. Following References [2] and [3], periodic boundary conditions for the field and particles quantities over all the sides have been chosen. In addition to the conventional periodic boundary condition, particles exiting from one side are readmitted on the opposite side with a random position and random thermal velocity. This eliminates the possibility that density waves, such as Langmuir waves, could exit from one side and re-enter on the opposite side.
5.6 Simulation Diagnostics

One of the advantages of using Particle-in-Cell methods is that a large number of output quantities are evaluated and are directly available for various uses. The user has information both on the distribution of the plasma particles and of the fields. The study of the neutralization process in this dissertation focuses on the analysis of the following quantities:

1. Charge density. Two charge density quantities are important for the neutralization problem: the net charge density, defined as the sum of the density of the beam, background electrons and background ions; and the electron charge density. A beam is called charge neutralized when the net charge density is equal to zero, or the electron charge density is equal to the beam charge density.

2. Electric field. The electric field is the driving force of the neutralization process. An electric field builds up to establish zero net charge density, when an imbalance of the net charge density is present. Strong electric field corresponds to high net charge density imbalance and low level of neutralization. In the two dimensional simulation, a parameter to characterize the beam neutralization is the radial average electric field of the beam, defined as

\[ <E_r> = \frac{2}{r^2_{\text{beam}}} \int_0^{r_{\text{beam}}} r \cdot E_r(r) dr. \] (5.16)

3. Electron average velocity. During the neutralization, the electrons not only need to spread across the beam, but also adapt their velocity to the beam propagation velocity. When the electron mean velocity is equal to the beam propagation velocity, the beam is called current neutralized. The electron average velocity can be calculated as:

\[ <v_e> = \frac{J_e}{\rho_e}, \] (5.17)
where the $J_e$ and $\rho_e$ are respectively the electron charge and current densities. Because, the movement in the $z$ direction is taken into account in the three dimensional configuration only, the study of the electron average velocity is completed in the three dimensional simulations only.

4. Electron phase space. The particle phase space consists of all values of particle position and velocities. The phase space is useful to detect eventual phase space mixing structures, such as vortices, that leads to the beam neutralization.

5. Electron velocity distribution function. The distribution function can be reconstructed from the knowledge of the computated particle velocity. Humps in the velocity distribution function can reveal wave-particle resonance phenomena, such as Landau damping, and beam instabilities [11]. The radial distribution function is calculated as:

$$f(v_r) = 2\pi \int_0^{3\cdot r_{beam}} r \cdot f(r, v_r) dr.$$  \hspace{1cm} (5.18)

To compare the distribution functions at different times, the velocity distribution function is normalized over the integral $\int_{-\infty}^{+\infty} f(v_r) dv_r$.

6. Electron trajectories. The orbits of selected ”computational” electrons can be tracked during the simulation. The study of particle orbits can reveal possible acceleration mechanisms.

7. Magnetic field. A moving beam produces a magnetic field in agreement with the Ampere’s law. The magnetic field in turn influences the propagation of the beam at high beam current values. The electron currents, that provide the beam neutralization, produce an additional magnetic field. In this dissertation, the magnetic field has been studied to determine its influence on the dynamics of the neutralization.
In addition to the quantities above, the conservation of the total momentum and of the total energy of the system needs to be monitored constantly during the simulation. In fact, the Particle-in-Cell method described in Chapter 2 conserves momentum to machine precision. However, the total energy is not conserved exactly. The fundamental reason is that the Particle-in-Cell method uses many particles per cell: there are infinite particle configurations resulting in the same value of the quantities projected to the grid. This degree of freedom is what causes the lack of exact energy conservation [21]. For this reason the total energy of the system needs to be monitored constantly.

5.7 The Choice of the Simulation Time Step

As pointed out in the previous section, one of a test of a computer simulation is that it conserves the total energy of the system. A simulation must be discarded, if it does not conserve the total energy, and a smaller time step needs to be used. All the simulations reported in this dissertation have been checked for energy conservation and they always preserved energy with less than 1\% variation. Figure 5.2 shows the typical evolution of the total energy of the system, as sum of the particle kinetic energies \( \frac{1}{2} \sum_{n_s}^{N_s} m_n v_n^2 \) and of the electromagnetic energies \( \frac{1}{8\pi} \sum_{g}^{N_g} (E_g^2 + B_g^2) \) for the simulation of the ion beam neutralization. The simulation of the neutralization process adds a further constraint on the choice of the time step. It is clear from the numerical dispersion relation of the implicit Particle-in-Cell method given in Chapter 2, that high frequency waves, such as the Langmuir waves, are numerically damped by the implicit Particle-in-Cell scheme. In fact, the neutralization process is characterized by large electron oscillations, and Langmuir waves are excited by these oscillations. Langmuir waves must not be numerically damped, because the Langmuir waves are an important phenomenon of the modeled system.

The numerical damping of the implicit Particle-in-Cell method depends on the
Figure 5.2: Evolution of the kinetic, electromagnetic and total energies. The total energy is perfectly conserved.
value of the de-centering parameter $\theta$ and on the choice of the simulation time step. As shown in Chapter 2, the numerical damping is minimum for $\theta$ equal to 0.5. Thus, $\theta$ equal to 0.5 has been chosen for all the simulations. Simulations with different time steps have been run to determine the time step that does not introduce numerical damping. A Langmuir wave, with wave number equal to $1 \omega_{pe}/c$, has been excited in a system with the same parameters as the NDCX simulations. The wave electric field has been simulated with an explicit Particle-in-Cell code, that does not numerically damp, and with implicit moment Particle-in-Cell code with two different time steps. Figure 5.3 shows the electric field of the Langmuir wave evolution. The Landau damping is absent when the NDCX simulation parameters are chosen. However, numerical damping is introduced in the case of the implicit moment Particle-in-Cell code, with large $\Delta t$. The Langmuir wave electric field is damped numerically (Figure
5.3) when a time step equal to 0.2 is chosen. However, no numerical damping is present when the time step is 0.01. Thus, the time step chosen for the all the simulations presented in this dissertation, is equal to 0.01. This value of the time step leads to optimal energy conservation and no numerical damping.

5.8 The Choice of the Grid Spacing

The explicit Particle-in-Cell methods must satisfy a numerical condition about the choice of grid spacing. This constraint arises from the condition of avoiding a numerical instability, called finite grid instability that arises because of the loss of information during the interpolation between the grid and the particles. The numerical constraint on the grid spacing is

\[ \Delta x < \varsigma \Lambda_D \]  \hspace{1cm} (5.19)

where \( \varsigma \) is a proportionality constant. The value of \( \varsigma \) is equal to one [14; 15] for the explicit Particle-in-Cell method, while there is no restriction on \( \Delta x \) for the implicit Particle-in-Cell methods, provided that the convergence condition is satisfied \( v_{\text{th}} \Delta t < \Delta x \) [21]. Thus, the implicit Particle-in-Cell method allows larger grid spacing than the ones allowed by explicit Particle-in-Cell scheme. However, the physics of the simulated system requires the spatial resolution over the Debye length in the implicit moment Particle-in-Cell simulations (as well as when using the explicit scheme). In fact, the interaction of the plasma and the beam is localized at the beam-plasma interface, where the boundary layer is characterized by scales of the order of Debye length. All the simulations carried out for this dissertation, resolve the Debye length, because it is important to describe accurately the physical interactions on the boundary layer between the beam and the plasma. A series of simulations has been carried out using different grid resolutions, always resolving the Debye length. Table 5.3 presents the grid resolution and the ratio between Debye Length \( \Lambda_D \) and the grid spacing \( \Delta x \) for
Table 5.3: Grid resolutions of the carried out simulations.

<table>
<thead>
<tr>
<th>Grid Resolution</th>
<th>BG Plasma Density/Beam density</th>
<th>$\lambda_D/\Delta x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>512 × 512</td>
<td>1</td>
<td>4.87</td>
</tr>
<tr>
<td>512 × 512</td>
<td>2</td>
<td>3.44</td>
</tr>
<tr>
<td>512 × 512</td>
<td>4</td>
<td>2.43</td>
</tr>
<tr>
<td>512 × 512</td>
<td>8</td>
<td>1.72</td>
</tr>
<tr>
<td>512 × 512</td>
<td>16</td>
<td>1.21</td>
</tr>
<tr>
<td>256 × 256</td>
<td>1</td>
<td>2.43</td>
</tr>
<tr>
<td>256 × 128 × 128</td>
<td>1</td>
<td>2.43</td>
</tr>
<tr>
<td>128 × 64 × 64</td>
<td>1</td>
<td>1.22</td>
</tr>
</tbody>
</table>

different configurations of the NDCX simulation. The two main grid configurations used in this dissertation, are 512 × 512 in the two dimensional configuration, and the 128 × 64 × 64 in the three dimensional configuration.

5.9 The Choice of the Number of Particles

Studies of the Particle-in-Cell methods has shown that there is a minimal number of particles required for convergence [43]. If $N_{PC}$ is the number of particle per cell, the minimum number of particles per cell must satisfy the inequality:

$$(\omega_{pe}\Delta t)^2 < N_{PC} \tag{5.20}$$

Because $\Delta t$ has been chosen to be very small (0.01), this inequality is always satisfied. However, an additional requirement is imposed by the physics of the neutralization, and by the need to describe the wave-particle interaction correctly. In fact, it is important that the population of particles that resonates with a propagating wave is statistically well represented by a large number of particles. As a rule of thumb, the Particle-in-Cell code used to model the interaction of particles and waves must use at least 100 particles per species per grid cell [43]. Because the neutralization
depends on accurate modeling of the wave particle interactions, all the simulations carried out for this dissertation have at least 100 particles per cell. This results in using 78,643,200 particles in the two dimensional simulations (512 \times 512 grid), and 157,286,400 in the three dimensional configuration (128 \times 64 \times 64 grid).
Chapter 6

Results of Simulations of the Beam Neutralization in the NDCX Configuration

Results of the simulations carried out for the NDCX settings are presented in this chapter. Results of simulations in the two and three dimensional configurations are reported. Charge densities, electric field, magnetic field, average electron velocity, electron phase space, electron velocity distribution function, and electron trajectories have been studied. In addition, it has been investigated if an equilibrium state is reached at the end of the neutralization transient. Properties of the equilibrium state are also investigated. Moreover, the effect of different background plasma densities have been also analyzed.

It has been found that the neutralization process is characterized by transient electron oscillations, eventually damped by a sheath around the beam-plasma interface, that opposes the oscillations. An oscillating sheath persists indefinitely at the beam-plasma interface that controls the flux of electrons, after the electron oscillations terminate and the beam is charge neutralized. This moving oscillating sheath forms a moving oscillating discontinuity (oscillating shock) in the charge density, the
electric field, and the average electron velocity in front of the beam’s head.

This chapter is organized as follows. Sections 6.1 and 6.2 show respectively the results, for the charge densities, and the electric field to study the dynamics of the charge neutralization. Section 6.3 presents the effects of different background plasma densities on the net charge density and the electric field evolution. The electron average velocity is studied in Section 6.4 to investigate the current neutralization. The configuration of the charge density, electric field, and electron average velocity after the neutralization transient ends, is analyzed in Section 6.5. Sections 6.6, 6.7 and 6.8 present the results of the electron phase space, electron velocity distribution, and the typical electron trajectories in the neutralization process. Finally, the results the evolution of the magnetic field are given in Section 6.9.

6.1 Charge Density

The charge density evolution in the two and three dimensional configurations are presented in this section. The net charge density (the sum of electron, Potassium and Barium densities) is used to investigate the charge neutrality of the beam: a positive or negative net charge density indicates that the beam is not neutralized, while zero net charge density means that the beam is charge neutralized.

6.1.1 Two Dimensional Simulations

Figure 6.1 presents a mosaic plot of the evolution of the net charge. Different tiles of the mosaic plot show the contour plots of the net charge density over a 2D cross section of the beam and surrounding plasma at different times, separated by a time interval of 0.5. The evolution is presented chronologically from left to right, and from top to bottom. The last tile (bottom-right) correspond to $t = 30$. The red color corresponds to positive charge, and therefore to a charged (not neutralized) beam.
The blue color corresponds to zero charge density, and therefore to a neutralized beam. The initial state \((t = 0)\) is shown in the top left tile of Figure 6.1. The beam in the center is in red color, because it is initially not neutralized, while the background plasma is blue because it is neutral. Proceeding from the top left tile to the right of Figure 6.1, the red circle representing the ion beam becomes first orange and then blue, the color representing the complete neutralization. The electrons from background plasma (blue) neutralize the beam, in approximately half plasma period (6 tiles of the mosaic). The neutralization electrons are localized in the proximity of the beam-plasma interface. The electrons in the plasma around the beam move to enter into the beam, and leave a net positive charge (absence of electrons) in the plasma around the beam. The background Barium ions are too heavy to move on the electron time scales and to neutralize this charge imbalance. The net positive charge around the beam is evident in tiles 2A to 2E as a red annulus. Looking at the fourth line of Figure 6.1, the beam is becoming red again as it was at \(t = 0\). This means that the beam is becoming positively charged because electrons are leaving the beam. It turns out that because of the electron inertia more electrons than necessary for neutralization, enter the beam, charging the beam negatively and building an electric field inside the beam that repels electrons. As electrons are expelled, the beam again becomes positively charged and accelerates electron back into the beam. This cycle between the neutralized and charged states, results in electron oscillation. However these oscillations are damped as can be seen in the last snapshot of Figure 6.1 when the beam does not get as positively charged as in earlier cycles.

The electron oscillations are also evident in Figure 6.2, that shows the evolution in time of the net charge density at three fixed points: at the center of the beam, at half the beam radius, and at the beam-plasma interface. The net charge density at the center of the beam, and at half the radius (blue and red color in the plot) oscillate roughly in phase. The net charge density at the beam-plasma interface (in green
Figure 6.1: Mosaic plot of net charge density evolution in the two dimensional geometric configuration. Different tiles, from left to right and from top to bottom, represent snapshots of the net charge density at $\Delta t = 0.5$ intervals. The red color represents positive net charge, while the blue color represents zero net charge and therefore a neutralized beam.
Figure 6.2: Evolution of the net charge density at three fixed points in the two dimensional geometric configuration. The net charge is evaluated at the center of the beam, at half the beam radius, and at the beam-plasma interface. The plots show charge density oscillations due to the neutralization process. The density oscillation at the beam-plasma interface is out of phase with the density oscillation inside the beam.
Radial net charge density spatial profile at times equal 14 (red line) and 16.75 (blue line). The figure shows a depletion of electrons at the beam-plasma interface and an excess of electrons inside the beam at $t = 14$; the opposite situation (depletion inside the beam, and an excess at the interface) occurs at $t = 16.75$.

Color), oscillates also but it is out of phase from the other oscillations. The electrons in proximity of the beam-plasma interface, move in opposite directions compared to the electrons inside the beam. The electron oscillations at all three fixed points, are damped during the first $10 \omega_{pe}^{-1}$, and then continue with a smaller amplitude.

The radial net charge density spatial profile at $t = 14$ and 16.75 are shown in Figure 6.3, and in Figure 6.4 for $t = 0, 15.25, 16, 16.75$ and 17.5. Figure 6.3 shows a depletion of electrons at the beam-plasma interface ($r/r_{beam} = 1$), and an excess of electrons inside the beam at $t = 14$. The opposite situation (electron depletion inside the beam, and excess of electrons at the interface) occurs at $t = 16.75$. This is in agreement with the results of Figure 6.2, where the charge density oscillations at the
Figure 6.4: Radial net charge density spatial profile at $t = 0, 15.25, 16, 16.75$ and $17.5$. 
Figure 6.5: Contour plot of the net charge density in the 3D configuration at different times. The absence of iso-surfaces means that the net charge density is zero, and consequently the beam is neutralized. The beam is completely neutralized at time 31, and presents a discontinuity in the net charge density in the proximity of the beam’s head.

beam interface, and inside the beam, were shown to be out of phase.

6.1.2 Three Dimensional Simulations

Figure 6.5 shows different snapshots for four iso-surfaces (+ 0.053, + 0.03, -0.03, -0.053) plots of net charge density for the 3D simulations. Iso-surfaces with positive and negative net charge densities are shown. Surface represented for the charge densities equal to zero (neutralized case) are not shown. The red and blue colors represent positive and negative charge densities, respectively. The beam is moving from left to right in the Figure 6.5. Initially, the plot shows the beam is not neutralized (only
the ion beam is a red ellipsoid) and the background plasma has no net charge density and therefore is not shown. The beam becomes negatively charged (blue) at \( t = 1.50 \). A red shell surrounds the ellipsoid, representing the depletion of electrons around the beam. The same phenomenon was observed in the two dimensional simulations. The beam continues to experience electron oscillation at \( t = 10.50 \). An enhanced electron density region with a bow shape appears in front of the head of the beam. The beam is completely neutralized at \( t = 31 \) and therefore the beam is not shown by the iso-surfaces. The same bow-shaped region that was seen at \( t = 10.50 \), appears in front of the beam at \( t = 31 \) but with red color, indicating a depletion of electrons.

Figure 6.6 shows the net charge density evolution along \( z \) axis in the \((z,t)\) plane. The beam is initially centered at \( z = 0 \), and moves from left to right. Each horizontal line of the plot represents the charge density along the \( z \) axis. Each column represents the time evolution of the net charge density at a specific point, placed on \( z \) axis lines. The red and blue colors represent a positive and negative net charge density; while the yellow and orange colors represent near zero net charge density. The beam is completely red (positively charged) at the \( t = 0 \). After one plasma period, the beam becomes blue and negatively charged. The oscillations last until \( 35 \omega_{pe}^{-1} \) and the beam is longitudinally neutralized (yellow and orange colors). There is a region in front of the beam’s head with oscillating net charge density between positive and negative values: an oscillating sheath.

The electron density evolution along the \( z \) axis is shown in Figure 6.7. In this case, the yellow color represents an electron density twice the initial electron density (red color). The beam becomes completely yellow around \( t \approx 35 \).

Figure 6.8 shows the transversal neutralization of the beam, i.e. the net charge density evolution along the \( x \) axis (perpendicular to the beam propagation direction), placed at the center of the beam and moving with the beam, is shown. It is clear that the beam undergoes electron oscillations in the transversal direction also, and it
Figure 6.6: Net charge density evolution along the $z$ axis. The beam is initially centered at $z = 0$ and moves from left to right. The dashed lines show the beam’s head and tail.
Figure 6.7: Electron charge density evolution along the $z$ axis. The beam is initially centered at $z = 0$, and proceeds from left to right.
Figure 6.8: Net charge density evolution along the $x$ axis, moving with beam.
Figure 6.9: Beam charge density evolution along the $z$ axis. The beam is initially centered in $z = 0$ and moves from left to right. It is completely neutralized at around $t \approx 20$. Figure 6.8 shows that the neutralization process starts from the head of the beam, and then propagates to the tail.

The neutralization process does not have an effect on the beam ion dynamics, because the Potassium ions are too heavy to respond to the electric field perturbation that occur on the electron time scales. Figure 6.9 presents the beam density evolution on the $z$ axis. The beam is initially centered at $z = 0$, and moves from left to right. The red color represents the ion beam, while the blue color represents the background plasma. It is clear from Figure 6.9 that the beam proceeds undisturbed, and the neutralization process does not have any noticeable influence on the beam propagation.
6.2 Electric Field

The evolution of the electric field are presented in this section in the two and the three dimensional configurations. The electric field is used to investigate the charge neutrality of the beam. The presence of an electric field inside the beam indicates that the beam is not neutralized, while zero electric field means that the beam is charge neutralized.

6.2.1 Two Dimensional Simulations

Initially, the electric field is zero at the center of the beam and grows linearly from the center of the beam, to the beam-plasma interface. The electric field reaches the maximum at the edge of the beam, and it decays after that, as the inverse of the distance from the beam center. The electric field spatial profile at $t = 0$ is shown in Figure 6.10.

Figure 6.11 shows a mosaic plot of the electric field intensity evolution, in the two dimensional configuration. Different tiles of the figure represent different contour plots of the electric field intensity at $0.5 \omega_{pe}^{-1}$ time intervals, similar to the mosaic plot of the net charge density shown in the previous section. The cronological order is from left to right, and from top to bottom. The red color represents a high intensity electric field, while the blue color indicates a zero electric field. It is important to note that the red color represents both negative and positive high intensity electric fields. The electric field becomes zero after only half plasma period, as is evident in the first tile of the second line of Figure 6.11, where the tile is completly blue (zero electric field). However, the electric field intensity starts oscillating as a consequence of the electron oscillations. After a brief transient, the electric field is dramatically damped, and it oscillates only with a small amplitude.

Figure 6.12 shows the spatial profile of the radial electric field at different times.
Figure 6.10: Radial electric field at $t = 0$. The electric field is zero at the center of the beam and grows linearly from the center of the beam to the beam-plasma interface. The electric field reaches the maximum at the edge of the beam, and it decays after that as the inverse of the distance from the beam center.
Figure 6.11: Mosaic plot of the electric field intensity evolution, in the two dimensional configuration. Different tiles, from the left to the right and from the top to the bottom, show the electric field intensity at time intervals of 0.5.
Figure 6.12: Spatial profile of the radial electric field at different times.

One important characteristic of the radial electric field spatial profile, is the change of sign in the proximity of the beam-plasma interface. For instance, the radial electric field at \( t = 7 \) is negative inside the beam \((r/r_{beam} < 1)\), and positive outside the beam \((r/r_{beam} > 1)\). The opposite situation occurs at \( t = 8.5 \). The radial electric field accelerates the electrons in opposite directions in the proximity of the beam-plasma interface. This phenomenon was also observed in the study of the charge density (see Figure 6.2).
6.2.2 Three Dimensional Simulations

The results of the three dimensional simulations for the electric field are presented in this subsection.

Figure 6.13 shows the evolution of the $z$ component of the electric field, in the $(z, t)$ plane. The beam is initially centered in $z = 0$ and is moving along the $z$ direction from left to right in the plot. The colors are red and blue for positive and negative electric field in the $z$ direction, respectively. The green color represents zero electric field. The electric field at $t = 0$ is outward (electrons due to their negative charge are accelerated inward) as shown in the figure by the red color on the right side of the beam ($z > 0$) and blue on the left side of the beam ($z < 0$). After a time lapse of $3 \omega_{pe}^{-1}$, an opposite configuration with the electric field pointing inward, occurs. The oscillation lasts for approximately $20 \omega_{pe}^{-1}$. After this transient, the oscillation of the electric field remains localized around the head of the beam.

Figure 6.14 shows the evolution of the $x$ component of the electric field along the $x$ axis (perpendicular to the beam propagation), moving with the beam. The goal is to study the evolution of the radial electric field, in the radial direction. As in Figure 6.13, the electric field is initially inward. The radial electric field oscillates until approximately $20 \omega_{pe}^{-1}$, after which the electric field is nearly zero inside the beam.

Figure 6.15 shows the electric field lines at $t = 0$, and at $t = 20$. The electric field during the neutralization transient moves from an open to a closed configuration of the field lines.

The evolution of the three dimensional electric field lines at $t = 14, 17, 20$ and $24$, is shown in Figure 6.16. The beam is moving in the $z$ direction (pointing upward in these plots). The color indicates the intensity of the electric field, with red color representing high intensity electric field and blue color representing low intensity electric field. The electric field lines, that are initially open, close around the beam,
Figure 6.13: Evolution of the $z$ component of the electric field in the $(z,t)$ plane. The beam is initially centered at $z = 0$ and moves from left to right. The dashed lines show the beam’s head and tail.
Figure 6.14: Evolution of the $x$ component of the electric field along the $x$ axis.

Figure 6.15: Electric field intensity at $t = 0$ and at $t = 20$ in the three dimensional configuration. During the neutralization transient the electric field moves from an open to a closed configuration of the field lines.
Figure 6.16: Electric field lines evolution. Different colors represent the intensity of the electric field. The beam is propagating in the $z$ direction.

as shown in Figure 6.15. The head of the beam is shielded at all times. The electric field, as shown in Figure 6.16, is not entering longitudinally in the beam, but it is deflected around at the beam’s head, and enters radially into the beam after the shield. The shield has a bow shape, that oscillates in intensity with time.

Details of the electric field around the beam at $t = 20$ are shown in Figure 6.17. The shield is present at the beam’s head and has a bow shape. The strong electric field (red color) is localized at the beam tail and it has primarily a radial component.

Figure 6.18 shows the electric field lines at $t = 17$ and 20. Colors represent the electric field component in the beam propagation direction ($z$ direction). Lines are red when the $z$ component of the electric field is positive, and blue when negative. The electric field in the $z$ direction is positive at the head of the beam, and negative
Figure 6.17: Electric field lines at $t = 20$, with colors representing the intensity of the electric field. The beam is moving from the bottom to the top of the figure.
at the tail at $t = 17$. The opposite configuration, with negative electric field at the head of the beam, occurs at $t = 20$. Thus, the electric field also undergoes through oscillations during the neutralization process. Similar oscillation of the electric field occurs in the radial direction also, as suggested by Figure 6.19. In this case, the color represents the electric field in the $x$ direction (red when the component is positive, and blue when the component is negative). The electric field is outward at the tail of the beam at $t = 17$, and inward at $t = 20$. 

Figure 6.18: $z$ component of the electric field at $t = 17$ and 20. Colors represent the intensity of the electric field component in the $z$ direction. The beam is moving in the $z$ direction.

\begin{center}
\includegraphics[width=\textwidth]{figure6_18}
\end{center}
Figure 6.19: \( x \) component of the electric field at \( t = 17 \) and 20. Colors represent the intensity of the electric field component in the \( x \) direction. The beam is moving in the \( z \) direction.
6.3 Net Charge Density and Electric Field with Different Background Plasma Densities

The simulation of the NDCX for different background plasma densities are presented in this section for the two dimensional configuration. Simulations have been carried out for background plasma density equal to 2, 4, 8, and 16 times the beam density.

Figures 6.20 trough 6.23 show the net charge density evolution for different background plasma densities. The net charge density initially oscillates in all the mosaic plots. However, the oscillation frequency depends on the background plasma and beam densities. Moreover, it is important to note that the sheath at beam-plasma interface is present in all the cases. For example, when the background density is higher, such as in Figure 6.23, the circle representing the presence of a sheath is weaker but still recognizable.

The evolution over time of the average radial electric field for different background plasmas is shown in Figure 6.24. The electric field when the background plasma density is equal to the beam density is shown in black color. The red, blue, and green colors represent the electric field with background plasma density equal to 4, 8 and 16 times the beam density. The average radial electric field oscillates with a frequency that depends on the beam and background plasma densities:

$$\omega_n = \sqrt{\frac{4\pi(n_{\text{beam}} + n_{\text{plasma}})q_e^2}{m_e}}.$$  \hspace{1cm} (6.1)

The damping of the average electric field is important when the background plasma and beam densities are close in value, while it is weaker when the background plasma density is higher than the beam density.
Figure 6.20: Mosaic plot of net charge density evolution in the two dimensional geometric configuration. The background plasma density is twice the beam density. Different tiles, from left to right and from top to bottom, represent snapshots of the net charge density at $\Delta t = 0.5$ intervals. The red color represents positive net charge, while the blue color represents zero net charge and therefore a neutralized beam.
Figure 6.21: Mosaic plot of net charge density evolution in the two dimensional geometric configuration. The background plasma density is 4 times the beam density. Different tiles, from left to right and from top to bottom, represent snapshots of the net charge density at $\Delta t = 0.5$ intervals. The red color represents positive net charge, while the blue color represents zero net charge and therefore a neutralized beam.
Figure 6.22: Mosaic plot of net charge density evolution in the two dimensional geometric configuration. The background plasma density is 8 times the beam density. Different tiles, from left to right and from top to bottom, represent snapshots of the net charge density at $\Delta t = 0.5$ intervals. The red color represents positive net charge, while the blue color represents zero net charge and therefore a neutralized beam.
Figure 6.23: Mosaic plot of net charge density evolution in the two dimensional geometric configuration. The background plasma density is 16 times the beam plasma density. Different tiles, from left to right and from top to bottom, represent snapshots of the net charge density at $\Delta t = 0.5$ intervals. The red color represents positive net charge, while the blue color represents zero net charge and therefore a neutralized beam.
Figure 6.24: Radial electric field with different background plasma densities.
6.4 Electron Average Velocity

The electron average velocity is an important quantity to determine if the beam is current neutralized. Current neutralization occurs when the electron average velocity is equal to the beam propagation speed. The results of the three dimensional simulations are analyzed because only the three dimensional simulations include the propagation of the finite beam in the $z$ direction. The electron average velocity is calculated using Equation 5.17. For reference, the beam propagation speed is equal to 0.004 ($c$ units).

Figure 6.25 shows the evolution of the $z$ component of the electron average velocity in the $(z,t)$ plane. Initially, average of the $z$ component of the velocity is roughly three times the beam propagation velocity, and oscillate in time between positive
and negative values (opposite directions). After the initial transient over $20 \omega_{pe}^{-1}$, the electron average velocity decreases considerably inside the beam. The high values of electron average velocity remain localized at the extreme points of the beam. However after the transient, the $z$ component of the average velocity continues to oscillate between the values of -0.004 and 0.004.

Figure 6.26 shows still the $z$ component of the electron average velocity, but in the $(x,t)$ on a reference system moving with the beam. As in Figure 6.25, the electron average velocity oscillates between positive and negative values. Thus the ion beam is not current neutralized.
Figure 6.27: Evolution of the net charge density in the \((z,t)\) plane, after the neutralization transient. The net charge density oscillates in the proximity of the beam’s head.

6.5 Equilibrium State

The neutralization process is characterized by the initial electron oscillations, as shown in the previous sections of this chapter. The time evolution of the physical quantities after the initial neutralization transient is terminated, are analyzed in this section. The goal is to investigate if a steady state or equilibrium is achieved.

Figures 6.27 and 6.28 show the values of the net and electron charge densities in the \(z\) direction, after the initial transient is over. It is clear from the two figures that the beam is completely neutralized. However, the densities still oscillate in a small region around the beam’s head.

The evolution of the \(z\) component of the electric field along the \(z\) axis, after
Figure 6.28: Evolution of the electron charge density in the \((z,t)\) plane \((r = 0)\), after the neutralization transient. The electron charge density oscillates in proximity of the beam’s head.
The initial neutralization transient is terminated, is shown in Figure 6.29. The $z$ component of the field is almost zero inside the beam (neutralized beam), but it is high at the beam’s head, and it keeps oscillating between positive and negative values.

Figures 6.30 and 6.31 show the spatial profile of the $z$ component of the electric field along the $z$ axis ($r = 0$), for $t$ over 55.25 to 56.5, and for $t$ 56.75 to 58.0, respectively. It is clear that the discontinuities of the electric field in front of the beam oscillate between positive and negative values also, after the neutralization transient is terminated.

The contour plot of the intensity of the electric field is shown in Figure 6.32. The beam is moving from the bottom to the top of the plot. The electric field contour
Figure 6.30: Spatial profile of $z$ component of the electric field from time 55.25 to time 56.5.
Figure 6.31: Spatial profile of the $z$ component of the electric field at six different times.
plot shows a V-shaped discontinuity in the proximity of the beam’s head (top part of
the plot).

Figures 6.33 and 6.34 show the $z$ component of the electron average velocity in
the $(z, t)$ and $(x, t)$ planes. The strong electron velocities are localized around the
beam’s head, and they oscillate between negative and positive values, similar to the
oscillations in the electric fields.

6.6 Electron Phase Space

Results for the phase space $(r, v_r)$ of the electron population are presented in this
subsection. The initial population is distributed uniformly in space, and it has a
**Figure 6.33:** Evolution of the electron average velocity along the $z$ axis after the neutralization transient.
Figure 6.34: Evolution of the average electron velocity in the direction $z$ along the $x$ axis after the neutralization transient
Figure 6.35: Number of electrons in the phase space \((r, v_r)\) at \(t = 0\).

Maxwellian distribution velocity, with no drift velocity, and thermal velocity equal to 0.003.

Figure 6.35 shows the initial distribution of the electrons. The phase space has been divided in \(200 \times 200\) phase space elements, and the number of electrons (a reduced sample of the whole electron population) has been counted for each phase space element. Figures 6.35 trough 6.38 show the number of particles for each phase space element at \(t = 0, 5, 10, 15\) and 20. The color key is shown on the right in each figure.

Figure 6.36 shows the phase space at \(t = 5\). The majority of electrons has negative radial velocity inside the beam radius \((r/r_{beam} < 1)\). On the other hand, the electrons have positive radial velocity, in the proximity of the beam-plasma interface \((r/r_{beam} \approx 1.2)\). There are two populations of electrons outside the beam radius. Both populations have positive radial velocity. However, one population has large
Figure 6.36: Number of electrons in the phase space \((r, v_r)\) at \(t = 5\).

spread in the velocities at a given \(r\) (bulk electrons outside the beam), where as the other one has a very small velocity spread (filament of Figure 6.36). This second population, is composed of the electrons that are reflected back at high velocity (roughly ten times the thermal velocity) at beam-plasma interface. The electrons are reflected due to a sheath in the proximity of the beam-plasma interface.

Figure 6.37 shows the electron phase space at \(t = 10\). The electrons have slightly negative radial velocity inside the beam radius, and positive radial velocity outside the beam. This means that the electrons inside the beam radius, are moving into the beam, while the electron outside the beam are reflected. The two filaments represent the successive reflections at the beam–plasma interface, due to a sheath.

At \(t = 15\) (Figure 6.38) the electron motion is in opposite directions. The electron mixing in the phase space is shown by the formation of a vortex structure inside the
Figure 6.37: Number of electrons in the phase space \((r, v_r)\) at \(t = 10\). The electrons have slightly negative radial velocity inside the beam radius, and positive radial velocity outside the beam. The two filaments represent the successive reflections at the beam-plasma interface, due to a sheath.
beam radius \((r/r_{beam} < 1)\). In fact, vortices in the phase space indicate a phase space mixing.

Figure 6.39 shows a sharp discontinuity at the beam-plasma interface \((r/r_{beam} = 1)\). The electrons inside the beam are almost thermalized around the velocity equal to zero, while the velocity is on average negative with a smaller velocity spread, outside the beam radius.

### 6.7 Electron Velocity Distribution Function

The initial velocity distribution of the background plasma electrons is a Maxwellian with thermal velocity, \(v_{the} = 0.003\).

Figures 6.40 trough 6.43 show the evolution of the distribution function at \(t =\)
Figure 6.39: Number of electrons in the phase space \((r, v_r)\) at \(t = 20\)
Figure 6.40: Electron velocity distribution at $t = 5$.

5, 10, 15 and 20. The initial distribution function is also shown for comparison.

Figure 6.40 shows the radial distribution function at $t = 5$. The electrons inside the beam radius have negative radial velocity, and create the hump in the left part of the distribution. The electrons outside the beam radius have positive radial velocity, and contribute toward the right hump of the distribution function. The high velocity filament of Figure 6.36 leads to the long tail of the distribution function.

The majority of the electrons at $t = 10$ has positive radial velocity. The peak in the distribution function in Figure 6.41 represents the previously reflected particle populations, and the long tail is due to the most recently accelerated electrons.

Figure 6.42 shows the electron velocity distribution at $t = 15$. In this case, the majority of the electrons has negative radial velocity. The two peaks close to the top of the distribution are two populations of electrons reflected in the previous cycles.
**Figure 6.41:** Electron velocity distribution $t = 10$. 
Figure 6.42: Electron velocity distribution at \( t = 15 \).
Figure 6.43: Electron velocity distribution at time equal to $t = 20$.

Figure 6.43 is the plot of the electron velocity distribution at $t = 20$. The majority of the electrons has negative radial velocity, with two visible peaks representing the reflected electron populations at the beam-plasma interface.

6.8 Electron Trajectories

Figure 6.44 shows the trajectory of a selected number of electrons in the two dimensional simulation. The blue triangle is the initial electron position, while the red triangle is the electron position at the end of the simulation. The black dots are the electron positions at different times with time intervals equal to 0.25. The entire simulation covers a time range $0 < t < 21$. All the trajectories of Figure 6.44 show an oscillating behavior. This is due to the fact that the dynamics of the electrons is
Figure 6.44: Selected electron trajectories during the neutralization process.
driven by the oscillating field of the beam, and then by the oscillating sheath at the beam-plasma interface.

6.9 Magnetic Field Evolution

The magnetic field evolution is studied in this section. Figure 6.45 shows the magnetic field at $t = 20$. The figure shows the magnetic field lines, that are tangent to magnetic field vectors. The color key for the intensity of the magnetic field is also given. The magnetic field is localized around the beam. The magnetic field lines form circles in the plane perpendicular to the beam propagation, i.e. the magnetic field primarily has an azimuthal component only. The intensity of the azimuthal component is not constant along the beam propagation direction, but it varies sinusoidally. If the values of the electric and magnetic fields are compared from Figure 6.45 and 6.17, it is found that peak values of the electric and magnetic fields at $t = 20$, are respectively $6.2 \times 10^{-3}$ and $7.1 \times 10^{-5}$, i.e. the intensity of the magnetic field is less than the intensity of electric field by two orders of magnitude.

Figure 6.46 shows the magnetic field lines at $t = 11, 14, 20$ and $24$. The magnetic field is azimuthal in all four cases. However, the position along the beam where the magnetic field reaches its peak, varies in time. In fact, the magnetic field produced by the beam propagation, is modulated by the neutralization electron currents. The electron current moving into the beam reinforces the magnetic field, because it moves in opposite direction to the beam, and has opposite charge. On the contrary, the electrons moving longitudinally out of the beam, decrease the magnetic field. This phenomenon is evident in Figure 6.47: the $y$ component of the magnetic field along the $x$ axis, moving with the beam, is shown in the $(x, t)$ space.

The magnetic field strength first increases because of the electron neutralization current, and then decreases because of the current going in the opposite direction. The
Figure 6.45: Magnetic field lines at $t = 20$. The color key for the intensity of the magnetic field is also given. The beam is moving in the $z$ direction from left to right in the picture. It is important to note that the intensity of the magnetic field is less than the intensity of the electric field by two orders of magnitude.
Figure 6.46: Magnetic field lines evolution. The beam is moving in the $z$ direction. The magnetic field is azimuthal in all cases shown here.
Figure 6.47: $y$ component of the magnetic field ($B_y$) along the $x$ axis (reference system is placed at the center of the beam and is moving with the beam). The magnetic field only has an azimuthal component and the intensity is modulated over time by the neutralization electron current.
phenomenon is oscillatory and has a maximum at $t = 8$. The magnetic field is not as heavily damped as the electric field (see Figure 6.14), but it continues oscillating.
Chapter 7

Discussion of the Neutralization Dynamics in the NDCX Configuration

This chapter answers the questions introduced in Chapter 1, that motivated this dissertation:

1. What is the dynamics of the neutralization process? Is it a transient phenomenon? Does it reach a steady state?

2. What are the effects of different background plasma densities?

3. What is the effect of the magnetic field? Does it have an effect on the neutralization dynamics?

The simulation results presented in Chapter 6 showed that the neutralization of an ion beam, moving in a plasma, is a transient phenomenon occurring over the time scale of tens of background plasma periods. When the ion beam is introduced in a plasma, the electrons from the background plasma start to move into and out of the ion beam. These large electron oscillations are damped by the formation of an electrostatic sheath forming at the beam-plasma interface. The sheath regulates the flux
of electrons, admitting into the beam some of them, and reflecting the others. After the electron oscillations are damped out and the beam is neutralized, an oscillating shock front is formed as result of the sheath oscillation and of the beam forward propagation. The oscillating shock regulates the flux of electrons between two plasmas (the neutralized beam and the background plasma) with different densities and temperatures.

The goal of this chapter is to analyze in detail the dynamics of the neutralization process, the effects of different background plasma densities and of the magnetic field in the NDCX configuration. Section 7.1 presents the dynamics of the neutralization process, including the electron oscillations, the formation of an oscillating sheath, and of an oscillating shock. The effects of different background plasma densities and of the magnetic field during the neutralization process are analyzed in Sections 7.2 and 7.3.

7.1 Ion Beam Neutralization Dynamics

The results of Chapter 6 showed that the neutralization process is characterized by three phenomena:

1. Initial electron oscillations into and out of the beam. The beam has a quasi-periodic pulsation that alternates the beam net charge, passing through a full neutralization only for one instant.

2. Sheath formation on the interface between the beam and the background plasma. The sheath first dampens the electron oscillations, and then persists after the neutralization is completed, regulating the electron flux between two regions (neutralized beam and background plasma) with two different densities and temperatures.
3. Formation of an oscillating shock by the forward motion of the oscillating sheath associated to the beam.

These three phenomena are investigated in the following sections.

### 7.1.1 Electron Oscillations

When an ion beam is injected in a plasma, the positively charged ion beam creates an outward electric field, as shown in Figure 7.1 a). The electrons respond quickly to the beam electric field, entering into the beam and neutralizing it. However, because of electrons inertia, more electrons enter the beam, than necessary to neutralize the beam, resulting in an excess of negative charge inside the beam, and in an electric field pointing radially inward. The reverse electric field causes electrons to move out of the beam, as shown in Figure 7.1 b). This motion of electrons into-the-beam and out-of-the-beam generates a periodic oscillation of the electrons. These electron oscillations
have been observed in both, the two and three dimensional simulations of Chapter 6. For instance, Figure 7.2 shows the quasi-periodic change in time, from not-neutralized to fully-neutralized states. As discussed in Chapter 6 (Equation 6.1), the electron oscillation frequency is close to the plasma frequency, of a plasma with density equal to the sum of the beam and of the background plasma densities. This oscillation frequency coincides with the oscillation frequency corresponding to the background plasma density in the case of the NDCX, where the background plasma density is two orders of magnitude higher than the beam density. These oscillations have been observed in previous simulations [31], and predicted by analytical calculations [4], but they have not been confirmed by the experiments. It should be noted that it is very difficult to observe the electron oscillations, because of their very high frequency, such as $10^9$ Hz in the case of the NDCX.

### 7.1.2 Oscillating Sheath

In the absence of collisions, such as in the NDCX configuration, and of any damping mechanism, the electron oscillation would continue indefinitely resulting at best only in the beam neutrality in the mean. However, there is experimental evidence in the NDCX [2; 3; 7], and in other neutralization experiments in the context of ion propulsion [68], that the ion beam is completely neutralized, after it passes through a preformed plasma. (This is usually inferred by looking at the divergence of an ion beam immersed in a plasma, which does not increase, proving that the beam is fully neutralized.) The simulations of the beam-plasma interaction reported in References [31], [33], and [32], also showed the perfect beam neutralization after an initial transient. Although the first simulations were aimed to show that neutralization can be achieved, and not to the analysis of the neutralization dynamics, the importance of beam-plasma boundary layer physics was immediately recognized. For instance, it was observed by Buneman and Kooyers [31] that the *advancing head of the beam acts*
Figure 7.2: Mosaic plot of the contour plot of the net charge density. Different tiles, from left to right and from top to bottom, represent snapshots of the net charge density at $3.9 \times 10^{-10}$ s intervals. The red color represents positive net charge, while the blue color represents zero net charge and therefore a neutralized beam. Initially, the beam oscillates between the fully-neutralized and not-neutralized states.
as an electron reflector. The head seems to become more and more diffuse: there appears to be a forward acceleration in space of the first ions, perhaps due the plasma pressure. Dunn and Ho [32] reported that there are excess electrons injected and these excess electrons return to the injection plane. They are reflected by an electron oscillating sheath that feeds the right number of electrons at the right velocity into the ion beam to provide complete neutralization. This second regime may be characterized as the "oscillating-electron-sheath" regime.

In this dissertation, the presence of a sheath at the beam-plasma interface is reported both in the two and three dimensional simulations. For instance, Figure 7.3 shows the presence of a sheath at the beam-plasma interface in the electric field intensity plot. The electric field, represented by arrows, has opposite directions at the interface of the beam and the background plasma. The thickness of the sheath is typically of the order of ten Debye lengths.

Two physical mechanisms contribute to the formation of the sheath at the beam-plasma interface:

1. Plasma with different densities and temperatures are put in contact. A boundary layer is naturally created to regulate the electron flux between the plasma regions with different densities and temperatures.

2. The higher mobility of the electrons compared to the ions creates a depletion of electrons around the beam. The depletion of electrons around the beam builds up an electric field that reflects some electrons.

The electron phase space plots of Chapter 6 clearly indicate that the neutralization process is enabled by the formation of sheaths. The electron oscillations are terminated by the flux of electrons moving in opposite directions in the proximity of the beam-plasma interface. For instance, the vortex structure in the electron phase space shown in Figure 7.4 shows the mixing of the electrons in the proximity of the beam-plasma interface ($r/r_{beam} \approx 1$).
Figure 7.3: The contour and quiver plots of the electric field show a sheath at the beam-plasma interface. The electric field is represented by arrows and has opposite directions at the interface of the beam and the background plasma.
Figure 7.4: The electron phase space shows the electrons undergoing phase mixing in proximity of the beam-plasma interface ($r/r_{\text{beam}} \approx 1$).
Figure 7.5: Discontinuity in the longitudinal electric field, charge density and electron average velocity in the proximity of the beam front at \( t = 58 \).

### 7.1.3 Oscillating Shock

The three dimensional simulations, reported in Chapter 6, showed that the beam undergoing the neutralization process forms an oscillating shock in proximity of the beam head, after the neutralization transient is over. The properties of the beam-plasma system, such as the charge density, the electric field, and the electron average velocity, change abruptly across the shock. Figure 7.5 shows the discontinuities in the electric field in the longitudinal direction, in the net charge density, and in the electron average velocity in the \( z \) direction at \( t = 58 \). The discontinuities are localized in the proximity of \( z \approx 0.95 \).

Moreover, the three dimensional simulations also showed the characteristic shock V shape common to shock phenomena. For instance, Figures 7.6 and 7.7 show this
Figure 7.6: Electric field lines at $t = 50$. The color represents the intensity of the electric field. The beam is shown in the transparent pink color. The beam moves in the $z$ direction from the bottom to the top of the figure. The V-shaped discontinuity of the electric field intensity is clear in the proximity of the beam head.

shape in the electric field lines and in the electron average velocity at $t = 50$.

7.1.4 Oscillating Shock Formation

The shock formation in the proximity of the beam head has been previously observed in other three dimensional Particle-in-Cell simulations [69; 70] aimed at investigating the beam neutralization in the ion thrusters for space propulsion. It was found that the shock formation depends strongly on the electron thermal velocity. Specifically it was found that the shock forms when the ratio of the electron thermal velocity and beam drift velocity $\eta = v_{\text{the}}/v_{\text{beam}}$ is less than 1.7. In addition, it has been suggested that the shock formation might be due to a phenomenon similar to the trapping of
Figure 7.7: Electron average velocity quiver plot on a mid-plane of the 3D domain at $t = 50$. The beam is completely neutralized and the discontinuity in the velocity is clear in the proximity of the beam head (in the transparent pink color).
electrons and ions in the potential of the ion acoustic waves, that generate double layer structures, reminiscent of the shock [71]. However, the authors recognized the fact that ions, because of their high mass and inertia, can not adjust their position in the short electron time scales to participate in the shock formation as supposed by this theory.

An alternative theory of the formation of the shock is proposed in this dissertation. Specifically, it is proposed that a shock forms when the disturbance propagates faster than the signal speed [72]. In a gas, the signal speed is the sound speed of the gas [72], where as in a plasma the signal speed depends on the Alfven and the sound speed [73; 74]. It is proposed that signal speed in the case of the ion beam neutralization is the Langmuir wave group velocity.

In a collisionless plasma, the plasma oscillations propagate by Langmuir waves [59; 75]. During the beam neutralization, the sheath oscillations described in the previous sections, propagate by Langmuir waves into the unperturbed plasma in the same way. In fact, the thermal motion of the electrons carries information about the sheath oscillation from the beam-plasma interface into in the undisturbed background plasma, and the sheath oscillation propagates as a wave. The dispersion relation for the Langmuir waves, the so-called Bohm-Gross equation, is [75; 76]:

$$\omega^2 = \omega_{pe}^2 + 3k^2v_{the}^2. \tag{7.1}$$

The group velocity of the Langmuir waves is:

$$v_g = \frac{d\omega}{dk} = \frac{3k}{\omega}v_{the}. \tag{7.2}$$

The propagation velocity of the Langmuir waves becomes zero, when the electron thermal velocity of the plasma tends to zero.

The shock forms when the beam speed is greater than the Langmuir wave propagation speed. In fact, when the beam exceeds the speed, with which the sheath oscillations in front of the beam travel, the beam overtakes the Langmuir waves. The
Figure 7.8: Scheme of the formation of a shock due to the beam propagation and to the Langmuir waves.

Overtaken waves create a bow wave: a single wave made up of all the sheath oscillations waves that would have propagated ahead of the beam but could not move fast enough. This simple physical mechanism is shown in Figure 7.8.

The simulation results, that are shown in Figure 7.9, are very similar to the cartoon picture of Figure 7.8. In Figure 7.8, the dashed lines represent the Langmuir waves, overtaken by the beam that is propagating forward. The shock has a circular shape at the tail of the beam, retaining the original propagation shape of the Langmuir waves, while the overtaken Langmuir waves form the characteristic shock V shape at the front of the beam. The sheath oscillations are localized around the beam-plasma boundary layer, and are characterized by the wave number of approximately equal to 0.1 (see for instance Figure 7.5) and by an angular frequency described by Equation 6.1. Using the simulation parameters, $k$ can be estimated as $k \approx 2\pi/(0.1) = 62.328$, $\omega = \sqrt{\omega_{pe}^2 + 3k^2v_{the}^2} \approx 1.0$, and $v_{the} = 0.00342$ from the simulation parameters. This
Figure 7.9: Electric field magnitude at $t = 50$. The dashed lines represent the Langmuir waves, overtaken by the beam that is propagating forward.
results in a group velocity \( v_g = 3 \cdot \frac{62.832}{1.0} \cdot 0.00342^2 = 0.0022 \), where the beam velocity \( v_b = 0.004 \). The shock angle \( \theta_S \) can be calculated as \( \sin^{-1}(v_g/v_b) = 33 \) degree, and it is in good qualitative agreement with the shock angle of Figure 7.9.

### 7.2 The Effect of Different Background Plasma Densities

Results of a series of simulations carried out using different background plasma densities were reported in Chapter 6. Figure 6.24 shows the average radial electric field evolution for background plasma densities equal to 4, 8, and 16 times the beam density. Figure 7.10 compares the average radial electric field evolution in a system with \( n_{\text{beam}} = 1.0 \) and 0.5, and \( n_{\text{plasma}} = 1.0 \). It is clear from Figure 7.10 that the background plasma and beam densities have two effects on the neutralization process in the NDCX configuration:

1. The electron oscillations during the neutralization have higher frequency when the sum of the background plasma and beam densities, \( n_{\text{plasma}} + n_{\text{beam}} \), is higher, in agreement with Equation 6.1 in Chapter 6.

2. The damping of the oscillations is important when the background plasma and beam densities are close in value, while it is weaker when the background plasma density is higher than the beam density.

It is important to note that complete beam neutralization in the NDCX configuration can be provided by background plasma with the same density as that of the beam. Thus, plasmas with considerably higher density, such as in the NDCX, are not strictly necessary for the neutralization purpose.

The temperature of the background plasma also affects the neutralization process. Figure 7.11 shows a comparison of the evolution of the average electric field in the
Figure 7.10: Average radial electric field evolution for two systems with $n_{\text{beam}} = 1.0$ and 0.5, and $n_{\text{plasma}} = 1.0$. 
Figure 7.11: Average radial electric field evolution for two NDCX configurations with background plasma $T = 3$ eV and 20 eV. The damping of the average radial electric field increases with the temperature of the background plasma.

beam for background plasma with temperature of 3eV and 20 eV. The damping of the electric field is faster when the background plasma temperature is higher. Background plasma with higher temperature creates sheaths with higher electric field at the beam-plasma interface, and thus to a higher electron mixing that leads to faster neutralization.

7.3 The Effect of the Magnetic Field

The results of Chapter 6 showed that two concurrent phenomena participate in the creation of the magnetic field: first, the beam motion itself generates an azimuthal magnetic field around the beam; second, the neutralizing electron currents generate
an additional magnetic field. The results of Chapter 6 show that the magnetic field only has azimuthal component and is modulated by the neutralization currents.

It useful to compare the value of the electric and magnetic forces in order to determine the importance of the magnetic field. It has been found in the simulations that the typical ratio between the electric and magnetic forces $F_E/F_B$ is:

$$F_E/F_B = \frac{vB}{cE} \approx \frac{1E - 3 \cdot 1E - 3}{1 \cdot 1E - 2} = 1E - 4$$  (7.3)

Thus, the electric field forces acting on the particles in the NDCX simulations is typically ten thousand times stronger than the magnetic field forces.

Additional simulations, where the magnetic field effects are neglected, and the Poisson equation is solved, instead of the Maxwell’s equations, have been carried out for the same simulation set-up to demonstrate that the magnetic field effects are indeed negligible. Figure 7.12 shows the average radial electric field evolution for an electrostatic and for a fully electromagnetic simulation. The results of the two simulations match perfectly, leading to the conclusion that the magnetic field effects in the current NDCX can be neglected, and a simpler electrostatic model of the plasma can be used effectively, saving computational time.
Figure 7.12: Average radial electric field evolution, simulated with an electrostatic and a fully electromagnetic PIC method. Results of the two simulations agree very well.
Chapter 8

Verification and Performance of the Fully Implicit Particle-in-Cell Code

The fully implicit Particle-in-Cell method, described in the second part of Chapter 3, has been implemented in a one-dimensional, electrostatic skeleton code. The fully implicit Particle-in-Cell code has been verified against two test problems: the electron beam instability, and the Landau Damping problems. The computational performance of the fully implicit method has been evaluated using different number of particles, grid points and time step, and then compared to the performance of the explicit Particle-in-Cell method.

The results of the simulation for the electron beam instability problem are presented in Sections 8.1, and the Landau Damping problem in Section 8.2. The performance results of the fully implicit Particle-in-Cell method are then compared to the explicit Particle-in-Cell code performance in Section 8.3. Section 8.4 concludes the chapter, commenting the development of the fully implicit Particle-in-Cell method.
8.1 Electron Beam Instability Simulation

The electron beam instability, presented in Chapter 4, has been chosen as the first verification test for the fully implicit Particle-in-Cell method. Two electron beams, composed of 10,000 electrons, initially flow in opposite directions, with propagation velocities equal to \(+0.5 \, c\) and \(-0.5 \, c\), and thermal velocity equal to \(0.05 \, c\). A background of ions neutralizes the system, with \(\omega_{pe} = 1\). The simulation box \(L_x\) is equal to \(2\pi c/\omega_{pe}\) and the speed of light in vacuum \(c = 1\). A perturbation of the beam densities is initially applied to the electron positions \(x_p\):

\[
x'_p = x_p + 0.01 \times \frac{\cos(kx_p)}{k}
\]

(8.1)

where \(k\) is the wave number of the perturbation. The wave number of the perturbation has been chosen as \(k = 1\) in \(\omega_{pe}/c\) units. Figure 8.1 shows the phase space of the electron beam instability, simulated using the fully implicit Particle-in-Cell code. The perturbation starts growing at \(t = 10 \, \omega_{pe}^{-1}\), and the two beams are mixed at \(t = 20 \, \omega_{pe}^{-1}\). Figure 8.2 shows the electric field energy evolution in a semi-logarithmic plot for the fully implicit Particle-in-Cell method for two values of \(\theta = 0.5, 1\). An explicit Particle-in-Cell code was also used to simulate the same system for comparison. The growth rate of the electric field energy match for all three simulations (the two fully implicit PIC codes and the explicit PIC). The only difference is that the electric field energy saturates at lower level for the fully implicit Particle-in-Cell simulations. The fully implicit method with \(\theta = 1\) saturates at lower level than fully implicit method with \(\theta = 0.5\). This is an effect of the numerical damping introduced by the implicit Particle-in-Cell methods. In fact, the numerical damping is higher for \(\theta\) equal to 1, than \(\theta\) equal to 0.5, as shown in Chapter 2.
**Figure 8.1:** Phase space evolution of the electron beam instability, simulated using a fully implicit Particle-in-Cell method. The perturbation starts growing at $t = 10\omega_{pe}^{-1}$, and the two beams are completely mixed at $t = 20\omega_{pe}^{-1}$.
Figure 8.2: Electric field energy evolution in the two stream instability, simulated with the explicit and the fully implicit Particle-in-Cell codes and 2 values of $\theta$ (0.5 and 1.0). The growth rate of the instability is equal for all the three cases, but the fully implicit PIC codes saturate at lower level, due to numerical damping introduced by the implicit numerical scheme.
8.2 Landau Damping

The fully implicit Particle-in-Cell method has been tested on the Landau Damping problem, presented in Chapter 4. In this test, a Maxwellian plasma is initialized with electron plasma frequency $\omega_{pe} = 1$, and electron thermal velocity, $v_{the} = 0.5c$. The speed light in vacuum $c$ is equal to 1. The number of electrons and ions is 10,000. Length of the simulation box, $L_x = 2\pi c/\omega_{pe}$. A perturbation with wave number $k = 1$ in $\omega_{pe}/c$ units is excited in the system perturbing the electron positions:

$$x_p' = x_p + 0.01 \times \frac{\cos(kx_p)}{k}$$

(8.2)

The simulation time step $\Delta t$ is equal to 0.05. The decay rate, calculated with linear theory is equal to:

$$\gamma = -0.126\omega_{pe}$$

(8.3)

Figure 8.3 shows a comparison of the results, obtained with the fully implicit Particle-in-Cell method with $\theta$ equal to 0.5 and 1, and the linear theory. The simulations and the linear theory result are in good agreement. The Landau damping is slightly enhanced by the numerical damping for $\theta$ equal to 1.

8.3 Computational Performance of the Fully Implicit Method

The computational performance of the fully implicit Particle-in-Cell code has been evaluated, counting the number of FLOPS and the execution time, for 200 and 50 computational cycles of the electron beam instability test problem. A 2 GHz Intel Pentium 4 processor with 256 MB of RAM memory, and the Matlab (5.3 version) have been used for these tests, as in the previous computational tests for the implicit moment Particle-in-Cell code.
Figure 8.3: Simulation of the Landau damping problem using the fully implicit Particle-in-Cell code and comparison with the linear theory. Plot shows the spectral component $k = 1$ for the electric field.
Table 8.1: Number of FLOPS and execution time for 200 cycles of the fully implicit PIC method for different number of particles $N_p$, number of grid points $N_g$, and $\theta$ equal to 0.5, and 1.0. The time step is 0.1.

<table>
<thead>
<tr>
<th>$N_p$</th>
<th>$N_g$</th>
<th>$\theta$</th>
<th>FLOPS</th>
<th>EXECUTION TIME (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5000</td>
<td>64</td>
<td>0.5</td>
<td>8.9769e8</td>
<td>77.692</td>
</tr>
<tr>
<td>10000</td>
<td>64</td>
<td>0.5</td>
<td>1.7832e9</td>
<td>139.17</td>
</tr>
<tr>
<td>20000</td>
<td>64</td>
<td>0.5</td>
<td>3.5892e9</td>
<td>282.136</td>
</tr>
<tr>
<td>10000</td>
<td>128</td>
<td>0.5</td>
<td>1.8178e9</td>
<td>152.57</td>
</tr>
<tr>
<td>10000</td>
<td>256</td>
<td>0.5</td>
<td>1.8829e9</td>
<td>181.43</td>
</tr>
<tr>
<td>5000</td>
<td>64</td>
<td>1.0</td>
<td>1.0447e9</td>
<td>90.52</td>
</tr>
<tr>
<td>10000</td>
<td>64</td>
<td>1.0</td>
<td>2.0807e9</td>
<td>174.621</td>
</tr>
<tr>
<td>20000</td>
<td>64</td>
<td>1.0</td>
<td>4.1199e9</td>
<td>316.6350</td>
</tr>
<tr>
<td>10000</td>
<td>128</td>
<td>1.0</td>
<td>2.1148e9</td>
<td>178.621</td>
</tr>
<tr>
<td>10000</td>
<td>256</td>
<td>1.0</td>
<td>2.1459e9</td>
<td>196.482</td>
</tr>
</tbody>
</table>

The number of FLOPS and the execution time for different number of particles and grid points and for $\theta = 0.5, 1$ are tabulated in Table 8.1. As expected, the number of FLOPS and the execution time, increase with the number of particles, and of grid points. Moreover the computational cost also increases with $\theta$: a larger number of iterations is necessary when $\theta$ is equal to 1.

The performance of the fully implicit Particle-in-Cell code using different time steps are tabulated in Table 8.2. Performance is evaluated for 50 computational cycles of the electron beam instability problem with 10,000 particles, and with 64 grid points. In the fully implicit Particle-in-Cell method, the choice of the the time step determines considerably the number of FLOPS and the execution time. The number of iterations of the fully implicit Particle-in-Cell method increases with the time step.
Table 8.2: Number of FLOPS and execution time for 50 cycles of the fully implicit Particle-in-Cell method for different $\Delta t$.

<table>
<thead>
<tr>
<th>$\Delta t$</th>
<th>$\theta$</th>
<th>FLOPS</th>
<th>EXECUTION TIME (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.5</td>
<td>4.192e8</td>
<td>36.292</td>
</tr>
<tr>
<td>0.2</td>
<td>0.5</td>
<td>5.5442e8</td>
<td>42.3</td>
</tr>
<tr>
<td>0.4</td>
<td>0.5</td>
<td>7.53e8</td>
<td>55.51</td>
</tr>
<tr>
<td>0.6</td>
<td>0.5</td>
<td>9.599e8</td>
<td>67.86</td>
</tr>
<tr>
<td>0.8</td>
<td>0.5</td>
<td>1.1684e9</td>
<td>88.27</td>
</tr>
<tr>
<td>1.0</td>
<td>0.5</td>
<td>1.42e9</td>
<td>95.39</td>
</tr>
<tr>
<td>1.5</td>
<td>0.5</td>
<td>2.21e9</td>
<td>154.57</td>
</tr>
<tr>
<td>1.75</td>
<td>0.5</td>
<td>2.69e9</td>
<td>178.95</td>
</tr>
<tr>
<td>2.0</td>
<td>0.5</td>
<td>3.0529e9</td>
<td>201.58</td>
</tr>
<tr>
<td>2.25</td>
<td>1.0</td>
<td>4.6946e9</td>
<td>292.751</td>
</tr>
<tr>
<td>2.5</td>
<td>1.0</td>
<td>5.2720e9</td>
<td>320.581</td>
</tr>
<tr>
<td>3.0</td>
<td>1.0</td>
<td>6.7560e9</td>
<td>396.921</td>
</tr>
</tbody>
</table>
Table 8.3: Comparison of the number of FLOPS for the explicit (EXP.) and the fully implicit (F.I.) Particle-in-Cell methods.

<table>
<thead>
<tr>
<th>$N_p$</th>
<th>$N_g$</th>
<th>EXP. PIC FLOPS</th>
<th>F.I. PIC FLOPS</th>
<th>F.I./EXP.</th>
</tr>
</thead>
<tbody>
<tr>
<td>5000</td>
<td>64</td>
<td>2.147e7</td>
<td>8.9769e8</td>
<td>41.91</td>
</tr>
<tr>
<td>10000</td>
<td>64</td>
<td>4.2612e7</td>
<td>1.7832e9</td>
<td>41.84</td>
</tr>
<tr>
<td>20000</td>
<td>64</td>
<td>8.4883e7</td>
<td>3.5892e9</td>
<td>42.28</td>
</tr>
<tr>
<td>10000</td>
<td>128</td>
<td>4.2946e7</td>
<td>1.8178e9</td>
<td>42.32</td>
</tr>
<tr>
<td>10000</td>
<td>256</td>
<td>4.3631e7</td>
<td>1.8829e9</td>
<td>43.15</td>
</tr>
</tbody>
</table>

8.4 Comparison of the Performance with the Explicit Particle-in-Cell Method

The computational performance of the fully implicit Particle-in-Cell method has been compared with the performance of the explicit Particle-in-Cell code. Table 8.3 presents the comparison of the computational performances for 200 computational cycles (time steps) of the electron beam instability problem, with time step equal to 0.1. The fully implicit Particle-in-Cell method is on average 42.3 times more computationally expensive than the explicit Particle-in-Cell method. The ratio of the FLOPS of the two methods, is almost constant, and it does not depend on the number of particles and number of grid points. However this ratio would increase, if a larger time step is chosen, since the number of FLOPS of the fully implicit Particle-in-Cell method increases with the time step, while the FLOPS of the explicit Particle-in-Cell would remain approximately constant.

8.5 The Fully Implicit Particle-in-Cell Method Development

This final section answers the question posed in Chapter 1:
1. Is it possible to develop a fully implicit Particle-in-Cell method? Does it converge? If so, what is its computational cost?

A fully implicit Particle-in-Cell method has been developed in a simple one dimensional electrostatic version to prove that the fully implicit Particle-in-Cell method can be implemented. The Newton-Krylov Jacobian-Free Matrix-Free GMRes solver made possible the solution of the non-linear system composed of the coupled field and particle equations. Despite the concern that the fully implicit method might not converge [19], it has been shown that the successive fully implicit Particle-in-Cell iterations are convergent. The method has been tested using two test problems: the electron beam instability and the Landau Damping problems.
Chapter 9

Discussion and Summary of the Implicit Particle-in-Cell Methods for Ion Beam Neutralization Simulations

This final chapter discusses the computational performances, the computer memory requirements, and the advantages of the implicit Particle-in-Cell methods in the beam plasma interaction simulations. This chapter answers the following question posed in Chapter 1:

1. Is it convenient to use the implicit Particle-in-Cell methods to study the neutralization process in the NDCX configuration?

The implicit Particle-in-Cell methods are more computationally intensive than the explicit Particle-in-Cell methods, resulting on average 4 and 40 times more computationally expensive than the explicit Particle-in-Cell scheme. The implicit Particle-in-Cell methods also use more computer memory, because they necessitate the memory storage of auxiliary variables. For this reason, the explicit Particle-in-Cell codes can
run with more computational particles and grid points than the implicit Particle-in-Cell code.

The computational performances of the implicit Particle-in-Cell methods are summarized in terms of number of FLOPS and computer memory usage in Section 9.1. The convenience of using the implicit Particle-in-Cell methods in the ion beam neutralization problems, and the simulation of the future NDCX experiments are discussed in Section 9.2 and 9.3. Section 9.4 concludes this dissertation, suggesting future work.

9.1 Computational Performance of the Implicit Particle-in-Cell Methods

A one dimensional electrostatic version of the explicit, moment implicit, and fully implicit Particle-in-Cell methods have been implemented in the Matlab/Octave language to compare the three algorithms. The number of FLOPS has been chosen to characterize the computational performance of the Particle-in-Cell methods, since this quantity depends only on the algorithm, and on the code implementation, and it provides a good estimate of the computational cost. The three numerical schemes were analyzed using the electron beam instability problem as benchmark. Of course, the performance depends on the particular problem, since the number of the solver iterations depends critically on the nature of problem. However, the electron beam instability provides a rough but useful estimate of the different algorithms. The memory usage of the different methods have also been evaluated, to estimate the number of computational particles and grid points, the different Particle-in-Cell methods can support.
Figure 9.1: Number of FLOPS for different Particle-in-Cell methods, and for the number of grid points equal to 64, 128, and 256.

9.1.1 Number of FLOPS

The number of FLOPS of the implicit moment and fully implicit Particle-in-Cell method have been presented in Chapters 4 and 8. Figure 9.1 summarizes the results for the performance of the implicit Particle-in-Cell methods, and compares them to the explicit Particle-in-Cell performances. The number of computational particles is 10,000, and the number of grid points are 64, 128 and 256. The implicit moment and the fully implicit Particle-in-Cell simulations are on average 4 to 40 times computationally more expensive than the explicit Particle-in-Cell simulations. Moreover, the performance of the implicit moment Particle-in-cell code depends largely on the number of grid points, and less so on the number of particles. On the other hand, the opposite situation is true for the fully implicit Particle-in-Cell method: the number
of FLOPS depends largely on the number of particles.

9.1.2 Computer Memory Usage of the Implicit Particle-in-Cell Simulations

The number of computations is not the only factor that determines the computational performance of the Particle-in-Cell methods. The amount of computer memory used by the numerical processor must be considered also, as pointed out by Bowers [77]. Implicit Particle-in-Cell methods consume more computer memory than the explicit Particle-in-Cell method. The reason is that the implicit Particle-in-Cell methods use auxiliary variables to store the estimate of the particles and moments (charge, current, pressure densities) quantities as intermediate variables. Because of the limited computer memory (typically 3 Giga Bytes per processor), the implicit Particle-in-Cell methods can support smaller grid points, and a smaller number of particles, when compared with the explicit Particle-in-Cell method.

Table 9.1 shows the computer memory requirements for storing the particles (position, velocity, and weight), the moments of the distribution function (charge, current density) and the fields (electric and magnetic field) quantities for different Particle-in-Cell methods. It is assumed that all the variables are stored in the floating-point double precision format (8 bytes). A $256 \times 128 \times 128$ grid and 300 particles per cell are considered as a typical example of three dimensional electromagnetic Particle-in-Cell simulation. The memory usage has been expressed in Giga Byte (GB). In the Particle-in-Cell methods, 99% of the computer memory is dedicated to the storage of particles positions, velocities and weights, and a small 1% to the moments of the distribution function and to field quantities. The implicit moment Particle-in-Cell method uses approximately 3.5 times the memory of the explicit Particle-in-Cell method for storing the moments. However, the memory used to store the moments of the distribution functions is negligible when compared with the memory needed.
for particles quantities. Therefore, the memory used for the implicit moment and explicit Particle-in-Cell methods is approximately the same. On the contrary, the fully implicit Particle-in-Cell method uses auxiliary variables to store particle positions and velocities, requiring almost double the computer memory than that required by the explicit and implicit moment Particle-in-Cell methods. Therefore, the explicit and the implicit moment Particle-in-Cell simulations require approximately the same amount of computer memory, while the fully implicit Particle-in-Cell method uses almost twice the memory of the other two methods. This large memory requirement limits the fully implicit moment method to use a smaller number of computational particles and grid points.

### 9.2 The Convenience of the Implicit Particle-in-Cell Methods in Neutralization Modeling

One of the disadvantage of using the implicit Particle-in-Cell with large time steps is that the numerical scheme produces a numerical damping of the Langmuir waves. The numerical damping of the Langmuir wave must be avoided when modeling the beam plasma interaction, because the Langmuir waves are an essential part of the beam neutralization physics. A small time step needs to be used to avoid the numerical damping of Langmuir waves, making the use of implicit Particle-in-Cell in the
current formulations, not computationally convenient for modeling the neutralization dynamics. In fact, the time step for describing correctly the neutralization process is small enough that explicit Particle-in-Cell methods still retain the numerical stability and can be used efficiently.

Moreover, the sheath on the beam plasma interface, develops over a spatial scale that is of the order of the Debye length, and the physics occurring over these scales also needs to be captured. Although the implicit Particle-in-Cell does not have to resolve the Debye length to be numerically stable (the explicit PIC has to), the Debye length must be resolved by the grid, because the physics under investigation requires it.

In summary, the physics of the neutralization process imposes two constraints on the choice of the time step and the grid spacing: the plasma period and the Debye length of the background plasma needs to be well resolved by the time step and grid spacing to correctly describe the neutralization physics. These two constraints make the implicit Particle-in-Cell methods in the current formulations, not computational advantageous for the neutralization modeling. The explicit Particle-in-Cell method can be used instead, saving the computational overhead of the implicit schemes.

9.3 Implicit Particle-in-Cell for Modeling Future NDCX Experiments

The choice of the future NDCX experiment parameters are currently being discussed at LBNL [78]. It is almost certain that the future NDCX experiments at LBNL will make use of ion beams with higher energies (few MeV), and with higher currents (few tens of mA).

As shown in Chapter 5, the increase of beam energy and current imply an increase of the beam propagation velocity, and of the beam density. A higher background
plasma density will be necessary to provide an increased number of electrons for the neutralization, because the beam density will increase. However, it has been shown by the simulations reported in this dissertation that the background density equal to beam density is already sufficient of provide perfect neutralization in approximately tens of plasma periods. The FEPS plasma in the current NDCX configuration already provides plasma densities capable of neutralizing beams with higher density.

A second effect of the increased higher beam current is the increase of the magnetic field effect on the neutralization. Because the current will be increased by an order of magnitude, the magnetic field will still not have an effect on the beam neutralization process in the next NDCX. An electrostatic model of the plasma will be adequate to model the next NDCX.

### 9.4 Future Work

Different formulations of the implicit Particle-in-Cell method might be developed for modeling the neutralization phenomenon in the future. A Particle-in-Cell method that retains the Langmuir wave physics when using large step must be implemented. An adaptive mesh refinement (AMR) approach probably can be used to resolve the Debye length only at the beam-plasma interface while allowing large grid spacing where it is not necessary to resolve the Debye length [79].
References


Author’s Biography

Stefano Markidis graduated from Politecnico di Torino in 2002 with a Master of Science degree in Nuclear Engineering. For three years Stefano worked as computational scientist for the Los Alamos National Laboratory before relocating to Champaign, Illinois, to pursue Ph.D. study in Nuclear, Plasma and Radiological Engineering. Stefano was awarded a R&D 100 award in 2005. His main interests are computational physics and high performance computing on massively parallel computers.