Particle in Cell and Hybrid Simulations of the Z Double-Post-Hole Convolute Cathode Plasma Evolution and Dynamics

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February 25, 2013
Abstract

The Z-accelerator at Sandia National Laboratories (SNL), is a high-current pulsed power machine used to drive a range of high energy density physics (HEDP) experiments [1]. To achieve peak currents of $>20\text{MA}$, in a rise time of $\sim 100\text{ns}$, the current is split over four levels of transmission line, before being added in parallel in a double-post-hole convolute (DPHC) and delivered to the load through a single inner magnetically insulated transmission line (MITL). The electric field on the cathode electrode, $>10^7\text{Vm}^{-1}$, drives the desorption and ionisation of neutral contaminants to form a plasma from which electrons are emitted into the anode-cathode (a-k) gap. The current addition path in the DPHC forms magnetic ‘null’ regions, across which electrons are lost to the anode, shunting current from the inner MITL and load. In experiment, current losses of $>10\%$ have been measured within the convolute; this reduces the power delivered to the load, negatively impacting the load performance, as well as complicating the prediction of the Poynting flux used to drive detailed magneto-hydrodynamic (MHD) simulations [2,3]. In this thesis we develop 3-dimensional (3D) Particle-in-Cell (PIC) and hybrid fluid-PIC computer models to simulate the plasma evolution in the DPHC and inner MITL. The expected experimental current loss at peak current was matched in simulations where Hydrogen plasma was injected from the cathode electrode at a rate of $0.0075\text{mlns}^{-1}$ ($1\text{ml}=10^{15}\text{cm}^{-2}$), with an initial temperature of $3\text{eV}$. The simulated current loss was driven by plasma penetrating the downstream side of the anode posts, reducing the effective a-k gap spacing and enhancing electron losses to the anode. The current loss at early time ($<10\text{MA}$), was matched in simulations where space-charge-limited (SCL) electron emission was allowed directly from the cathode; to match the loss over the entire current pulse, a delay model is motivated. Here, plasma injection was delayed after the start of SCL emission, based on realistic plasma expansion velocities of $\sim 3\text{cm}\mu\text{s}^{-1}$. The PIC model, which was necessary to accurately simulate the kinetic behaviour of the lower density plasma and charged particle sheaths, was computationally intensive such that the spatial resolutions achieved in the 3D simulations were relatively poor. With the aim of reducing the computational overhead, allowing finer spatial resolutions to be accessed, we investigate the applicability of hy-
brid techniques to simulating the cathode plasma in the convolute. Our PIC model was both implemented in the resistive MHD code, Gorgon, where part of the plasma was modelled in the single fluid approximation, and extended to include an inertial two-fluid description of the plasma. The hybrid models were applied to the DPHC simulations, the results from which are used to motivate a three component model; here, the densest part of the convolute plasma is modelled using the single fluid MHD approximation, transitioning to a fully kinetic PIC description of the lower density plasma and charged particle sheaths, linked by a two-fluid description.
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Chapter 1

Introduction

1.1 The Z Pulsed Power Machine

The Z-accelerator at Sandia National Laboratories (SNL) is a high current pulsed power machine used for a range of high energy density physics (HEDP) and materials experiments. It is the world’s most powerful X-ray source demonstrating over 200TW X-ray powers from a wire array Z-pinch load, equivalent to greater than 10% wall socket to X-ray conversion efficiency [1].

The Z-accelerator began life in 1985 as the Particle Beam Fusion Accelerator II (PBFA II) and was initially designed as a high voltage (10-30MV) ion beam driver for Inertial Confinement Fusion (ICF) research. In 1996, components of the machine were modified to allow high current (18-20MA) experiments. Here, the machine was used to drive wire array Z-pinch loads, to study X-ray energy and power scaling. The success of these shots resulted in the accelerator never being converted back to an ion diode drive configuration, leading to the machine subsequently being renamed Z [4]. In 2003, the accelerator was refurbished, the ZR project, where components of the machine were redesigned specifically for Z-pinch applications. Here, the aim was to both increase the peak current that could be delivered to the load (up to 26MA), by increasing the initial energy storage (new capacitors in the Marx banks) and improve reliability [4]. In addition to wire arrays, Z has also been used to carry out a range of other HEDP
experiments with applications covering basic ICF research [5,6], radiation effects [7] and materials testing [8].

A schematic of the Z machine is shown in Figure 1.1. The design methodology used to convert PBFA II for use as a low impedance Z-pinch driver was reviewed in [9–11]. The pulsed power machine was designed to generate, temporally compress and transport electrical energy initially stored in 36 Marx banks, at a radius of 33m, to a load on the axis. As shown in Figure 1.1, Z consists of 36 identical modules arranged uniformly around the azimuth. Starting at the outer edge of the machine, the Marx banks consist of a set of capacitors that are charged in parallel to 70-90kV, with a total energy storage of up to 22MJ [12]. The capacitors are discharged in series, generating peak voltages of $\sim 3$MV, applied to two levels of water filled coaxial capacitors, on a time scale of $\sim 2\mu s$. The coaxial lines are discharged into a second set of water filled lines, through laser triggered gas switches [9]. Using laser triggering ensures good synchronicity between the 36 modules, where jitters are on the order of 2-3ns. Conversely, individual laser triggers on each set of lines gives flexibility in the pulse shaping. For example the machine can be run in long pulse mode, where the nominal 100ns rise time is increased to 300ns. Taking this further, the pulse shape can be precisely tailored for isentropic compression experiments, where the aim is to compress a sample of material using the magnetic field associated with the current, without shocking the material [8].

The second set of water lines are discharged through self-breaking switches into bi-plate lines, which transport the voltage pulse, now with a full-width half-maximum (FWHM) of $\sim 100$ns, to the insulator stack at a radius of 1.6m [11]. This section of the machine, known as the water convolute, transitions the geometry from the cylindrical water lines, to the radial vacuum section. The insulator stack provides the transition from this water filled pulse-forming (PF) section to the vacuum section of the machine, in which the experiment is carried out [12]. The insulator stack, which consists of a series of plastic rings with surfaces angled at 45 degrees, separated with metallic discs, was designed using a combination of circuit, electrostatic, electromagnetic (EM) and Particle in Cell (PIC) modelling, to ensure that it did not break down for the duration of the voltage pulse [11].

In order to achieve the fast rise times required for Z-pinch applications, the total inductance of the vacuum section of the machine was minimised by splitting it into four
levels. Below a radius of $\sim 1.3\text{m}$, the electric field strength, $>10^7\text{Vm}^{-1}$, is sufficient to break down the electrode, forming a cathode plasma from which a space-charge-limited (SCL) electron current is drawn [13]. The magnetic field associated with the bound current results in electron Larmor radii which are smaller than the anode-cathode (a-k) gap and the sheath is insulated, such that the four levels of transmission lines comprising the radial disk feed operate as magnetically insulated transmission lines (MITLs); the operation of MITLs will be discussed in detail in chapter 2. Note that the a-k gaps in the radial lines, Figure 1.1, are reduced proportionally with the radius, in order to give a near uniform vacuum impedance [14].

At a radius of 10cm, the double-post-hole convolute (DPHC) begins. This is shown schematically in Figure 1.2; the standard Z convolute consists of two levels of twelve anode (blue) posts (white), slotted through holes in the cathode (red), arranged uniformly around the azimuth. Note that a nine post-hole variant of the DPHC has been fielded in experiments [15]. The convolute geometry is such that the bound current entering from the four level radial disk feed is added in parallel and delivered to a single inner MITL, which starts at a radius of 5cm. The pulse is transported along the inner MITL and delivered to the load on axis, which in short-pulse mode, receives a peak current of $\sim 20\text{MA}$ with a 100ns rise time. In Figure 1.2, we have shown the right angled in-
Figure 1.2: A schematic of twelve post, double-post-hole convolute (DPHC) used to add current in parallel from the four level radial disk feed and deliver it to the single inner MITL.

ner MITL geometry, which transitions from radial to coaxial geometry, such that the Z-pinch load can be lifted above the convolute for improved diagnostic access. For the configuration shown in Figure 1.2, the a-k gaps at the start of the DPHC feed input lines are 1cm, reducing to 6mm in the radial part and 4mm in the coaxial part, of the inner MITL. Various inner MITL electrode geometries have been fielded dependent on the specific load type [3].

The current addition path in the DPHC results in regions of zero magnetic field strength, which are known as magnetic 'nulls' [16]. For each of the 12 layers of two anode posts and cathode holes there are three such nulls; two on the upstream sides (away from the load) of the anode posts and one between the anode posts on the second line from the top (level B line). As no current flows on axis, there is an additional central null which is uniform about the azimuth. Results from EM simulations of the DPHC will be presented in chapter 4. The magnetic nulls are clearly shown in slices of the simulated magnetic field, Figure 4.6, here. Apart from the central null, the nulls occur where the polarity of the field is reversed due to the direction of the bound current in the electrode, as will be shown in Figure 4.7.
1.2 Current Loss in the Z Double-Post-Hole Convolute and Inner Magnetically Insulated Transmission Line

Experimentally, the bound current in the anode electrode is measured using a series of B-dots. In Figure 1.3, the current measured within the radial lines at a radius of ∼70cm (the total current shown is a sum of the measurements made on the four levels) is compared to the current measured at the start of the inner MITL, at a radius of ∼6cm, for a typical Z-pinch shot; note that the current has been plotted on Z machine time. Here, we have adopted the nomenclature of [2]; specifically, we refer to the current measured in the radial lines as the MITL current, and the current measured at the start of the inner MITL as the convolute current. Note that in the majority of the literature, the convolute current is referred to as the load current; we reserve this label for the current that is actually delivered to the load and is typically not measured in experiment. From Figure 1.3, we see that the convolute current is smaller than the MITL current; current has been ‘lost’ within the convolute. This difference between the convolute and MITL currents is referred to as the current loss. These traces are from Z shot 1786, which was a 2cm diameter, 1cm long, 300 wire tungsten wire array load with a total mass of 6mg [2]. In this shot, the current loss was ∼4MA at peak current, corresponding to ∼18% of the peak MITL current. Pre-refurbishment, the typical measured current loss was ∼2MA corresponding to ∼10% of the peak MITL current [16]. The current loss is sensitive to the load type and is generally larger for higher impedance loads, such as these 2cm diameter, compact wire arrays [17]. Note that the current measured at the insulator stack, at a radius of ∼1.6m is consistent with the MITL current, such that the current loss is constrained to the DPHC [2].

In addition to the measured convolute current loss, a further, undiagnosed multi-mega current loss within the inner MITL has been inferred from detailed comparisons of coupled circuit and 3-dimensional (3D) simulations of wire-array experiments on Z [2,3]. The magnitude of this loss was found to be dependent on the geometry of the inner MITL electrodes, with the highest losses corresponding to the right-angled bend configuration.
Figure 1.3: A comparison of the MITL and convolute currents measured in a typical Z-pinch experiment, demonstrating the multi-MA current loss that occurs within the DPHC.

shown in Figure 1.2 [3].

The current losses within the convolute and inner MITL limit the power that can be delivered to the experimental load through the Poynting flux [2]. For the majority of applications, maximising the power delivered to the load by minimising the current loss, is desirable. For example, wire array Z-pinches have been proposed as an alternative X-ray radiation source to indirectly drive ICF capsules [5]. The radiated X-ray power and therefore the hohlraum temperature, is a strong function of the power that can be delivered to the load [3].

Understanding the current loss is also important for gaining an accurate theoretical understanding of the experimental loads. The current loss complicates the prediction of the Poynting flux used to drive detailed 3D magneto-hydrodynamic (MHD) simulations of the wire array loads; accurate prediction of the Poynting flux is important to decouple uncertainties in the implosion physics from uncertainties in the driving circuit [2, 3]. In [3], it is stated that the power delivered to the load is an uncertainty potentially as large as the MHD implosion dynamics. Measured current losses can be parameterised for inclusion in such circuit models, however this does not represent a fully predictive capability for optimising new experimental designs on current and future facilities [2, 3].

Current addition in convolutes is and will continue to be a key component of the design of current and future higher power facilities. Understanding and minimising the current loss is therefore important to minimise the physical size (set by the peak current) and therefore cost of these facilities to achieve their goals e.g. fusion gains.
For the majority of pulsed power driven fusion schemes e.g. wire array and gas-puff Z-pinch schemes, it is predicted that a peak current of 60MA will be required to achieve ignition and significant gain [5]. This represents a greater than two times increase in the theoretical peak current on Z (26MA). Between Z and ZR the theoretical peak current was increased from ~20 to 26MA; here, the convolute a-k gaps were increased to accommodate the larger peak voltage and the angle of the lines was increased for better diagnostic access. However, on the whole the electrode geometry was consistent with the pre-refurbishment design [15]. Considering that the loss current increased from 10 to up to 20% , for this 30% increase in the peak current [2,15–17] between Z and ZR, we see that the scaling of the current loss is a large uncertainty in the design of the next generation of accelerators.

1.3 Thesis Outline

The current loss occurring within the DPHC is believed to be driven by the evolution of plasma formed on the electrodes during the high voltage discharge. This thesis can be split into two main parts. In the first part, we investigate the current loss mechanisms in the Z DPHC and inner MITL using numerical simulation techniques, specifically 3D PIC simulations of the electrode plasma and charged particle sheath evolution and dynamics. This work was motivated by the goals of developing a model that could predict and ultimately aid in the re-design of the convolute to minimise the current losses, as well as improve and justify the parameterisations used for the current loss in equivalent circuit models to more accurately predict the Poynting flux delivered to 3D MHD simulations of the experimental loads [2,3].

Both LSP [15,16] and Quicksilver [12,14,18] 3D PIC simulations of the Z and ZR DPHC have been reported. The simulations presented in this thesis have been carried out using our own PIC code, which was developed over the course of the project. This was a significant undertaking and was motivated by the desire to move away from commercial codes, where the physics algorithms are typically used as a 'black box'. An additional motivation for our DPHC simulation work was therefore to provide an independent comparison of the published simulation results. The simulations of the inner MITL were motivated by the inferred current losses found in [2,3], combined with a lack of published results regarding the plasma and charged particle sheath evolution.
and dynamics in this part of the machine.

The computational overhead of fully kinetic simulations of the plasmas in the Z DPHC and inner MITL were significant. Moving to higher current facilities, the electrode plasma density is expected to increase, which will be even more stressing for a fully kinetic plasma model. The second part of the thesis was motivated both by the desire to develop a practical design tool for current and next generation high current pulsed power systems and practically achieve higher spatial resolutions to address some concerns identified in the accuracy of the plasma transport in the relatively poorly resolved kinetic simulations. Here, we investigate the applicability of hybrid kinetic-fluid models to the DPHC and inner MITL simulations. Assuming collisionality, we investigate treating part of the plasma using both a single fluid MHD and inertial two-fluid description. A kinetic description was maintained in the lower density parts of the plasma and the charged particle sheath, where the fluid approximation was not valid. Our PIC code formed the basis for the kinetic part of these models, where it was both implemented in the Imperial College MHD code Gorgon and extended to include a two-fluid description of the plasma. This work was further justification for the decision to develop our own PIC code.

1.4 Synopsis

In chapter 2, the theory of electrode plasma formation and evolution and power flow in MITLs, relevant to the operation of the Z radial lines, DPHC and inner MITL, will be reviewed. The proposed current loss mechanisms and results from published circuit and PIC simulations of the DPHC and inner MITL are also outlined here.

The PIC code developed to carry out detailed 3D kinetic simulations of the plasma and charged particle sheaths in the Z DPHC and inner MITL and used to form the basis of the hybrid fluid-kinetic models, is described in detail in chapter 3. Using the theory developed in chapter 2, the code design choices will be physically justified by considering the parameters of the plasma and sheaths expected to form in the convolute.

Results from 3D fully kinetic simulations of the DPHC using the PIC code described in chapter 3, will be presented in chapter 4. Here, the measured current loss was reproduced by explicit inclusion of plasma on the cathode electrode. We will focus on
the role of the evolution and dynamics of this plasma in enhancing the current loss in the Z DPHC. Current loss within the inner MITL will also be investigated in the 3D simulations, as well as a separate series of higher resolution 2D kinetic simulations.

Assuming the electron and ion components of the convolute plasma were sufficiently collisional, the applicability of a single fluid MHD model (Gorgon) to simulating the plasma evolution and dynamics is investigated in chapter 5. Here, the additional physics included in the field solution and code modifications made to allow accurate and stable simulation of the relatively low density and temperature convolute plasma will be described. The implementation of the PIC model described in chapter 3 in Gorgon, to form the hybrid model, will also be outlined here; tests of the coupling between the fluid and kinetic components of the plasma through a common field solver are discussed and the methods and pitfalls of transferring plasma between the MHD and PIC descriptions will be reviewed.

In chapter 6, an inertial two-fluid plasma model extension of the PIC code described in chapter 3, will be outlined with the focus on mitigating inadequacies identified in applying the single fluid MHD description in chapter 5. Results from test simulations of the Z DPHC and inner MITL using the hybrid model will be used to justify its applicability.

Finally, the conclusions of the thesis are reviewed and drawn in chapter 7. The direction of future work will also be outlined here.
Chapter 2

Magnetically Insulated Transmission Line Theory and Current Loss in $Z$

2.1 One Dimensional Lossless Transmission Line Theory

Transmission lines are used to transport high frequency EM waves. They consist of a cathode and anode electrode separated by a dielectric material or vacuum and can have a range of electrode geometries, including parallel plate and coaxial. The simplest description of a transmission line assumes that it is infinitely long, has a uniform anode-cathode (a-k) gap spacing i.e. is one dimensional (1D) and is lossless i.e. the resistance of the electrodes is negligible [19].

In these cases, a small section of the transmission line, $\Delta x$, can be modelled with an equivalent circuit comprised of a series inductor and parallel capacitance to model the self-inductance per unit length, $L$, and capacitance per unit length, $C$, of the line respectively. Defining the voltage and current on the line at time $t$ and position $x$, $V(x, t)$ and $I(x, t)$, over the small distance $\Delta x$, the voltage drop across the self-inductance,
\[ (V(x + \Delta x, t) - V(x, t))/\Delta x = \partial V/\partial x, \] is described by Eqn.(2.1) [19].

\[
\frac{\partial V}{\partial x} = L \frac{\partial I}{\partial t} \tag{2.1}
\]

The current in the conductors is also a function of \( x \) due to the capacitance between the anode and cathode. For a lossless line, the bound currents in the cathode and anode are equal and opposite. The change in the current over the small distance \( \Delta x \) is given by \((I(x + \Delta x, t) - I(x, t))\Delta x = \partial I/\partial x\), which is equal to the current carried by the capacitance, \( C\Delta x (\partial V/\partial t) \) to give Eqn.(2.2) [19].

\[
\frac{\partial I}{\partial x} = C \frac{\partial V}{\partial t} \tag{2.2}
\]

Together, Eqn.(2.1) and Eqn.(2.2) are known as the telegrapher equations. Differentiating Eqn.(2.1) with respect to \( t \) and Eqn.(2.2) with respect to \( x \) and equating the results gives Eqn.(2.3) [19].

\[
\frac{\partial^2 V}{\partial t^2} = \frac{1}{LC} \frac{\partial^2 V}{\partial x^2} \tag{2.3}
\]

This is a wave equation describing the voltage wave along the line, which travels with a velocity of \( v = 1/\sqrt{LC} \). The general solution to Eqn.(2.3) is a sum of waves travelling along the line from left to right, \( V_1 \) and right to left, \( V_2 \), both at a speed of \( v \), as in Eqn.(2.4) [19].

\[
V(x, t) = V_1(vt - x) + V_2(vt + x) \tag{2.4}
\]

The line can be characterised by a ‘vacuum’ impedance \( Z_0 = V(x, t)/I(x, t) = \sqrt{L/C} \). For a finite length line terminated by a different impedance, \( Z_1 \), the voltage wave will be partially reflected and transmitted, according to the coefficients, Eqn.(2.5-2.6) [19].

\[
R = \frac{Z_0 - Z_1}{Z_0 + Z_1} \tag{2.5}
\]

\[
T = 1 - R = \frac{2Z_0}{Z_0 + Z_1} \tag{2.6}
\]
For $Z_0 = Z_1$, $T = 1$ and $R = 0$, so the wave will be fully transmitted. In the limit
$Z_1 >> Z_0$, $T = 0$ and $R = 1$ and the wave will be completely reflected and is the case
for an open circuit termination. In the other limit, $Z_1 << Z_0$, $T = 0$ and $R = -1$ and
is the case for a short circuit.

Circuits comprising sections of ideal transmission line, characterised by a length and
impedance, can be used to approximate the operation of real pulsed power systems [20].
In this work, we have used such a model to simulate the Z vacuum radial lines, as will
be discussed in section 3.5 in the next chapter.

2.2 Cathode and Anode Plasma Formation

The presence of electrode plasmas in high-voltage pulsed power systems is well estab-
lished through direct observation [21] and indirect arguments relating to the large, un-
bound electron currents measured in vacuum transmission lines [22]. An electron may
escape from a metallic cathode electrode into vacuum, if it’s energy is larger than the
work function, $\varphi$, of the electrode material. For example, by heating the electrode, elec-
trons in the conduction band can gain enough energy to escape, constituting thermionic
emission [23].

In the presence of a large applied electric field, the trapping potential barrier is
lowered and given finite width, such that electrons with energy below $\varphi$ can quantum
mechanically tunnel through the barrier. The current drawn by this field emission pro-
cess is described by the Fowler-Nordheim equation [23] and to first order is independent
of temperature [24].

For a typical pulsed power machine, the electric field stress at the cathode can exceed
$10^7$Vm$^{-1}$ and is sufficient for field emission of electrons [12]. However, the currents
predicted by field emission theory are one to four orders of magnitude smaller than
those observed experimentally [22]. These are instead on the order of space-charge-
limited (SCL) emission, described in one dimension by the well-known Child-Langmuir
relation [23]. The experimental measurements can be explained by the presence of a
plasma with a density of between and $10^{13}$ and $10^{17}$cm$^{-3}$, which is quickly established,
< 10ns, on the cathode electrode surface [24]. The plasma constitutes a zero work
function surface from which electrons are emitted into the vacuum gap [25].
The formation and evolution of electrode plasmas can inhibit performance through plasma expansion driven gap shorting and impedance collapse, as well as cause hardware damage [21]. The electrode plasma generation mechanism is a complicated process and is not fully understood; however, relating to electron and ion beam diodes, as well as MITL applications, a large amount of experimental and theoretical work to understand these processes has been carried out.

The cathode and anode plasma generation mechanisms are different, however they are both sourced from neutral contaminates that are absorbed on the electrode surfaces [24]. It is well known that pulsed power machines are not clean, where contaminant molecules are absorbed in oxide layers of aluminium and stainless steel electrodes, as well as metallic inclusions. An extensive review of electrode contamination, plasma formation and cleaning techniques in pulsed power systems is given by Cuneo in [21]. There are estimated to be over 100 monolayers (ml), where \(1 \text{ml} = 10^{15} \text{particles cm}^{-2}\), of hydrocarbons, \(C_nH_m\), \(H_2\), water, \(H_2O\), \(CO\) and \(CO_2\), bound on the electrode surfaces of a typical pulsed power machine. These species are consistent with spectroscopic measurements of cathode and anode plasmas, as well as vacuum system inventories [21].

### 2.2.1 Cathode Plasma Formation and Evolution

The plasma breakdown process at the cathode electrode is believed to be initiated by enhanced field emission of electrons from localised spots on the cathode surface. These are typically metallic whiskers, or other microscopic features at which the electric field is enhanced [24]. The contaminant layers are bound by Van der Waals forces, which are much weaker than metallic bonds. As such, collisions between the field emission electrons and contaminant atoms are energetic enough to break the bonds, leading to stimulated desorption of the neutral contaminants [21]. A dense neutral gas layer, with a density of up to \(10^{19} \text{cm}^{-3}\), is formed above the electrode surface, which is ionised by the field emission electrons to form a plasma. These conditions can lead to explosive plasma emission. Here, ions are accelerated from the plasma back into the cathode, heating the electrode surface further and enhancing thermionic electron emission. In addition, the positive ion space charge increases the local electric field at the cathode surface, enhancing field emission of electrons [26]. The plasma shields the cathode electrode
from the external electric field in the transmission line; the plasma therefore acts as a zero work function surface and electrons are emitted into the a-k gap from the plasma, with currents on the order of SCL emission [27]. This current is supplied by the plasma which is continually replenished by current flow through a sheath formed between the plasma and the cathode electrode surface [26].

A further mechanism proposed for replenishing the cathode plasma is unipolar arcs. Here, large electron currents arc from the electrode surface to the plasma and back to the electrode, at localised enhanced electron emission regions. These arcs have large current densities which Ohmically heat the electrode, vaporising the electrode material and releasing plasma [26].

Experiments on coaxial MITLs at 1MA and 1MV, measured cathode plasma densities of order $10^{16}\text{cm}^{-3}$ and temperatures of up to 3eV [16]. As the external retarding electric field is screened by the plasma electrons, the cathode plasma ions can expand away from the cathode surface under the influence of the plasma pressure gradients [26]. In the limit of zero magnetic field, this is on the ambipolar diffusion time scale [27]. As the majority of electrode contaminants contain Hydrogen, the a-k gap closure by the cathode plasma is thought to be dominated by protons; this is the least massive ion species and is able to cross the a-k gap within the pulse duration, which is typically of the order of 100ns. This is consistent with spectroscopic measurements of the plasma in the ZR convolute [17]. Here, strong continuum emission with absorption features was measured, most notably the hydrogen H-alpha lines at 6563 Angstroms. Measurements of the location of the continuum emission as a function of time also indicated that plasma originates on the cathode and travels from the cathode to the anode with an apparent velocity of $>7\text{cm}\mu\text{s}^{-1}$ [17]. This work will be discussed further in section 2.6.2, in relation to the current loss mechanism within the convolute.

The apparent expansion velocity measured on Z was larger than experiments on other pulsed power machines, where typical plasma expansion velocities between 1-3cm$\mu$s$^{-1}$ have been measured [17, 27]. Charged states of carbon and oxygen, as well as heavy metal ions, have also been observed in the cathode plasmas. However, these more massive ion species expand on slower time scales compared to protons [21].

A theoretical model of the cathode plasma behaviour in a space-charge limited 1D planar diode was developed by Shefer et al [27]. Assuming a supply of neutral atoms,
Figure 2.1: One dimensional planar diode with plasma cathode showing gas layer $0 < x \leq x_0$, plasma layer $x_0 < x \leq \bar{x}$ and vacuum gap containing space-charge limited flow $\bar{x} < x < L$.

plasma was formed throughout the discharge, where a simplified electron impact ionisation source was postulated to represent a range of complicated bulk and plasma-surface interactions.

As shown in Figure 2.1 (reproduced from [27]), the a-k gap, $L$, was split into three regions. A vacuum gap ($\bar{x} < x < L$) containing SCL electron flow, a source free plasma layer ($x_0 < x \leq \bar{x}$) and a neutral gas and plasma source layer ($0 < x < x_0$) where $x_0 << \bar{x}$ was assumed [27]. Here, the plasma ions expand under the influence of plasma pressure gradients, as the external retarding electric field was screened by the dense plasma [26].

Under SCL conditions the diode electric field is approximately zero at the emitting plasma surface, such that the electrons enter the gap ($\bar{x} < x < L$), at a rate determined by their random flux as in Eqn.(2.7). Here, $n_s$ is the density of the plasma at $x = \bar{x}$, $V$ is the voltage, $\alpha$ is a constant and $v_e = (3k_BT_e/m_e)^{1/2}$ is the characteristic electron velocity in the Maxwellian distribution characterised by the electron temperature, $T_e$ [27].

$$n_s v_e = \alpha V^{3/2} / (L - \bar{x})^2 = \Gamma e_0$$  \hspace{1cm} (2.7)
In the source free plasma layer \((x_0 < x \leq \bar{x})\) the continuity equations are given by Eqn.(2.8) [27].

\[
\frac{\partial n}{\partial t} = -\frac{\partial \Gamma_i}{\partial x} \\
\frac{\partial n}{\partial t} = -\frac{\partial \Gamma_e}{\partial x}
\]  

(2.8)

In the diffusion approximation the fluxes are given by Eqn.(2.9), where in this region the density \(n = n_e = n_i\) and the current is continuous, \(\Gamma_e - \Gamma_i = \Gamma_{e0}\). Here, \(\mu_{e,i}\) and \(D_{e,i}\) are the electron and ion mobility and diffusion coefficients, respectively [27].

\[
\Gamma_i = \mu_i n E - D_i \frac{\partial n}{\partial x} \\
\Gamma_e = -\mu_e n E - D_e \frac{\partial n}{\partial x}
\]  

(2.9)

The electric field, \(E\), in Eqn.(2.9) can be removed by combining the electron and ion fluxes to give an expression for the ion flux as in Eqn.(2.10). Here, \(D_a = (\mu_i D_e + \mu_e D_i) / (\mu_i + \mu_e)\) [27].

\[
\Gamma_i = -D_a \frac{\partial n}{\partial x} - \left( \frac{\mu_i}{\mu_i + \mu_e} \right) \Gamma_{e0}
\]  

(2.10)

At \(x = 0\), it is assumed that \(\Gamma_i = -\Gamma_{e0}\) i.e. that the current is returned to the cathode through the ion flux only. This is a valid assumption as long as the potential drop in the cathode sheath is much larger than the electron thermal energy [27].

To study the temporal evolution of the plasma, it was assumed that the total current is quasi-stationary at all times, \(\Gamma_e(x, t) - \Gamma_i(x, t) = \Gamma_{e0}(t)\), where \(\Gamma_{e0}(t)\) is the instantaneous electron flux extracted from the plasma boundary. This is justified since the evolution takes place on the slow ambipolar diffusion time scale and the electrons are highly mobile in comparison [27].

The plasma was evolved numerically by discretising Eqn.(2.10) into a series of planes of width \(\Delta x\). To close the solution, the plasma density in the source region \((0 < x < x_0)\), \(n_0\), was calculated from the ion continuity equation here, as in Eqn.(2.11). Here, \(n_a\) is the neutral density, \(\Gamma_0\) is the flux and \(\langle \sigma v \rangle_i\) is the integrated cross-section for the effective electron impact ionisation rate [27].
\[ \frac{\partial n_0}{\partial t} = -\frac{\partial \Gamma_0}{\partial x} + n_0 n_a \langle \sigma v \rangle_i \] (2.11)

Assuming that the source layer is in quasi-equilibrium (\(\partial n_0/\partial t = 0\)), then the number of particles in the source layer can be written as in Eqn.(2.12). Here, 
\[ G = \frac{n_0 x_0}{\int_0^{x_0} n(x) dx}, \]
describes the non-uniformity of the plasma density in the source region [27].

\[ N_0 = \frac{G \Gamma_0 \Delta x}{n_a x_0 \langle \sigma v \rangle_i} \] (2.12)

Starting with all the particles in the source layer, the model was evolved by small steps forward in time \(\Delta t\). At each step, the new position of the plasma surface was calculated and the vacuum electron flux, \(\Gamma_0\), recalculated accordingly. In general, the above model predicts an initial phase of rapid plasma expansion into the gap, followed by a slower expansion to steady state. For a fully ionised source free plasma layer steady state corresponds to an exponential density profile. The initial rapid expansion is a strong function of the electron temperature through the diffusion coefficients, \(D \propto T_e^{5/2}\), so that the initial expansion was driven by ambipolar diffusion. The ion current was found to decrease as a function of time so that \(J_i \to 0\) for all \(x\) as the system evolved to steady state. The initial rapid expansion phase predicted by the Shefer model is consistent with experiment, where the plasma layer was predicted to expand at 1-3cm\(\mu\)s\(^{-1}\) [21,27].

### 2.2.2 Anode Plasma Formation

Formation of plasma at the anode electrode follows from thermal and stimulated desorption of neutral contaminants, due to bombardment from electrons emitted from the cathode plasma and accelerated across the a-k gap. Typically, the electrode surface is quickly heated above 700K, the threshold for thermal desorption to dominate stimulated processes. The desorbed neutral layer is ionised by an electron avalanche [21]. As for cathode plasmas, the main constituent observed in anode plasmas is hydrogen [26]. As the anode neutral production rate is dominated by thermal desorption, for a given electron flux on the anode surface, plasma generation is reduced for materials with higher specific heats [21].
As for the cathode plasma, the anode plasma shields the electrode from the line electric field and acts as a zero work function surface for SCL ion emission into the vacuum gap. The anode plasma expansion is driven by the ions and as such typically evolves on a slower time scale than the cathode plasma.

In addition to electrons, photons can provide the energy required to desorb electrode contaminants and photo-ionise them [21]. For example, UV radiation emitted during Z-pinch plasma implosions is thought to enhance electrode breakdown close to the load in wire array experiments [28].

2.3 Magnetically Insulated Transmission Line Theory

As discussed in section 1.1 of chapter 1, the electric fields generated across the a-k gaps during the current pulse, in the vacuum radial lines, DPHC and inner MITL of Z are sufficient to initiate electrode breakdown and cathode plasma formation, by the mechanisms described in the previous section. With the cathode plasma acting as a zero work function surface, electrons will be emitted into the vacuum gap and accelerated by the electric field; the behaviour of the emitted electrons will depend on the strength of the magnetic field. If the field is relatively weak, such that the electron Larmor radii are larger than the a-k gap spacing, then the electrons will cross the a-k gap and impact the anode, decoupling a part of the accelerator current from the load [25]. This is undesirable for the majority of applications, where the aim is to maximum the current delivered to the load. However, if the magnetic field strength is relatively high, the electron orbits will be deflected back towards the cathode electrode, magnetically insulating the electrons. In this case, an electron sheath will be formed across the a-k gap, consisting of electrons, $\vec{E} \times \vec{B}$ drifting in the direction of power flow, towards the load. The total bound anode current, $I_a$, will be split between a bound current in the cathode electrode, $I_c$ and a current carried by the electrons comprising the sheath, $I_e = I_a - I_c$ [29].

Neglecting the expansion of the cathode and anode plasmas and assuming they remain tightly bound to the electrode surfaces, the electron sheath flow in a uniform,
constant vacuum impedance transmission line evolves as follows. When the machine is fired, the EM wave generated in the pulse-forming circuit propagates along the transmission line towards the load. When the strength of the normal component of the electric field at the cathode electrode exceeds $\sim 240\text{kVcm}^{-1}$, a plasma is formed as described above and electrons are emitted into the a-k gap. Before the EM wave front reaches the load, the magnetic field in the line is generated by the displacement current and is typically too small to insulate the electrons; the electrons cross the a-k gap and impact the anode. The current drawn from this loss front is sufficient to deflect the electrons upstream of the loss front away from the anode. At this time the line is said to be self-limiting. As the sheath is insulated behind the loss front, the front itself propagates along the line. The loss front propagation speed is less than the speed of light due to the finite electron mass and can be estimated from the average velocity of the electrons in the flow layer [25].

When the EM wave reaches the load, if the load impedance is larger than the self-limited impedance, typically the line will continue to operate in this self-limited mode. However, if the load impedance is smaller than the self-limited impedance, then typically a re-trapping wave will propagate back along the line from the load, returning (re-trapping) electrons from the sheath to the cathode electrode. In this case, the operational impedance of the line is increased closer to the vacuum impedance [30].

A precise description of the dynamics of the relativistic electron sheath flow and its coupling to the electromagnetic fields requires the solution of a closed set of three dimensional partial differential equations. In general this can only be achieved numerically, a method for which will be discussed in detail in chapter 3. However, the important characteristics of magnetically insulated electron flow can be studied analytically by making a range of simplifying assumptions. The resulting models provide equations for the electrical properties of the MITLs, which agree well with experimental measurements and computer simulations. Beginning with the simplest case of uniform vacuum impedance along the MITL, these models will be reviewed in the following section.

On Z, where the radial lines transition into the convolute, as well as within the convolute itself and the inner MITL, the vacuum impedance of the transmission lines is not uniform. In these cases, the electron sheath dynamics are more complicated, exhibiting instability formation which limits the applicability of analytic models developed for
uniform lines. The operation of non-uniform vacuum impedance MITLs, specifically the formation of vortices in the electron sheath, will be reviewed in section 2.5.

2.4 Uniform Vacuum Impedance MITLs

We will first consider the simplest case of a MITL with uniform vacuum impedance. As discussed in section 2.1, the vacuum impedance of a transmission line is a function of its inductance and capacitance, \( Z = \sqrt{L/C} \), which is related to the physical geometry of the electrodes comprising the line [19]. As discussed in section 1.1 of chapter 1, the \( Z \) vacuum radial lines from the insulator stack (\( r=1.6m \)) to the start of the DPHC (\( r=10cm \)), have an a-k gap spacing which reduces as a function of the radius. This was done in order to maintain a close to uniform vacuum impedance, which as will be discussed below, aimed to reduce the fraction of current carried in the electron sheath [13]. The vacuum impedance of a radial line can be derived from that of a parallel plate line, with the width replaced by the circumference and as such is a function of the radius, \( Z(r) \sim 60d/r \), where \( d \) is the a-k gap spacing and \( r \) the radius. Here we see that if \( d \propto r \), then \( Z \) will be constant [31].

The presence of the electron sheath in the MITL modifies its electrical properties. The first two MITL models considered derive these properties by restricting the orbits the electrons in the sheath can take.

2.4.1 Parapotential Model

The parapotential model restricts the electron orbits to the simplest possible case, that of a straight line travelling parallel to the electrode surface. The work of Creedon [32,33] on these laminar flows assumed that the electric and magnetic forces were dominant, with the electrons in the flow moving in straight lines along equipotential surfaces on which their total energy and axial canonical momentum were identically zero [32]. The charge density of the electron flow layer in this model has been shown to be strongly peaked at the vacuum-sheath interface [34].

This model was generalised by Lawconnell and Neri [35], to allow non-zero total energy and axial canonical momentum, along the straight line parapotential orbits.
This was found to provide flexibility in specifying the distribution of the electrons in the sheath.

### 2.4.2 Quasi-laminar Model

In the quasi-laminar model [36, 37], the electrons are assumed to follow cycloid-like orbits, beginning on the cathode and reaching the edge of the electron flow layer, before returning to the cathode. The relativistic Child-Langmuir law [23] is applied at the cathode and Poisson’s equation used to calculate the potential within the a-k gap. The electron flow is derived assuming conservation of energy and canonical momentum in the electron orbits, which is justified by the small initial electron velocities at the cathode surface compared to in the a-k gap, where the electrons are accelerated by the gap electric field [37].

### 2.4.3 Pressure Balance Model

The parapotential and quasi-laminar models of the electron sheath make specific assumptions about the electron orbits. Kinetic PIC simulations predict that the electron orbits are a mixture of the straight line and cycloid-like orbits assumed in the parapotential and quasi-laminar models, respectively [25]. The electron flow has been investigated independently of the electron orbits, using simple electric and magnetic pressure balance arguments [29].

The pressure balance MITL model, developed by Mendel et al. [29], will be described using the parallel plate line geometry shown in Cartesian coordinates in Fig.(2.2).
d the a-k gap spacing and $d_a$ the width of the electron sheath. The line has a width, $w$, along the y-axis, which is directed into the page.

In equilibrium, the electron sheath remains at a constant separation from the electrodes. In this case, the electric and magnetic pressures at the cathode and anode are related as in Eqn.(2.13) [29]. Here, the $a$ and $c$ indices refer to quantities at the anode and cathode electrodes respectively. This is known as the pressure balance equation and is derived in [30].

$$\frac{B_a^2}{2\mu_0} - \frac{\epsilon_0 E_a^2}{2} = \frac{B_c^2}{2\mu_0} - \frac{\epsilon_0 E_c^2}{2} \quad (2.13)$$

$$E_a^2 = c^2 (B_a^2 - B_c^2) \quad (2.14)$$

The second relation in Eqn.(2.14), assumes that the cathode is a SCL emitter of electrons [29]. This assumption does not imply the charge density of the electron sheath, $\rho_c$, is distributed across the gap according to the classical relation, $\rho_c \propto x^{2/3}$ [23]. Instead, the model assumes there is sufficient space charge in the gap to force the electric field normal to the cathode surface to be zero, $E_c = 0$ [25]. As such, additional electron emission or electron current loss to the anode and return to the cathode, is allowed to adjust the space charge in the gap and enforce this condition [30]. Note that the SCL condition means that the model cannot describe current re-trapping.

As justified in [29], the model also assumes the anode is not a SCL emitter of ions, the kinetic pressure of electrons at the electrodes is negligible and the MITL is efficient. Efficiency is defined as the ratio of the extracted to injected anode current, with this assumption supported by a range of experimental studies [29]. Replacing the magnetic fields at the anode and cathode electrodes in Eqn.(2.14) with $B_a = \mu_0 I_a/w$ and $B_c = \mu_0 I_c/w$ yields the pressure balance relation in terms of the bound currents, Eqn.(2.15). Here, the vacuum impedance of the line is $Z_0 = (\mu_0/\epsilon_0)^{1/2} d/w$ [25]. This expression also holds in radial disk transmission lines, where the width of the line, $w$, is replaced by $2\pi r$ in cylindrical coordinates, such that the vacuum impedance is a function of the radius, $r$ [31].

$$E_a d = Z_0 (I_a^2 - I_c^2)^{1/2} \quad (2.15)$$
Taking the potential at the cathode to be zero, \( V_c = 0 \), in the presence of the electron sheath space charge, the voltage across the line can be expressed as Eqn.(2.16). Here, \( V_s \) is the potential at the position of the vacuum-sheath interface, \( d_s \), and \( V \) is the voltage at the anode [29]. The space charge correction factor, \( V_s \), is small for strongly insulated flows and becomes more important for systems with larger vacuum electron sheaths.

\[
V = \int \vec{E} \cdot d\vec{l} = E_a (d - d_s) + V_s \tag{2.16}
\]

A specific expression for \( V_s \) can be derived by assuming the charge density in the electron sheath, \( \rho_c \), is constant [29]. In this case, the electric field as a function of distance across the a-k gap is given by Eqn.(2.17).

\[
E(x) = \frac{\rho_c x}{\epsilon_0} \tag{2.17}
\]

Here, \( E_a = E_s = \rho_c d_s/\epsilon_0 \) and \( V_s = \rho_c d_s^2/2\epsilon_0 \) (= \( \int_{d_s}^{d} E(x) \, dx \)), where \( E_s \) is the electric field at \( d_s \). Note that \( E_a = E_s \) as \( \rho_c = 0 \) for \( d > x > d_s \) [25]. Substituting for \( d_s \), Eqn.(2.18), in the previous expression for \( V_s \) yields Eqn.(2.19).

\[
d_s = \frac{\epsilon_0 E_a}{\rho_c} \tag{2.18}
\]

\[
V_s = \frac{\epsilon_0 E_a^2}{2\rho_c} \tag{2.19}
\]

Assuming SCL emission at the cathode, \( E_c = 0 \), the Newton-Lorentz equation of motion for electrons close to the cathode electrode yields an approximate expression for the z-component of the electron velocity, \( v_z (x) = eB_c x/m_e \), where \( m_e \) is the electron mass. From conservation of the electron energy, \( v_x^2 (x) + v_z^2 (x) = e\rho_c x^2/m_e\epsilon_0 \); substituting the approximate expression for \( v_z \) into this equation and replacing the magnetic field at the cathode with \( B_c = Z_0 I_c/cd \) yields Eqn.(2.20) [29],

\[
v_x (x) = x \sqrt{\frac{e\rho_c}{m_e\epsilon_0} - \frac{e^2 \epsilon_0 Z_0^2 I_x^2}{m_e^2 c^2 d^2}} \tag{2.20}
\]

For a physical solution of Eqn.(2.20) to exist, the charge density must satisfy the equality, Eqn.(2.21).
Constant voltage contours from the Mendel MITL voltage expression, Eqn.(2.22). The axes are the bound anode and cathode currents, $I_a$ and $I_c$, multiplied by the line vacuum impedance, $Z_0$, such that all quantities are in MV.

$$\rho_c \geq \frac{\varepsilon \varepsilon_0 Z_0^2 I_c^2}{m_e c^2 x^2} \quad (2.21)$$

Taking the lower limit of Eqn.(2.21) and combining it with Eqn.(2.15), Eqn.(2.16), Eqn.(2.18), Eqn.(2.19) and Eqn.(2.21), yields the final expression for the voltage on the line, Eqn.(2.22), including the approximate space charge correction term [25].

$$V = Z_0 \left( I_a^2 - I_c^2 \right)^{1/2} - \frac{m_e c^2}{2e} \left( \frac{I_a^2}{I_c^2} - 1 \right) \quad (2.22)$$

This expression is useful for estimating the voltage at a point along a MITL from experimental measurements of the bound currents $I_a$ and $I_c$ [38]. Similar expressions to Eqn.(2.22) have been obtained from the other MITL models, specifically the parapotential and quasi-laminar schemes discussed above. In general, the expressions differ only in the form of the space charge correction term. Therefore, for strongly insulated systems where this term is small, the results from the different models do not differ significantly. A review of the different models and voltage expressions, as well as a comparison of the models with a range of experimental data, is given in [39].

Constant voltage contours of Eqn.(2.22) are plotted in Fig.(2.3), showing the allowed combinations of cathode and anode currents. The left asymptote is referred to as saturated flow, corresponding to the minimum cathode current at which the line can
operate. In this case, the electron sheath extends across the entire a-k gap, \( d_s = d \). At the other extreme is super insulated flow, where the electron sheath is bound tightly to the cathode electrode [25].

In the above derivations, the charge density of the electron sheath was assumed to be constant. Other distributions can be chosen, generating expressions similar to Eqn.(2.22), differing by only a scaling factor in the space charge correction term [25]. This freedom was exploited in [25], where an explicit scaling factor was included in the numerator of the final term of Eqn.(2.22). This factor was approximated by a cubic polynomial and fitted to data from PIC simulations of a uniform impedance MITL; the rescaled model voltage predictions were found to fit experimental data more closely [25].

The minimum of each curve in Fig.(2.3) is unique and corresponds to the minimum total current, \( I_a \). It was originally postulated that the minimum current solution corresponded to the self-limited flow, at which a line operates behind the loss front. Other authors postulated self-limited flow occurred at the minimum energy solution [25], which lies close to the minimum current solution. However, the rescaled model presented in [25], demonstrated that self-limited flow occurs slightly to the left of the minimum current solution, in the saturated region of the solution space.

Using the pressure balance model, further expressions, describing for example, the mean electron drift velocity and sheath thickness, in terms of the line current and voltage, can also be derived as in [25,29].

2.4.4 Flow Impedance Modelling

The presence of the electron sheath space charge within the MITL a-k gap alters the impedance of the line compared to the vacuum impedance. For modelling dynamic systems, it is therefore useful to define an operational impedance, known as the flow impedance [40]. The electric flow impedance, \( Z_f \), is defined as the vacuum impedance taking the distance between the anode and the mean position of the electron sheath space charge as the a-k gap [30].

Again considering the parallel plate MITL geometry in Fig.(2.2), the centroid of the sheath space charge is defined as in Eqn.(2.23), where \( Q(x) \) is the charge per unit length across the a-k gap, with \( Q_a = Q(d) \) and \( Q_c = Q(0) \) the charge per unit lengths enclosed...
at the anode and cathode electrodes, respectively. The total gap spacing is \( d \) and the distance from the centroid of the sheath space charge to the anode is \( d_c \).

\[
\int_{Q_a}^{Q_c} x dQ / \int_{Q_c}^{Q_a} dQ = d - d_c \tag{2.23}
\]

Making a change of variables to units of impedance, \( R(x) = \sqrt{\mu_0/\epsilon_0 x/w} \), in Eqn.(2.23), yields Eqn.(2.24). Here, the vacuum impedance of the line is \( Z_0 = R(d) = \sqrt{\mu_0/\epsilon_0 d/w} \). Evaluating the integral in the numerator using integration by parts gives Eqn.(2.25).

\[
\int_{Q_a}^{Q_c} RdQ / \int_{Q_c}^{Q_a} dQ = Z_0 - Z_f \tag{2.24}
\]

\[
\int_{Q_c}^{Q_a} RdQ = \int_0^{Z_0} \left( \frac{dQ}{dR} \right) RdR = Z_0Q_a - \int_0^{Z_0} Q(R) dR \tag{2.25}
\]

The last term in the above expression is proportional to the voltage across the line, \( V_a = \int_0^{Z_0} cQ(R') dR' \). Combining this with Eqn.(2.24) and Eqn.(2.25), gives expressions for the electric flow impedance, Eqn.(2.26) and Eqn.(2.27), in terms of the line parameters.

\[
V = Z_0cQ_c + Z_f c(Q_a - Q_c) \tag{2.26}
\]

\[
Z_f = \frac{V_a - Z_0cQ_c}{c(Q_a - Q_c)} \tag{2.27}
\]

Typically, the flow impedance ranges between \( Z_0/2 \) and \( Z_0 \). The first term of Eqn.(2.26) represents the contribution of the charge on the cathode to the voltage, whilst the second term is the contribution from the charge within the electron sheath, \( Q_a - Q_c \) [30]. This contribution is equivalent to a shell of charge \( Q_a - Q_c \), of infinitesimal thickness, located at the position of the sheath space charge centroid \( d_c = d - d_f \), or in terms of impedance, \( R = Z_0 - Z_f \). As defined above, it follows that the flow impedance is the vacuum impedance of the line with the electrodes located at the positions of the anode and the charge shell. Considering the charge to exist in a thin shell is useful for modelling a range of systems [40].
A simplified form for the flow impedance can be obtained by again assuming pressure balance in the flow layer, which in terms of the anode and cathode currents and charges can be expressed as \( I_a^2 - c^2 Q_a^2 = I_c^2 - c^2 Q_c^2 \). The electric field at the cathode is \( cQ_c \), such that the SCL emission condition is now \( Q_c = 0 \), yielding \( cQ_a = (I_a^2 - I_c^2)^{1/2} \). Substituting this expression into Eqn.(2.27), gives the simplified relation, Eqn.(2.28) [40].

\[
Z_f = \frac{V}{cQ_a} = \frac{V}{(I_a^2 - I_c^2)^{1/2}}
\]  

(2.28)

Mendel et al. used this scheme to model a number of systems, including a MITL impedance transition and voltage adder [40]. A second, magnetic flow impedance, \( Z_m \), can also be defined from the centroid of the current density within the MITL a-k gap, as in Eqn.(2.29). Here, \( A_a \) is the magnetic vector potential at the anode. In general, the position of the current density centroid will lie closer to the anode than that of the charge density, due to the higher electron velocity near the vacuum-sheath interface, meaning \( Z_m \leq Z_f < Z_0 \). When the charge distribution can be approximated by a single layer of infinitesimal thickness, as discussed above, \( Z_m = Z_f \) [30].

\[
cA_a = Z_m I_a + (Z_0 - Z_m) I_c
\]  

(2.29)

### 2.4.5 Generalised Models

Ottinger et al [30] have developed a MITL model which relaxes some of the assumptions made in the pressure balance model. Here, the electron sheath was modelled as a one dimensional electron fluid; the electron pressure in the sheath was retained and non-zero values of the electric field allowed at the cathode electrode. As such, the model could treat electron emission and re-trapping at the cathode [30]. The model has been parameterised for incorporation into the Bertha [20] transmission line circuit code. Here, the goal was to accurately model dynamic MITL systems without reverting to the more computational expensive PIC method. The results of this model are consistent with the pressure balance theory in the SCL emission limit, \( E_c = 0 \) [30].

A similar fluid model was used to study the effects of collisions on the MITL electron sheath. Here, collisional effects due to rapidly oscillating electric fields were included through a general collisional term in the fluid equations. The collisional model results
were found to lie close to predictions of the collisionless pressure balance, parapotential and quasi-laminar theory. The effect of the collisions was to drive the expansion of the electron sheath; this effect is expected to be more important as the length of the MITL increases, as electrons will be given more time to collisionally expand across the a-k gap [39].

2.5 Non-uniform Vacuum Impedance MITLs

So far, we have considered only MITLs with uniform vacuum impedance and voltage. Systems with non-uniform vacuum impedances give rise to non-linear effects in the electron sheath [40]. As such, analytic treatment of the electron flow dynamics is complicated, with numerical simulation providing valuable insights.

For radial transmission lines, the vacuum impedance is a function of the radius, \( Z_0 \sim \frac{60d(r)}{r} \). As discussed above, on \( Z \), from the insulator stack, \( r = 1.6 \text{m} \), down to \( r \approx 20 \text{cm} \), the a-k gap, \( d \), decreases proportionally to the radius, giving a slow change in the vacuum impedance of the line. At 20cm, the line transitions to a constant a-k gap of 1cm, such that the vacuum impedance increases relatively rapidly with reducing radius [13]. In these regions, where the electrons in the sheath are drifting up the vacuum impedance gradient, the electron sheath is predicted to detach from the cathode electrode [13, 31]. These dynamics of the electron layer can be analysed using the pressure balance theory outlined in section 2.4.3. Taking the strongly insulated limit of Eqn.(2.22), \( I_e \ll I_a \), i.e. \( I_e \sim I_a \), yields Eqn.(2.30), where the vacuum impedance has been substituted in the second expression [31].

\[
I_e(r) \sim \frac{V^2}{2I_aZ_0^2} = \frac{V^2r^2}{I_a d(r)^2}
\]

At larger radii, where the vacuum impedance changes slowly (as \( d \propto r \)), the electron sheath layer remains bound to the cathode electrode. However, as the radial coordinate reduces, \( I_e \) must also reduce in order to maintain pressure balance (i.e. satisfy Eqn.(2.22)); this is achieved by re-trapping electrons in the cathode electrode [31]. LSP [31] and Quicksilver [13] PIC simulations of the \( Z \) feed lines do in fact predict electron re-trapping for \( r > 20 \text{cm} \). As will be discussed in more detail in the next section,
the simulations actually predict enhanced re-trapping due to electron vortices formed in the flow layer. For larger gradients in the vacuum impedance, electron re-trapping alone cannot maintain pressure balance; the electron sheath detaches from the cathode, moving closer to the anode electrode, such that its charge centroid maintains a gap spacing of $d(r) \propto r$ i.e. a constant flow impedance. [41]. For $r < 20\text{cm}$, PIC simulations of the Z feed lines show the layer to be composed of two components; an attached layer with re-trapping and a layer which has lifted away from the cathode to maintain pressure balance [13,31]. The electron flow layer may also detach from the cathode in regions of reducing electric field in the flow direction, for example due to EM wave reflections from an under matched load. A reduced electric field lowers the electron drift velocity $|v_E| = E/B$, reducing the Lorentz force and causing the layer to lift away from the cathode [42].

Similar electron sheath dynamics are also predicted to occur in systems involving voltage addition. Induction Voltage Adder (IVA) technology [43], is used to drive high voltage (10s MVs) electron and ion beam diodes. Here, voltage waves from a series of $N$ PFLs, at $\sim 1\text{MV}$, are added in series on a central stalk to generate a potential of $N\text{MV}$s at the load. In negative polarity, the central stalk is the cathode, which operates as a MITL. The electron flow has similar dynamics to that described for uniform vacuum impedance MITLs, existing in a sheath that remains closely bound to the cathode [44]. Typically, the Mendel voltage relation, Eqn.(2.22), is directly applicable and used to calculate the line voltage from the measured bound anode and cathode currents in experiment [38].

IVAs are used in positive polarity to drive ion beam diodes. Now, the outer electrode is the cathode and the central stalk, the anode [44]. Due to the voltage addition, each gap is at a different potential, such that electrons emitted in different gaps have different energies. The electron flow layer remains attached to the electrode it was created on, but as it enters the next gap, at larger potential, the flow lifts away from the surface, moving closer to the anode in order to maintain EM pressure balance [44]. The flow in the second gap therefore consists of two layers; an electron sheath attached to the cathode consisting of locally emitted particles and a ”launched flow” from the first gap [45]. For accelerators with several gaps, there are multiple flow layers [44].

Analytic treatments of multiple laminar flow layers, where the layers do not interact,
have been reported [40,46]. However, two dimensional PIC simulations show the formation of electron vortices, leading to mixing of the flow layers [45]. In positive polarity IVA simulations, vortices are seen to form in the attached layer at the upstream end (start) of each gap. Here, electric field enhancements on the sharp corner where power is fed into the gap, lead to enhanced SCLE of electrons. This excess space-charge sets up an electric field in the flow layer, parallel to the electrode which acts to slow down electrons behind it, reducing the electron velocity and consequently the magnetic part of the Lorentz force, causing the flow to lift off and move away from the cathode electrode surface [42].

2.5.1 Detached Sheath Instability and Electron Vortices

As discussed above, in MITLs with non-uniform vacuum impedance, in order to maintain pressure balance, part of the electron sheath can detach from the cathode electrode. The detached electron sheath is susceptible to the diocotron instability [47]; this instability is common to charged particle beams propagating in crossed electric and magnetic fields and results from the interaction of waves excited on the free surfaces of the charged particle layer [31,47,48].

The instability results in the electron sheath breaking up to form electron vortices [47]. These consist of collections of electrons that $\vec{E} \times \vec{B}$ drift counter clockwise about the centre of the vortex, due to the electric field associated with the vortex space-charge. In addition, the whole vortex structure $\vec{E} \times \vec{B}$ drifts in the direction of the power flow due to the line electric field. Vortex formation in the electron sheath is seen to occur in PIC simulations of the Z radial lines and DPHC [13,31], as well as in the attached and launched flow layers of positive polarity IVAs [44,45].

In simulation, the vortices typically become detached from the bound part of the electron sheath, drifting above it in the a-k gap. In these cases, the vortices are seen to have a large effect on the surrounding electron flow. The electric field associated with the vortex space-charge opposes the applied line electric field at the cathode, suppressing electron emission [44]. Electrons at the downstream edge of the vortex can also be returned to the cathode electrode; here, the vortex provides an efficient electron re-trapping mechanism [31]. As the vortex drifts above the attached flow, it draws electrons
from this region, with the upstream and downstream electron flow wrapping counter clockwise around the vortex [44].

Two dimensional electron vortices have been studied analytically [45,49]. In [49], the vortex radius, \( R \), is assumed to be smaller than the collisionless skin depth, \( \lambda = c/\omega_p \), where \( \omega_p \) is the electron plasma frequency. In this limit, the vortices are not diamagnetic and do not affect the external magnetic field [50]. Church et al [45], studied the vortices using relativistic electron fluid equations, in the limit \( R \approx \lambda \). Here, the vortices are predicted to be diamagnetic and have a maximum radius of \( 2^{3/2}\lambda \) [45]. This result was found to agree well with two dimensional PIC simulations [45], where vortices in positive polarity IVA accelerators are predicted to be diamagnetic [44]. These results have also been used to incorporate the average effects of electron vortices into analytic MITL layered flow models. Here, the launched flow layer thickness is set based on this maximum vortex radius and is used to model positive polarity IVAs and other non-uniform MITL systems [44].

Electron vortex formation in the electron sheath is a common feature of PIC simulations of the Z radial lines and DPHC [13, 14, 31]. A specific example of where they have been predicted to affect the current loss is in the magnitude of the electron sheath current entering the convolute, which will be discussed further below. Here, the current predicted to enter the convolute was \( \sim 50\% \) higher than that predicted from the Mendel pressure balance theory due to the unstable electron sheath [31]. Additionally, field reversal at the cathode due the electric field associated with the vortex space charge, was considered as a mechanism to draw ions from the plasma into the a-k gap, potentially further enhancing the electron flow current. This was included in LSP simulations of the Z radial lines, but was found to have little effect on the prediction for the current entering the convolute [31].

2.6 A Review of Current Loss Mechanisms and Modelling

In this section, the proposed current loss mechanisms within the Z DPHC and inner MITL and models used to describe and study them will be reviewed. These range from
2.6.1 Circuit Modelling

As discussed in section 1.2 of chapter 1, detailed simulations of experimental loads on Z, such as the wire array Z-pinch, require a circuit model of the accelerator to model the Poynting flux delivered to the load and the electrical coupling between the load and the accelerator [2].

For computational efficiency, the vacuum section and part of the water lines is typically modelled with the simple circuit representation shown in Figure 2.4 (reproduced from [2]). This Thevenin equivalent circuit is a reduced form of more advance circuit models that include all of the components of the machine. The equivalent voltage source required to drive the circuit can either be calculated by the more complete model or reconstructed from electrical records from a given shot [2].

In this equivalent circuit, the current loss within the convolute is modelled as an electron flow loss and is included as a variable resistance to ground after the 13.1nH inductor representing the radial lines, in parallel with the load inductance, as shown in Figure 2.4. The effective resistance of this loss follows from considering the electron flow entering the convolute from the radial lines [2]. As described above, the electric field stress on the cathode electrodes in the radial lines exceeds 240kVcm$^{-1}$, such that...
a plasma is formed on the electrode surfaces. Electrons emitted from the plasma into
the vacuum a-k gaps are insulated by the magnetic field and $\vec{E} \times \vec{B}$ drift down the lines
towards the convolute [13,31].

This insulation is lost at the magnetic nulls in the convolute, which as described in
the previous chapter, are formed by the current addition path. As such, electrons from
the sheath can cross the a-k gap at the nulls and impact the anode, shunting current
from the load. This is the origin of the electron flow loss [2,14,16]. In experiment, post
shot damage on the anode electrodes is consistent with the electron deposition at the
positions of the nulls [16].

Such electron flow losses at a single magnetic null have been studied theoretically and
experimentally. In these experiments, the bound anode and cathode currents were mea-
sured upstream and downstream of the null [51]. Experimentally, the flow impedance,
$Z_f$, defined in Eqn.(2.31), relating these measurements, was found to be approximately
constant throughout the power pulse. Here, $I_{total}$ and $I_{cathode}$ are the total current mea-
sured upstream of the loss and the bound cathode current measured downstream of the
loss, respectively. Note that, $Z_f$, is non-linearly dependent on the current loss. As $I_{total}$
is the sum of the currents flowing in the cathode and electron sheath prior to the loss,
it can be identified with the return current flowing in the anode [2].

$$Z_f = \frac{V}{\sqrt{I_{total}^2 - I_{cathode}^2}} \quad (2.31)$$

Comparing Eqn.(2.31) with the flow impedance derived from Mendel’s pressure bal-
ance theory in the SCL emission limit, Eqn.(2.28) [40], we see they are very similar,
demonstrating the loss is related to electron motion in crossed electric and magnetic
fields.

In the Thevenin circuit model, it is assumed that all of the electron flow current is
lost to the anode, such that the electron flow loss can be represented by the effective
resistance given in Eqn.(2.32). For $Z_r$, Figure 2.4, the electron flow losses from the four
level radial transmission lines at the convolute magnetic nulls are lumped together into a
single flow impedance, $Z_f$. Initially, this was set to a constant value of around 0.25$\Omega$ in
order to match the experimental current loss at stagnation. More sophisticated imple-
mentations of the model used a time varying flow impedance, which was reconstructed

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from electrical measurements for the specific shots of interest [2].

\[ R = Z_f \left( \frac{I_{\text{total}} + I_{\text{cathode}}}{I_{\text{total}} - I_{\text{cathode}}} \right)^{1/2} \]  

(2.32)

Transmission line circuit models of the Z vacuum section, used to design and predict the electrical performance of the machine, treat the convolute loss in a similar manner; the loss current is included as a shunt resistor at the downstream end of the convolute [52, 53]. The resistance of this element is calculated assuming that all of the vacuum electron current emitted in the radial lines is lost in the convolute [52]. This assumption precludes the possibility for vacuum current to be re-trapped in the cathode electrode [10], a phenomena which has been observed in PIC simulations of electron flow in the Z radial lines [13, 31]. The magnitude of the vacuum electron current is approximated from the electrical parameters of the circuit transmission element using a modified form of the Mendel pressure balance voltage, Eqn.(2.22). Here, the vacuum impedance, \( Z_0 \), is replaced with \( Z_0 \left( 1 - vt/g \right) \), where \( v \) is the cathode plasma expansion velocity, \( t \) the time and \( g \) the a-k gap spacing, to account for the finite cathode plasma expansion during the current pulse [52]. Typically, an expansion velocity of 2.5cmµs\(^{-1}\) is used, consistent with experimental measurements [16]. In the model, the magnetic flux is assumed to diffuse through the plasma closing the gap, such that the changing line impedance does not modify the transmission line element parameters [10]. The results of the circuit model show good agreement with experimental results up to peak current, after which time an additional 0.3Ω shunt resistance near the convolute is required to achieve a closer fit [52].

A more detailed circuit model of Z than the Thevenin equivalent shown in Figure 2.4, used to drive MHD (Gorgon) simulations of wire-array Z-pinches, has been developed by Jennings et al. [2]. Here, the requirement for an improved model came from the need to reduce uncertainties in the Poynting flux being delivered to the load and allow simulated voltages and currents to be compared to the experimental electrical histories to further constrain the MHD load model [2]. A schematic of the model is shown in Figure 2.5 (reproduced from [2]).

The vacuum radial lines from the insulator stack to the convolute were modelled as four separate ideal, lossless transmission lines. The voltage and current waves along
the lines were evolved via an implicit solution of the telegrapher equations, Eqn.(2.1) and Eqn.(2.2). The inductance and capacitances used for the lines in the circuit model were calculated from EM Gorgon simulations. Here, the lines were split into 1.4mm sections along the radial direction and driven with a linear rising voltage; the inductance and capacitance of each segment could then be inferred from the simulated voltage and currents. The voltage source used to drive the radial lines was applied in the water transmission lines and was constructed from the stack voltage measurements by translating them back in time [2].

To represent the electron flow losses at the magnetic nulls in the convolute, separate electron flow losses were included at the end of each of the four transmission lines; these are labelled as $R_{A-D}$ in Figure 2.5. A separate effective resistance was calculated for each line using Eqn.(2.32), with a flow impedance calculated from the line parameters at the convolute. Specifically, Mendel’s pressure balance relation for the voltage, Eqn.(2.22), which relates the electron flow current to the voltage, $V$, the total current, $I_a$, the current in the cathode, $I_c$, and the vacuum impedance of the line, $Z_0$, was used to rewrite the definition of flow impedance, Eqn.(2.31), to provide a function of known or derived parameters from the circuit model, Eqn.(2.33). Note that the model again assumed that all of the electron flow current was lost within the convolute; as will be discussed

Figure 2.5: A schematic of the transmission line circuit model of the Z vacuum radial lines, convolute and inner MITL.
below, this assumption is consistent with 3D PIC simulations of the convolute [2].

\[ Z_f = \frac{Z_0}{2} + \frac{Z_0}{2} \left( 1 - \frac{2mc^2V}{eZ_0^2I_c^2} \right) \] (2.33)

The vacuum impedance was further modified to include the cathode plasma expansion, as described above [52]. The four levels of transmission line were coupled together through series inductors with values to represent the convolute geometry. The convolute was then coupled to the MHD load simulation through a single transmission line, representing the inner MITL; the inductance and capacitance profile of this line was again derived from Gorgon EM simulations [2].

The circuit model was applied to Gorgon simulations of a compact tungsten wire-array. Comparing the simulated and experimentally measured stack and load currents, the inclusion of the electron flow losses at the ends of the radial lines, was found to give better agreement between the simulation and measurement at early times (<4MA). Note that without the electron flow loss, both the experimental and simulated traces showed the load current to be lower than the stack current at these times; this is a result of the finite propagation time of the EM wave along the lines and not a current loss in the sense discussed above. Including the electron flow loss increased the difference between the stack and load currents in the simulations and was closer to the experiment [2].

At later times (>10MA), the simulation under predicted the current loss. The simulated loss could be increased by increasing the cathode plasma expansion velocity in the definition of the vacuum impedance; however, even with unreasonably high velocities, the experimental loss near peak current could not be matched. At these times, the electron flow loss was found to be minimal due to the increasing current improving the magnetic insulation in the radial lines. To match the experimental loss, it was therefore necessary to include a separate convolute loss resistance in the circuit. This was inferred by translating the stack voltage to the position of the convolute current measurement. Above, ∼10MA the resistance was seen to suddenly collapse to around 0.4Ω around halfway up the current pulse, until stagnation, after which time it further decayed [2].

The inferred convolute resistance was parameterised by assuming that resistive plasma had been able to expand across the a-k gap in the convolute. It was argued that electron deposition on the anode was sufficient to form a plasma that expanded
with velocity, $v$, starting at time $t_0$, across one of the magnetic nulls of width, $g_c$ and area, $A$. From this, a phenomenological loss resistance was defined, as in Eqn. (2.34), where the loss was described as a combination of a SCL electron current (first term) and a current flowing through a plasma with resistivity, $\eta$, (second term). This was distinct from and applied separately to the electron flow losses at the ends of the radial lines discussed above [2].

$$R_{\text{plasma}} = \frac{d^2}{2.34 \times 10^{-6} A \sqrt{V}} + \frac{\eta (g_c - d)}{A}$$

$$d = g - \min (g_c, v (t - t_0))$$ (2.34)

The inferred convolute resistance could be fitted by assuming a gap spacing of 1.5 cm, a plasma expansion area of 15 cm$^2$, an expansion velocity of 21 cm$\mu$s$^{-1}$ and plasma resistivity of 0.035 $\Omega$. It was noted that the last two parameters were high; however, the expansion velocity was consistent with 3D PIC simulations of the convolute plasma [15], whilst the plasma resistivity was strongly dependent on the chosen area. As such, these parameters represented one possible combination that could be used to fit the data [2].

Including the additional resistive loss in the circuit model gave improved agreement between the simulated and measured stack and load currents up to peak current. However, after stagnation, the simulation still significantly underestimated both of these currents. The discrepancy was due to an over prediction of the convolute voltage, where during this time the voltage was maintained by the rapidly increasing inductance of the load as it imploded. It was concluded that the discrepancy was either due to the MHD model inaccurately describing the load implosion, or the load current measurement overestimating the current that was actually delivered to the load [2].

In [2], it was concluded that the latter case was the most probable; here, the MHD model was constrained by a range of radiation and radiography measurements. Including an additional electron flow loss in parallel with the load in the inner MITL part of the circuit model driving the MHD simulations was found to give excellent agreement between the simulations and the whole range of electrical and implosion diagnostics. The choice of an electron flow loss to model this additional, undiagnosed current loss within the inner MITL, was made in the absence of the known current loss mechanism [2].

The current at the load is typically not measured in experiment. A series of current
scaling experiments on Z, showed the X-ray power to have sub $I^2$ scaling, which is expected from simple physical arguments based on the kinetic energy of the load [28]. Here, the convolute current, which is measured at the start of the inner MITL ($r \sim 6\text{cm}$), was taken to be the current delivered to the load on axis. It is therefore possible that the experimentally inferred scaling was effected by an additional current loss occurring within the inner MITL radius [2]. However, more recent scaling studies have shown X-ray power and energy scaling closer to the expected $I^2$ [54].

The inferred inner MITL loss was found to be strongly dependent on the electrode geometry; the largest losses were found for the right-angled bend configuration fielded on early experiments. This prompted it to be replaced with a conical electrode shape, which gave a smoother impedance transition from the convolute to the load and a reduced predicted current loss, for later experiments [3].

### 2.6.2 Particle-in-Cell Simulations

In parallel to the circuit modelling discussed above, the current loss within the Z DPHC has been studied using detailed 3D kinetic PIC simulations. Quicksilver [12,14,18] and LSP [15, 16], simulations of both the Z and ZR DPHCs have been reported. In the Quicksilver studies of the Z convolute, [12,14] the current loss was treated as an electron flow loss. As such, it was assumed that plasma was formed on the cathode electrode, but that it remained tightly bound during the current pulse. In this way, SCL electron emission was allowed directly from the cathode electrode once the strength of the normal component of the electric field exceeded the electrode breakdown threshold. The earlier simulations [12], did not model the full current pulse; instead, the simulations were terminated with a resistive load, representative of a wire-array Z-pinch load at various times during the current rise and implosion. These simulations were driven with a voltage pulse that rose to a representative value in a few nanoseconds and then levelled off. An insulated electron sheath was observed to form in the radial lines; this insulation was lost in the convolute where the electrons were able to impact the anode by travelling across the magnetic nulls. This steady state current loss was assumed to be representative of the experimental loss, when the load impedance passed through the value used in the simulation [12]. Later, the model was modified to simulate the entire current
pulse [14]. In a similar way to the circuit model developed in [2], the four level radial
disk feed driving the convolute was modelled out to the insulator stack with a series of
ideal transmission lines, driven by an effective voltage derived from the measured stack
voltage [14]. Again, the current loss was treated as an electron flow loss, with SCL elec-
tron emission allowed directly from the cathode electrode. This methodology was also
used to simulate the electron flow loss in the modified ZR convolute electrode geometry;
here, the transmission line circuit model was also modified to account for the changes
made to the coupling of the water lines to the insulator stack in the refurbishment [18].

Equivalent LSP simulations of the electron flow loss over the full current pulse, in
the Z [16] and ZR [15] DPHCs have been reported. In both the Quicksilver [14,18] and
LSP [15,16] simulations, the wire array load was modelled as a time varying inductance,
using the well-known zero dimensional (0D) implosion model [55]. Here, the wire array
is modelled as a solid liner of fixed mass and length [16]. The current at the load from
the PIC simulation is used to calculate the magnetic force on the liner and update its
velocity and radial position [55]. With a fixed current return path radius, the change in
inductance of the load is calculated from the expression for a coaxial transmission line.
This is used to update the load voltage, which represents the reflected component of the
voltage pulse from the load impedance [16]. The liner motion is terminated at a specified
final radius, usually with a 10:1 convergence ratio [14]. This simple load model does
not include many of the physical phenomena present in real wire array loads, which are
reviewed in [56] and [57]. However, the electrical properties of the load are reproduced
with sufficient accuracy to warrant its use [55].

As was found in the initial Quicksilver simulations [12], the Quicksilver [14,18] and
LSP [15,16], electron flow current loss simulations predicted that a magnetically insu-
lated electron sheath was formed in the radial lines. This insulation was lost in the
convolute at the magnetic nulls; current was shunted from the load by electrons im-
pacting the anode across the magnetic nulls. However, as was found in the coupled
circuit-MHD simulations in [2], the absolute magnitude of the electron flow current
losses around peak current, predicted from both the Quicksilver and LSP simulations,
were significantly lower than the measured current loss [14,16,18]. The magnitude of the
electron flow current loss predicted by both codes could be increased slightly by includ-
ing SCL proton emission from the anode. Here, an anode plasma was assumed to form
on the electrode were the temperature exceeded 700K, the threshold for thermal desorption and ionisation of neutral contaminants. As for the cathode plasma, this plasma was assumed to remain tightly bound to the electrode for the duration of the current pulse; the plasma acted as a zero work function surface for SCL proton emission. The enhanced electron flow current loss in this case, followed from the increase in the SCL electron current drawn from the cathode due to the presence of the positive ion space charge; in models of SCL emission in a 1D a-k gap, this is equivalent to the well-known bi-polar flow [23].

Both the driving circuits used in the Quicksilver [14, 18] and LSP [16] simulations assumed ideal transmission lines. As such, these did not include the electron flow current emitted at larger radii in the radial feed lines [14]. In the Z radial lines, the electric field stress exceeds the threshold for cathode plasma formation, $\sim 240 \text{kV cm}^{-1}$, below a radius of $\sim 1.3 \text{m}$ [13]. The PIC simulation domain typically extends to below 20cm. As such, the models could have under predicted the loss current by under predicting the magnitude of the electron flow current entering the convolute from the radial lines. As discussed in section 2.5, PIC simulations of the Z radial disk feeds, representing the convolute and load with an equivalent circuit model, showed strong insulation in the vacuum electron layer where the anode electrode is tapered to give a slowly varying vacuum impedance [13, 31]. Where the lines transition to a constant 1cm a-k gap, launched electron flow and vortex formation were predicted [13, 31]. These non-linear sheath dynamics were found to further increase the average vacuum current injected into the convolute from the feed lines by a factor of three to four, compared to that predicted by the Mendel pressure balance theory using the simulated line parameters [13]. Note that this is also true of the circuit models described in previous section, which use the Mendel relations to calculate the electron flow current entering the convolute. As such, later Quicksilver simulations varied the geometry of the radial feed electrodes at the simulation domain boundary to match the electron flow current in the convolute simulations, with that predicted from separate PIC simulations of a larger extent of the radial lines [18]. However, even accounting for this additional injected electron flow current, the current losses predicted from the Quicksilver PIC simulations were still significantly lower than measured in experiment [14]. Note that this result i.e. the insufficiency of treating the convolute current loss with only an electron flow current
loss, is consistent with the results from coupled circuit-MHD load simulations [2] and
detailed transmission line circuit models [52, 53], described above.

Current losses in the Z DPHC, consistent with measured values of $\sim 1.5\text{MA}$ at peak
current, were predicted by LSP PIC simulations including the evolution of a Hydro-
gen plasma from the cathode electrode [16]. Here, a fully ionised plasma was injected
into the vacuum cell next to the electrode by desorbing neutral particles at a fixed rate
and randomly ionising them within the cell. Additionally, SCL proton emission was
allowed from the anode electrode if the temperature exceeded 700K due to heating by
electron bombardment. The cathode plasma reached a peak density and temperature
of $\sim 10^{16}\text{cm}^{-3}$ and 3eV. The enhanced current loss over the electron flow current sim-
ulations described above, came from the plasma penetrating the downstream (towards
the load) sides of the anode posts, reducing the effective a-k gap. Here the plasma at
a density of $\sim 3\times 10^{13}\text{cm}^{-3}$ acted as an effective cathode, emitting electrons at the SCL
limit. The reduced effective a-k gap allowed electrons to cross from the plasma region
to the anode and enhanced the electron current loss. The plasma penetration came
partly from plasma drifting along magnetic field lines connecting the cathode holes up-
stream (away from the load) of the anode posts and collecting downstream of the posts.
Plasma penetration was also observed from the cathode plasma on the upstream side of
the anode posts at the positions of the magnetic nulls [16].

The magnitude of the simulated current loss at peak current was found to be a
strong function of the neutral desorption rate; the experimentally measured values,
$\sim 1.5\text{MA}$, were obtained with relatively low rates of between 0.005 and 0.0075$mnl^{-1}$
[16]. Here, one monolayer ($ml$) $=10^{15}\text{cm}^{-2}$ [21]. The LSP Hydrogen plasma model
was later modified to simulate the modified ZR DPHC [15]. As was described for the
electron flow current loss simulations, as well as the electrode geometry, the transmission
line circuit model was modified accordingly. Additionally, the OD load model was
replaced with a simple snow-plough model to simulate nested wire-array implosions.
The measured current losses on ZR were matched with the same low neutral desorption
rates of between 0.005 and 0.0075$mnl^{-1}$ [15]. In the Z case [16], the simulation was
run through stagnation and the current loss inferred from an A to B comparison of the
simulations included the cathode plasma and SCL electron emission only. In contrast,
in the ZR simulations [15], the simulated MITL and convolute currents were matched
to the experimental traces, were in general apart from early times, good agreement was found. Additionally, the simulations were not run through stagnation but terminated just before peak current. The plasma evolution and dynamics in the ZR convolute were consistent with the results on Z; specifically, the enhanced current loss in the plasma case came from plasma penetrating the downstream sides of the anode posts reducing the effective a-k gap, allowing electrons to cross from the plasma to the anode electrode [15]. It should be noted that the peak plasma densities in the ZR convolute simulations were over ten times higher than the Z convolute case. Also, the plots of the simulated plasma density in [15], indicate that plasma was only sourced on the inside edges of the cathode holes. This was in contrast to the Z simulations [16], where plasma was also sourced in a small part of the radial lines. The LSP ZR study also included simulations of the nine post-hole variant of the convolute geometry. Here the plasma penetration on the downstream side of the top post was reduced, but enhanced at the bottom post [15]. It should be noted that although a cathode plasma creation model is outlined and results from 1D electrostatic Quicksilver simulations have been reported [18], no results from Quicksilver simulations of the DPHC, including a cathode plasma have been published. However, the author has discussed some general features of the Quicksilver simulation results with Pointon [58].

As discussed in section 2.2, spectroscopic measurements of the plasma in the ZR convolute found strong continuum emission with absorption features [17]. The diagnostic was located at the same position as the convolute B-dot i.e. at the start of the inner MITL, in the anode at a radius of approximately 6cm. This allowed a view of the a-k gap on the downstream side of the anode posts. Measurements of the locations of the continuum emission indicated that the plasma was formed on the cathode and travelled from the cathode to the anode with an apparent velocity of \(>7\text{cm}\mu\text{s}^{-1}\). It was noted that this was higher than the expected 1-2\(\text{cm}\mu\text{s}^{-1}\) from other experiments; it was suggested that the observed emission was from an ionisation wave propagating ahead of the hydrodynamic motion of the cathode plasma [17]. However, this high apparent closure velocity was also consistent with the LSP simulations, were high effect gap closure velocities followed from the plasma penetrating into the gap by flowing along the field lines from the upstream inside edge of the cathode electrode [2,15].

Stark broadening of the hydrogen H-alpha absorption feature was used to determine
a time resolved plasma electron density. The plasma density history was found to be dependent on the load impedance history and ranged between $10^{16-18}\text{cm}^{-3}$ \cite{59}. This was consistent with typical densities found in the LSP simulations of the ZR convolute \cite{15}.

A lithium tracer placed on the anode posts was also used to constrain the axial position of the continuum emitter in the top post hole. In these experiments, the bulk of the emission was found to come from below the centre of the cathode hole \cite{17}; this was consistent with the location of the plasma penetration into the downstream side of the top anode post found in the LSP simulations \cite{15,17}.

### 2.7 Chapter Summary

Detailed circuit models of the Z radial lines and DPHC and inner MITL, coupled to 3D MHD (Gorgon) models of the wire array Z-pinch loads, found that although an electron flow current loss improved the early time (<4MA) agreement of the simulation with experiment, it was not sufficient to reproduce the current loss near peak current. This same conclusion was drawn from 3D LSP and Quicksilver PIC simulations of the convolute, including only SCL electron and ion emission from the cathode and anode electrodes, respectively. The LSP simulations where a fully ionised Hydrogen plasma was injected from the cathode electrode, could reproduce the measured current loss at peak current with relatively low plasma injection rates \cite{15,16}. Alternatively, in \cite{2}, the measured convolute impedance was parameterised assuming an anode plasma expanding across and resistively shorting one of the magnetic nulls.

The formation of a Hydrogen plasma and its penetration into the a-k gap from the cathode on the downstream side of the anode posts is consistent with spectroscopic measurements made of the plasma in the ZR convolute \cite{17,59}. Here, a Hydrogen plasma with a peak density of $\sim 10^{18}\text{cm}^{-3}$ was inferred from the Stark broadening of the H-alpha absorption feature and the positions of the optical emission were consistent with the plasma crossing the a-k gap from the cathode to the anode, with a relatively high velocity of $>7\text{cm\mu s}^{-1}$ during the current pulse \cite{17}. The presence of a Hydrogen plasma was also consistent with the expected neutral contaminant inventory on the electrode, where the plasma forms via ionisation of desorbed contaminant molecules \cite{21}.
We therefore chose to investigate the current loss in the DPHC and inner MITL, through detailed kinetic simulations of the cathode plasma evolution and dynamics. The PIC code developed for this task is described in the next chapter. Here, the electrode plasma and MITL theory reviewed in this chapter will be used to physically justify the design choices made in the PIC model. The DPHC and inner MITL simulation results will be presented in chapter 4. Here, the Mendel pressure balance theory derived in section 2.4.3, will be used to analyse the resulting sheath dynamics; we will also find the formation of vortices in the electron sheath, due to the non-uniform vacuum impedance of the Z lines, to which the discussion in section 2.5.1, will be applicable. The model of the cathode plasma in a 1D gap reviewed in section 2.2.1, will be used to justify the cathode plasma creation model described in the next chapter and applied to the DPHC and inner MITL simulations in chapter 4.

The theory of ideal transmission lines outlined in section 2.1, formed the basis of the circuit model used to self-consistently model the voltage wave transport in the radial lines and injection into the PIC model of the convolute.
Chapter 3

Particle In Cell Model

To investigate the current losses occurring within the Z DPHC and inner MITL, we simulated the evolution of cathode plasmas and charged particle sheaths formed by the ionisation of neutral contaminants desorbed from the electrodes during the current discharge. The complicated 3D electrode geometry necessitated the use of numerical simulation techniques.

Electrons and ions emitted from the plasma on the cathode and anode electrodes form sheaths which range in density from $10^{12}$ to $10^{13}$ cm$^{-3}$ and as discussed in section 2.5.1, in non-uniform impedance transmission lines, are vulnerable to instability formation [14, 16]. As such, to accurately model their evolution a kinetic model is required; specifically a solution of the collisionless Vlasov equation, Eqn.(3.1). Here, the particles comprising the sheath, with charge $q$ and mass $m$, are described by a six dimensional time dependent distribution function $f(\vec{x}, \vec{v}, t)$, where $\vec{x}$ are the three spatial coordinates and $\vec{v}$ the three velocity coordinates. The ensemble average electric, $\vec{E}$ and magnetic, $\vec{B}$, fields in the Lorentz force include both externally applied and self-consistently generated fields [60].

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{x}} + \frac{q}{m} (\vec{E} + \vec{v} \times \vec{B}) \cdot \frac{\partial f}{\partial \vec{v}} = 0 \quad (3.1)$$

Direct numerical simulation of Eqn.(3.1) requires the distribution function, $f$, to be discretised in both position and velocity space and is both complicated to implement
and computationally intensive to solve in 3D. For this study, we therefore pursued an alternative particle based solution scheme, namely the Particle in Cell (PIC) method. Here, in place of direct numerical simulation of the kinetic equation, a system of ordinary differential equations (which are characteristics of the Vlasov equation) [61] to evolve the momenta, Eqn.(3.2) and positions, Eqn.(3.3), of a collection of ‘macroparticles’ are solved. Here, $\vec{x}$, $\vec{v}$ and $\vec{p}$ are the macroparticle position, velocity and momentum vectors, respectively [62].

$$\frac{d\vec{p}}{dt} = \frac{q}{m} \left( \vec{E} + \vec{v} \times \vec{B} \right)$$  \hspace{1cm} (3.2)

$$\frac{d\vec{x}}{dt} = \vec{v}$$ \hspace{1cm} (3.3)

Combined with Maxwell’s equations to evolve the electric and magnetic fields, the desired evolution of the charged particle sheath in the DPHC and inner MITL can be self-consistently modelled. Note that the PIC scheme is a Monte-Carlo (MC) method in the sense that the distribution function is statistically sampled by a relatively small number of macroparticles, where each macroparticle represents a large number, typically $\sim 10^9$, of ‘real’ particles [62]. As such, the PIC method typically produces noisier results than an equivalent ‘quiet’ direct simulation, with the trade-off for improved particle statistics in the PIC simulation being longer run times [63]. The PIC method is used extensively within the pulsed power community to study and improve the operation of existing, as well as design new, pulsed power systems.

### 3.1 Applicability of the PIC Method to Simulating Plasmas in the Convolute

For simplicity, it would be desirable to use a single numerical method to simulate both the charged particle sheaths and plasma present in the convolute. The PIC method is applicable to plasma simulation and is used extensively by the laser plasma community [62]. To understand whether the method is applicable to the plasmas of interest in the convolute, which range in density from $10^{13}$ to $10^{17}\text{cm}^{-3}$, with temperatures between...
and 10eV [16, 17], we must consider the numerical spatial and temporal resolutions required to obtain stable and accurate results from the model.

3.1.1 Explicit Versus Implicit Differencing

The differential equations comprising the PIC model are solved numerically using finite difference techniques [62]. The constraints on the resulting spatial and temporal steps, $\Delta x$ and $\Delta t$, for a stable solution, are dependent on the type of differencing used to discretise the model equations. Implicit differencing casts the variables at the new time step in terms of the dependent variables also at the new time. In contrast, explicit differencing casts the variables at the new time in terms of known values of the variables at the current time step. For stability, implicit differencing allows larger spatial and temporal steps to be taken than explicit differencing, meaning that implicit methods can access a wider range of plasma parameters for the same resolution [64].

The improved stability properties of implicit differencing comes at the cost of increased complexity, where typically a system of linear equations must be solved. Compared to simpler explicit algorithms, implicit algorithms are therefore more difficult to efficiently parallelise to take advantage of the scaling available on modern High Performance Computing (HPC) facilities. As such, the additional computational overhead of taking smaller steps in an explicit model can be offset by efficiently running on multiple processors simultaneously.

It is important to note that although implicit schemes do not need to resolve all of the physical length and time scales of the plasma to be stable, they will not necessarily accurately capture the evolution of the system compared to an explicit scheme, which forces these length and time scales to be resolved. In this study we have therefore focussed on efficient parallel implementation and exclusively used explicit differencing to solve the model equations.

3.1.2 Cell Size and Time Step Constraints

Using a spatial grid to calculate the inter-particle forces gives the macroparticles an effective size [62]. Analytic analysis has been carried out to study the interaction of finite size particles, including spatial grid and finite time stepping effects [65, 66], with
a review given in [62]. Neglecting grid effects, the interactions of finite size particles can be investigated by replacing the charge in point particle interactions, \( q\delta (\vec{x} - \vec{x}) \), with \( qS (\vec{x} - \vec{x}) \), where the point particle and charge cloud centre are collocated at \( \vec{x} \). The shape factor, \( S \), represents the finite extent of the particle and differs for each interpolation scheme. As an example, consider the dispersion relation for Langmuir wave oscillations. For point particles \( \omega^2 = \omega_{pe}^2 \) and there is no wavelength dependence. For finite particles this is modified as, \( \omega^2 = S^2 (k) \omega_{pe}^2 \), where \( S (k) \) is the Fourier Transform (FT) of the particle shape factor. Here, the effect of the finite particle size is to introduce a wavelength dependence, \( \lambda = 2\pi/k \), into the dispersion relation, which for a first order interpolation scheme, gives the largest deviation from the point particle result when \( 2dx \sim \lambda \) i.e. when the wavelength is approximately equal to the particle size [62].

The effect of the spatial grid is to generate a component of the force which depends on the particle positions within a cell. This is a non-physical grid force, which is non-invariant under grid displacements [62]. Analysis of the grid force is given in [65, 67], and is again reviewed in [62]. Here it was found that the effect of the grid was to couple perturbations at wavevector \( k \) with those at \( k \) differing by \( 2\pi/\Delta x \), where \( \Delta x \) is the grid cell size, leading to instability growth.

The energy and momentum conservation properties of the PIC model are dependent on the choice of interpolation scheme used to map the particle currents to the grid and the grid EM fields to the particles [62, 63, 68]. For computational efficiency, it would be desirable to first average the staggered EM fields to common positions on the mesh, such that a single set of interpolation fractions for each particles could be used for all of the field components. Unfortunately, when the computational cell size, \( \Delta x \), is larger than the Debye length, \( \lambda_e \), of the plasma to be modelled1, such schemes are susceptible to the well-known numerical electron heating instability [62, 63]. The Debye length is given in Eqn.(3.4), where \( n_e \) is the electron number density, \( m_e \) is the electron mass, \( \epsilon_0 \) is the permittivity of free space, \( k_b \) is Boltzmann’s constant, \( e \) is the electron charge and \( T_e \) is the plasma electron temperature [69].

\[
\lambda_e = \left( \frac{\epsilon_0 k_b T_e}{n_e e^2} \right)^{1/2}
\]

(3.4)

The instability arises due to a discrepancy between the change in the electron ki-
netic, $\Delta K$ and the electric potential energy, $\Delta E$, over the simulation time step, $\Delta t$ and saturates when the numerical electron temperature in Eqn.(3.4) forces $\lambda_e \sim \Delta x$ [63,68]. Taking a typical peak convolute plasma density of $10^{16}$cm$^3$ and $\Delta x$ of 1mm, the instability will heat the electron macroparticles to $>100$keV, which is many orders of magnitude higher than expected plasma temperatures. From Eqn.(3.4), we see that the Debye length decreases with increasing number density and/or decreasing temperature. To extend the PIC model to accurately simulate the relatively high density and low temperature plasmas formed in the convolute, where the Debye length is typically less than 10$\mu$m, using practical spatial steps of 1mm, we interpolated the EM field components to the particles directly from the staggered mesh positions; this will be referred to as the energy conserving interpolation scheme and was sufficient to mitigate the numerical electron instability, even where $\Delta x >> \lambda_e$ [62,68]. As will be discussed in section 3.7.1.2, the downside of this choice was lower order interpolation in the directions parallel to each field component, as well as a larger computational overhead, as separate interpolation weights for each component of the electric field had to be calculated [18,68].

In the PIC model, stability constraints on the time step follow from resolving EM wave propagation across a computational cell and the electron plasma frequency [62]. For stability, the electromagnetic field solution must not permit an electromagnetic wave to propagate a distance of more than the smallest spatial length, $\Delta x_{min}$ in a single time step i.e. $\Delta t \leq \Delta x_{min}/c$ where $c$ is the speed of light [63]. This is known as the Courant condition and for typical spatial resolutions used in the convolute simulations enforces $\Delta t \sim 0.8$ps. Similarly for stability in the particle momentum and position update, the time step must enforce $\omega_{pe} \Delta t < 2$, where $\omega_{pe}$ is the electron plasma frequency, Eqn.(3.5) [62]. The plasma frequency increases with particle number density and so limits the plasma density that can be modelled. For the largest plasma densities of interest in the convolute, $\sim 10^{16}$cm$^{-3}$, this condition gives $\Delta t < 0.4$ps and is of the same order of magnitude as the time step enforced by the Courant condition.

$$\omega_{pe} = \left( \frac{n_e e^2}{m_e \epsilon_0} \right)^{1/2}$$  \hspace{1cm} (3.5)

The high currents achieved during the Z-accelerator discharge result in large magnetic field strengths; at peak current a magnetic field strength of 200T occurs at the
smallest feed radius of 2cm in the inner MITL. In order to accurately model guiding centre drift motions and to avoid aliasing of the electron orbits, the time step must enforce $\omega_{ce}\Delta t < 2$ i.e. at least three computational steps per cyclotron orbit. Note that the resolution of the electron cyclotron frequency $\omega_{ce}$, Eqn(3.6), is not an issue of stability, as the magnetic field does not alter the magnitude of the velocity, but one of accuracy [12, 70]. In the convolute simulations, this condition was more restrictive than both the Courant and plasma frequency and as such it was the electron cyclotron frequency that determined the simulation time step. Taking a typical peak magnetic field strength of 200T, a time step of $\Delta t < 0.06\text{ps}$ was required to enforce $\omega_{ce}\Delta t < 2$, which is approximately an order of magnitude shorter than the time step set by the Courant condition. However, this peak field only occurs at peak current, so by having a time step that dynamically decreases with increasing current, we could achieve practical simulation run times. Note that due to the larger mass of the ions, the ion cyclotron frequency $\omega_{ci}$ is always smaller than $\omega_{ce}$, such that it is the electrons macroparticles that govern the simulation time step.

$$\omega_{ce} = \frac{eB}{m_e} \quad (3.6)$$

### 3.1.3 Coulomb Collisions

In the basic PIC method, the macroparticles interact through electric and magnetic fields known at discrete positions on a numerical grid. For macroparticles with separations smaller than this grid length, the inter-particle force is modified compared to the Coulomb force law, with the force tending to zero for zero particle separation [62]. Macroparticles can pass smoothly through each other and the numerical collision cross-sections are modified. In this form, the PIC method is therefore most applicable to modelling low density and/or high temperature plasmas, where $L >> \lambda_D$ and $N_p >> 1$ and charged particle sheaths, where long range collective interactions dominate shorter range Coulomb interactions [63]. Here, $L$ is the length scale of interest and $N_p = n_e \frac{4}{3} \pi \lambda_D^3$, is the plasma parameter which is interpreted as the number of electrons within a Debye sphere and is a measure of the effectiveness of electronic charge screening of the ions. In these cases, the removal of the divergence in the Coulomb force is a desirable property.
of the PIC model \[62]\).

For higher density and/or lower temperature plasmas, Coulomb interactions within the Debye sphere have an important effect on the distribution functions of the plasma components and transport properties. In the weakly coupled limit, the Coulomb interactions can be approximated by a series of many small angle binary interactions, which dominate over the fewer large angle scattering events \[71]\; in this way, statistical averages can be taken and the interactions characterised by the electron-ion, $\tau_{ei}$, and ion-ion, $\tau_{ii}$, scattering times, Eqn.(3.7) and Eqn.(3.8), respectively \[72\]. Here, the number density, $n$, is in cm$^{-3}$ and the electron and ion temperatures, $T_e$ and $T_i$, are in eV. The Coulomb logarithm, $ln\Lambda$, was calculated as in \[73\].

$$\tau_{ei} = \frac{3.44 \times 10^5 T_e^{3/2}}{ln\Lambda Zn}$$

$$\tau_i = \frac{2.95 \times 10^7}{ln\Lambda} \left( \frac{m_i}{2m_p} \right)^{1/2} \frac{T_i^{3/2}}{Z^2 n}$$

Electron-electron and ion-ion interactions establish local thermodynamic equilibrium (Maxwellian velocity distributions) within each component of the plasma, on time scales given by $\tau_{ee} \sim \tau_{ei}$ and $\tau_{ii} \sim \tau_i$, respectively \[72\]. As the electron velocities are typically larger than the ions, $\tau_{ee} < \tau_{ii}$. Electron-ion interactions will establish thermodynamic equilibrium between the different components on a time scale of $\tau_{ei}$; as electron-ion interactions are relatively ineffective at exchanging energy, $\tau_{ei} > \tau_{ii}$. For a proton plasma, $\tau_{ee} : \tau_{ii} : \tau_{ei}^e$, $1 : \left( \frac{m_e}{m_i} \right)^{1/2} : \left( \frac{m_e}{m_i} \right)$. The momentum transfer times in electron-electron and ion-ion interactions are on the same time scale as the electron-electron and ion-ion energy exchange i.e. $\tau_{ee} \sim \tau_{ei}$ and $\tau_{ii} \sim \tau_i$. The momentum transfer from ions to electrons occurs on about the same time as the energy transfer, $\tau_{ei}^e$; ion-electron momentum transfer is small compared to ion-ion transfer and collisions with electrons have little effect on the form of the proton distribution function. In contrast, the transfer of momentum from electrons to ions occurs on the same time as the electron-electron momentum transfer, $\tau_{ee} \sim \tau_{ei}$; collisions of electrons with the ions will quickly deflect the electrons giving rise to an isotropic distribution of velocities that has important consequences for the transport \[71\].

The proton plasma formed in the convolute has a density range of $10^{13-16}$ cm$^{-3}$ at
temperatures between 1 and 10eV [16, 17]. The shortest collisional interaction times occur at high density and/or low temperature [72]. From Eqn.(3.7) and Eqn.(3.8), for a 1eV plasma in this density range, $\tau_{ei} \sim 4\text{ns} \rightarrow 7\text{ps}$ and $\tau_i \sim 250\text{ns} \rightarrow 0.4\text{ns}$ (note that $\tau_i \sim \left(\frac{m_i}{m_e}\right)^{1/2} \tau_{ei}$). At 10eV, the interaction times are longer, with $\tau_{ei} \sim 93\text{ns} \rightarrow 0.13\text{ns}$ and $\tau_i \sim 5.6\mu\text{s} \rightarrow 7.9\text{ns}$. A plasma is said to be collisionless if $\omega_{pe} \tau_{ei} \gg 1$ [62]. At 1eV, $\omega_{pe} \tau_{ei} \sim 700-16$ between plasma densities of $10^{13-16}\text{cm}^{-3}$, such that the condition is not valid for the higher density convolute plasma and Coulomb collisions within the Debye sphere are important for accurate simulation; the basic PIC model must therefore be extended.

Returning to the collisionless Vlasov kinetic equation, Eqn.(3.1), collisional interactions are included by adding an extra term to the right hand side, $(\partial f / \partial t)_{coll}$, which describes the rate of change of $f$ due to collisions [61]. For Coulomb collisions, a common form for this term is the Fokker-Plank (FP) integral, Eqn.(3.9), which is comprised of two parts to describe slowing down and diffusion in velocity space, respectively. In the weakly coupled limit the averages, $\langle \Delta \vec{v} \rangle$ and $\langle \Delta \vec{v} \Delta \vec{v} \rangle$ can be computed from the dynamics of binary Coulomb interactions [60].

$$\left( \frac{\partial f}{\partial t} \right)_{coll} = -\frac{\partial}{\partial \vec{v}} \left( f \langle \Delta \vec{v} \rangle \right) + \frac{1}{2} \frac{\partial^2}{\partial \vec{v} \partial \vec{v}} \left( f \langle \Delta \vec{v} \Delta \vec{v} \rangle \right)$$

A range of schemes to extend the PIC model consistent with the Vlasov-Fokker-Planck (VFP) equation have been developed [63, 74]. We adopted a binary collision algorithm, which randomly paired macroparticles within a computational cell and updated their velocities based on an energy dependent collision frequency. This is a MC scheme in the sense that each particle could scatter from every other particle in the cell and the scatterings represent a random sample of all the possible interactions [75, 76]. However, the scheme, which makes no assumptions about the particle distribution functions, could easily be made conservative as well as handle collisions between differently weighted particles [74].

The collision algorithm involved sorting and pairing the particles and as such represented one of the largest computational overheads in the simulations [76]. Again, considering a 1eV proton plasma, the shortest collision time is given by $\tau_{ei}$, which ranges between 4ns and 7ps for densities of between $10^{13-16}\text{cm}^{-3}$. As discussed in section 3.1.2,
the initial time step was set by the Courant limit, $\Delta t_{\text{init}} \sim 0.8\, \text{ps}$; during the convolute simulations, this step was reduced in order to resolve the electron cyclotron orbits. As such, the time step was always at least ten times shorter than $\tau_{\text{el}}$, such that the collision times were relatively well resolved. In fact, we found that the collision algorithm could be called less frequently [75] without effecting the results, as long as the time step gave at least ten steps for each collision time. In this way, the simulation run times could be reduced significantly.

3.2 Model Development

From the above considerations we can conclude that the energy conserving PIC method, including a Coulomb collision model, is applicable to modelling the plasmas and charged particle sheaths formed in the Z DPHC. For modelling charged particle sheaths in MITLs, the PIC method has been used extensively by the pulsed power community to aid the design and understanding of a wide range of pulsed power machines. As such there are a number of available PIC codes that have been developed specifically for pulsed power applications; of these both LSP [77], developed by Voss Scientific and licensed by ATK and Quicksilver [78], developed at Sandia National Laboratories (SNL), have been used to simulate the Z DPHC, as described in the previous chapter. Of these, LSP is the most sophisticated and contains a wide range of explicit and implicit field solvers and particle integrators. Quicksilver is a more standard explicit PIC code, of which the author has no practical experience.

The LSP code is controlled through a graphical user interface (GUI); as such many of the physics algorithms are operated as 'black boxes', typically with many user definable options. Although we did have a license for LSP, for this study we decided to develop our own PIC code. This was a significant undertaking, but was justified by the extra understanding gained and the ability to control and adapt the physics models; this was especially useful for the convolute simulations, where a number of the algorithms were experimental.

As will be discussed in the next chapter, fully kinetic PIC simulations of the convolute were computationally intensive. Having our own PIC code allowed us to investigate hybrid simulation techniques with the aim of reducing simulation run times and accessing
improved spatial resolutions, compared to a full kinetic PIC model of the plasma. To this end we implemented our PIC model in the 3D MHD code, Gorgon [79]. This work will be described in chapter 5. To address some of the shortcomings of the MHD approximations when applied to the convolute plasma, we also investigated an inertial two-fluid plasma model. The implementation of this model in our PIC code is described in chapter 6.

In the remainder of this chapter we will outline the elements of the PIC code and its development. Results from simulations of the Z DPHC and inner MITL using the code, to address the issue of current loss, will be presented in the next chapter.

3.3 Numerical Model

The PIC method was initially developed in the 1950s and 60s by Buneman [80] and Dawson [81]. As described above, the model represents the plasma and charged particle sheath with a number of simulation macroparticles, \(N_p\). The macroparticles carry the same charge to mass ratio as the physical particles, but have charges and masses that can be several orders of magnitude larger than their physical values [62]. Early simulations used several hundred particles, with particle-particle interactions computed by direct solution of Coulomb’s force law (an \(N^2\) operation for an \(N\) particle system). As the number of simulation particles increases, it is necessary to use a discrete grid to solve either the Poisson equation for electrostatic, or Maxwell’s equations for electromagnetic simulations [63]. Here, interactions between the particles are calculated by interpolating the macroparticle properties to the grid [62]. Extensive reviews of the standard PIC method are given in [62], [63] and [64]. Of these, [62] is the standard reference textbook.

The velocity, \(\vec{u}\), and position, \(\vec{x}\), of each macroparticle, indexed by \(i \in \{1, \ldots, N_p\}\), is evolved in time by solving the relativistic Newton-Lorentz equation of motion, Eqn.(3.10) and Eqn.(3.11), respectively. Here, \(\vec{u}\) is related to the particle 3-velocity, \(\vec{v}\), by \(\vec{u} = \gamma \vec{v}\), where \(\gamma = \left(1 + \frac{u^2}{c^2}\right)^{1/2}\) is the relativistic gamma factor. Note that in the relativistic case it is \(\vec{u}\) and not \(\vec{v}\) which is stored and updated for each macroparticle [62]. The electric and magnetic field strengths appearing in the Lorentz force in the velocity equation, Eqn.(3.10), are evolved in time by solving Maxwell’s equations, corresponding to Gauss’s law, Eqn.(3.12), Faraday’s law, Eqn.(3.13), the no magnetic monopole law, Eqn.(3.14)
and Ampere’s law including the displacement current, Eqn.(3.15). Here, \( \rho_p \) and \( \vec{j}_p \), are the total macroparticle charge and current density, which act as source terms in Gauss’s, Eqn.(3.12), and Ampere’s, Eqn.(3.15), laws respectively. The field equations are spatially differenced on a uniform grid, such that the electric and magnetic fields are known at discrete positions [63]. The macroparticle positions are continuous (to machine roundoff), where the fields used to calculate the Lorentz force in Eqn.(3.10), are interpolated from the grid to the macroparticle positions. Similarly, the source terms \( \rho_p \) and \( \vec{j}_p \) are grid quantities that are interpolated from the continuous macroparticle positions to the grid [62]. Note that in practice only Eqn.(3.13) and Eqn.(3.15) are explicitly solved to update the electric and magnetic fields; Gauss’s law is satisfied automatically by ensuring the macroparticle current and charge density interpolation satisfies the charge continuity equation, Eqn.(3.16) [68, 82] and the equations are differenced such that if Eqn.(3.14) is satisfied at \( t = 0 \) it will continue to be satisfied for all later times [63].

\[
\frac{d\vec{u}}{dt} = \frac{q_i}{m_i} \left( \vec{E} + \vec{u} \times \vec{B} \right) 
\]
(3.10)

\[
\frac{d\vec{x}_i}{dt} = \frac{\vec{u}_i}{\gamma} 
\]
(3.11)

\[
\vec{\nabla} \vec{E} = \frac{\rho_p}{\epsilon_0} 
\]
(3.12)

\[
\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} 
\]
(3.13)

\[
\vec{\nabla} \vec{B} = 0 
\]
(3.14)

\[
\vec{\nabla} \times \vec{E} = \mu_0 \vec{j}_p + \frac{1}{c^2} \frac{\partial \vec{E}}{\partial t} 
\]
(3.15)

\[
\frac{\partial \rho_p}{\partial t} + \vec{\nabla} \cdot \vec{j}_p = 0 
\]
(3.16)

Temporally, the system is evolved as an initial value problem. From a starting electromagnetic field and macroparticle distribution (typically vacuum in pulsed power simulations), the fields and particles are advanced forward in time by a small amount.
The simulation cycle to advance the solution forward by a single time step from a time $t^n$ to $t^{n+1} = t^n + \Delta t$, is shown schematically in Figure 3.1. Starting in the top box, the Lorentz force at the current time $F^n_p$ is used to update the macroparticle positions, $\vec{x}^n \rightarrow \vec{x}^{n+1}$ and velocities, $\vec{u}^{n-1/2} \rightarrow \vec{u}^{n+1/2}$. Note that the position and velocity are leap-frogged in time for second order accuracy. The macroparticle currents, $j^{n+1/2}$, are then calculated from the change in the particle positions and interpolated to the grid. Note that as the positions are known at times $n$ and $n+1$, the currents are defined at the midpoint $n+1/2$. At this stage, particles which have left the simulation domain or impacted an electrode are removed from the simulation. The macroparticle current, along with boundary sources to model EM waves injected by the circuit, are used to update the electric, $\vec{E}^n \rightarrow \vec{E}^{n+1}$ and magnetic, $\vec{B}^{n-1/2} \rightarrow \vec{B}^{n+1/2}$, fields. Again, note that the electric and magnetic fields are leap-frogged in time for second order accuracy. Coulomb collisions are included at this point which update the particle velocities. Finally, new particles are created and the grid electric and magnetic fields are interpolated to all active macroparticles; these are used to calculate the Lorentz forces ready for the next particle push. The cycle in Figure 3.1 is repeated many times, $N_t$, until the final simulation time is reached, $t_{\text{final}} = N_t \Delta t$ [62, 63].

The natural choice of coordinate system for the 3D convolute simulations was cylindrical $(r, \theta, z)$. The model could also be run in 2D cylindrical $(r,z)$ coordinates by assuming symmetry along the $\theta$-direction. In the remainder of this chapter the solution of the model equations in 3D cylindrical coordinates will be described.

To take advantage of modules and dynamic memory allocation for particle variables, our code was written in Fortran 95; the latter feature provided a significant reduction in run times compared to using arrays with fixed dimensions. We stored the particle variables in a series of 1D arrays in place of a linked list data structure, as we found the former was faster to run and could take advantage of vectorisation on modern CPU architectures.

### 3.4 Electromagnetic Field Solution

The electric and magnetic fields were updated using a central explicit difference of the Maxwell equations, Eqn.(3.13) and Eqn.(3.15). To ensure second order accuracy in the
Figure 3.1: A flow diagram of the steps taken during a time step of the PIC model.

Figure 3.2: The Yee mesh showing the staggered positions of the electric and magnetic field components.

evolution of the cross-product terms, the spatial gradients were calculated on a staggered Yee-mesh, Figure 3.2, where $i$, $j$ and $k$ are the spatial cell indices along the $r$-, $\theta$- and $z$-axes. The electric field, $\vec{E}$, and particle current density, $\vec{j}_p$, are defined on the cell edges whilst the magnetic field, $\vec{B}$, is defined on the cell faces [83].

The resulting difference equations for the electric field components are given in
Eqn.(3.17-3.19). Here, $\Delta t$ is the time step, $n$ is the time index and $\Delta r$, $\Delta \theta$ and $\Delta z$ are the spatial steps along the $r$-, $\theta$- and $z$-directions respectively [62]. Note that we included an Ohm’s law term in the current density, $\vec{j}_{Ohm} = \sigma \vec{E}$, where $\sigma$ is the electrical conductivity. This was used to model media with finite conductivity and was included implicitly for guaranteed stability [12].

$$E_{r,i+1/2,j,k}^{n+1} (1 + \mu_0 c^2 \Delta t \sigma_{i+1/2,j,k}) = E_{r,i+1/2,j,k}^n + c^2 \Delta t \left( \frac{B_{\theta,i+1/2,j,k+1/2}^{n+1} - B_{\theta,i,j,k-1/2}^{n+1/2}}{\Delta z} - \frac{B_{z,i,j+1/2,k}^{n+1/2} - B_{z,i,j,k-1/2}^{n+1/2}}{r_{i+1/2} \Delta \theta} - \mu_0 \vec{j}_{p,r,i+1/2,j,k}^{n+1/2} \right)$$

(3.17)

$$E_{\theta,i,j+1/2,k}^{n+1} (1 + \mu_0 c^2 \Delta t \sigma_{i+1/2,j,k}) = E_{\theta,i,j+1/2,k}^n + c^2 \Delta t \left( \frac{B_{z,i+1/2,j,k}^{n+1/2} - B_{z,i,j,k-1/2}^{n+1/2}}{\Delta r} - \frac{B_{r,i,j,k+1/2}^{n+1} - B_{r,i,j,k-1/2}^{n+1}}{\Delta z} - \mu_0 \vec{j}_{p,\theta,i,j+1/2,k}^{n+1/2} \right)$$

(3.18)

$$E_{z,i,j,k+1/2}^{n+1} (1 + \mu_0 c^2 \Delta t \sigma_{i,j,k+1/2}) = E_{z,i,j,k+1/2}^n + c^2 \Delta t \left( \frac{B_{r,i,j,k+1/2}^{n+1} - B_{r,i,j,k-1/2}^{n+1}}{r_i \Delta \theta} \right) - c^2 \Delta t \left( \frac{r_{i+1/2} B_{\theta,i+1/2,j,k}^{n+1/2} - r_{i-1/2} B_{\theta,i-1/2,j,k}^{n+1/2}}{r_i \Delta r} + \mu_0 \vec{j}_{p,z,i,j,k+1/2}^{n+1/2} \right)$$

(3.19)

The difference equations for the magnetic field are given in Eqn.(3.20-3.22). Second order accuracy in the time step was ensured by leap-frogging the electric and magnetic fields in time; the magnetic field led the electric field by half a time step. To calculate the Lorentz force in the particle push step, the magnetic field was therefore averaged to the full time step as $\vec{B}^{n+1} = \left( \vec{B}^{n+1/2} + \vec{B}^{n+3/2} \right) / 2$ [62].

$$E_{r,i,j+1/2,k+1/2}^{n+3/2} = \frac{E_{r,i,j+1/2,k+1/2}^{n+1} - E_{r,i,j+1/2,k}^{n+1}}{\Delta z} - \Delta t \left( \frac{E_{\theta,i,j+1/2,k+1/2}^{n+1} - E_{\theta,i,j+1/2,k}^{n+1}}{\Delta \theta} \right)$$

(3.20)

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\[ B_{\theta,i+1/2,j,k+1/2}^{n+3/2} = B_{\theta,i+1/2,j,k+1/2}^{n+1/2} \]
\[ - \Delta t \left( \frac{E_{z,i+1/2,j,k+1/2}^{n+1} - E_{z,i,j,k+1/2}^{n+1}}{\Delta r} - \frac{E_{r,\theta,i+1/2,j,k+1/2}^{n+1} - E_{r,\theta,i,j,k+1/2}^{n+1}}{\Delta z} \right) \] (3.21)

\[ B_{z,i+1/2,j+1/2,k}^{n+3/2} = B_{z,i+1/2,j+1/2,k}^{n+1/2} \]
\[ - \Delta t \left( \frac{E_{r,i+1/2,j+1/2,k}^{n+1} - E_{r,i,j+1/2,k}^{n+1}}{r_{i+1/2} \Delta \theta} - \frac{r_{i+1} E_{r,\theta,i+1/2,j+1/2,k}^{n+1} - r_i E_{r,\theta,i,j+1/2,k}^{n+1}}{r_{i+1/2} \Delta r} \right) \] (3.22)

The stability of the central differencing scheme can be analysed using a 1D wave equation, Eqn.(3.23) [63].

\[ \frac{\partial^2 \psi}{\partial t^2} = c^2 \frac{\partial^2 \psi}{\partial x^2} \] (3.23)

Centrally differencing Eqn.(3.23) yields Eqn.(3.24), where \( \Delta x \) is the cell size in the 1D system [63].

\[ \psi_j^{n+1} = \left( \frac{c \Delta t}{\Delta x} \right)^2 \left( \psi_{j+1} - 2 \psi_j + \psi_{j-1} \right) + 2 \psi_j^n - \psi_j^{n-1} \] (3.24)

Assuming sinusoidal solutions, \( \psi(x,t) = \exp(i(\omega t - kx)) \), where \( \psi_j^n = \exp \left( i \left( \omega t - \tilde{k} \Delta x \right) \right) \) and \( \tilde{k} \) is the numerical wavevector. Substitution into Eqn.(3.24) gives Eqn.(3.25) [63].

\[ \cos(\omega dt) = \left( \frac{cdt}{dx} \right)^2 \left[ \cos \left( \tilde{k} \Delta x \right) - 1 \right] + 1 \] (3.25)

For stability, \( c \Delta t/\Delta x \leq 1 \) or \( \Delta x \geq c \Delta t \), i.e. the wave cannot propagate across more than a single grid cell during a time step. In 3D, the stability condition, known as the Courant-Levy criterion, is given by Eqn.(3.26) [62]. In cylindrical coordinates, \( i \in \{1,2,3\} \) with \( \Delta x_i \in \{ \Delta r, r_{\min} \Delta \theta, \Delta z \} \), where \( r_{\min} \) is the smallest radial distance in the system. In the convolute simulations, an EM wave could propagate to the axis; in order to avoid impractically small time steps, \( r_{\min} \) was typically set to 1.9cm (the inner MITL cathode was at a radius of 2cm). As such, below this radius the EM field solution was transitioned to 2D cylindrical \( r-z \) coordinates, by assuming uniformity along the \( \theta \)-direction.

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The Maxwell equations, Eqn.(3.13) and Eqn.(3.15), are hyperbolic differential equations. The most accurate numerical solution using the differencing scheme described above is achieved with \( \Delta t = \Delta t_{\text{Courant}} \), assuming that the grid cell size resolves all of the EM wavelengths of interest. For example, consider a plane wave propagating in a 1D simulation. Here, \( \Delta t_{\text{Courant}} = \Delta x/c \), the transit time of the wave across a cell. For \( \Delta t < \Delta t_{\text{Courant}} \), numerically a grid node can have a finite electric and magnetic field at a time before the physical wave could reach the nodes position, reducing the simulation accuracy. For 2 and 3D simulations, \( \Delta t_{\text{Courant}} \) is always less than the transit time of an EM wave (travelling at a speed \( c \)), along one axis of the cell. Therefore, the most accurate solution is achieved with \( \Delta t = \Delta t_{\text{Courant}} \), i.e. the time step closest to the physical propagation time across a cell [84]. In practice, we typically set \( \Delta t = 0.5 - 0.9 \Delta t_{\text{Courant}} \) to reduce noise in the electric field solution when macroparticles were included.

### 3.4.1 Low Pass Spatial Filtering of the Electric Field

An issue identified in the convolute simulations was the formation of high frequency noise in the electric field; this is a common issue in PIC simulations including relativistic electrons. Unchecked, the amplitude of the noise was seen to grow during the simulation, eventually disrupting the electron sheath. This particle induced noise is introduced through the current term in Maxwell’s equations and is generated at the shortest possible wavelengths i.e. on the scale of the particle and cell size [85]. This issue can be mitigated by improving the particle statistics i.e. increasing the number of macroparticles or filtering the fields. In practice, the latter option is more efficient as the noise scales as \( \propto 1/\sqrt{N_{\text{particles}}} \), where \( N_{\text{particles}} \) is the number of macroparticles [86].

To remove the highest frequency modes, we implemented a low pass spatial filter, \( P(\lambda) \), which was applied to the electric field as in Eqn.(3.27), after each field update step. Here, \( \lambda \) is a difference operator, given in Eqn.(3.28), normalised to have a maximum Eigen value of unity at the grid wavelength i.e. the maximum wavevector \( k_{\text{max}} = 2\pi/\Delta x_{\text{min}} \), where \( \Delta x_{\text{min}} \) was the smallest grid spatial length (equal to \( r_{\text{min}}\Delta \theta \) in 3D) [85]. The factor, \( \alpha \), is a constant scaling parameter, that was typically set to 0.5 [86].
Figure 3.3: A plot of the low pass spatial filter function.

\[ P(\lambda) \vec{E} = (1 - \lambda)^2 (1 + 2\lambda) \vec{E} \]  \hspace{1cm} (3.27)

\[ \lambda \vec{E} = -\frac{\alpha (\Delta x_{\text{min}})^2}{4\pi^2} \vec{\nabla} \times \vec{\nabla} \times \vec{E} \]  \hspace{1cm} (3.28)

As an example, consider a plane EM wave propagating along the positive z-axis. With \( \alpha = 1 \), application of Eqn.(3.28) to the electric field, \( E_x = E \exp(ik_z z) \), gives

\[ \lambda E_x = \frac{k^2}{k_{\text{max}}^2} E_x \], as desired. The filter function \( P \), Eqn.(3.27), is plotted as a function of \( \beta^2 = k^2/k_{\text{max}}^2 \) in Figure 3.3, where we see the filter acts most strongly on the shortest wavelength modes \[85]\.

The filter removes energy from the highest frequency spatial modes which was permanently lost from the simulation. The total energy was tracked during the convolute simulations; as will be discussed in section 4.13 of the next chapter, the convolute simulations showed excellent energy conservation, such that the filtering did not appear to have a significant impact on this aspect of the model.

### 3.4.2 Electrode Boundary Conditions

A key aspect of the convolute simulations was the electrode boundary conditions. Figure 3.4 shows a slice of the Yee-mesh, Figure 3.2, in the r-z plane. The electrode, shown as the shaded region, was assumed to fill the entire cell. As such, the true electrode geometry was approximated by a series of 'stair-steps' \[87]\; the stair-stepping can be seen clearly in Figure 4.1 of chapter 4, which shows the simulated convolute electrode.
Figure 3.4: A slice of the Yee-mesh, Figure 3.2, in the r-z plane to demonstrate the electrode boundary conditions.

geometry.

In the convolute simulations, the majority of the electrode cells were treated as perfect conductors; here it was assumed that a current flowed instantaneously on the surface of the cell to neutralise any component of the electric field parallel to the conductor surface [87]. In practice, after the electric field was updated to the new time step, we cycled over the grid and tested for electrode cells; the parallel electric field components on the cell edges and perpendicular magnetic field components on the cell faces of the cell were then set to zero.

Additionally, electrode cells could be modelled as regions of finite conductivity [12]. The conductivities were defined at the cell centres, where the electrode was again assumed to fill the entire cell. The bound current term, $\vec{j}_{\text{bound}} = \sigma \vec{E}$, included in the finite differenced form of Ampere’s law, Eqn.(3.17-3.19), were defined on the cell edges. As such, the cell centred conductivities were spatially averaged to the cell edges, were only cells with non-zero conductivity were included in the average.

For the spatial resolutions used in the convolute simulations, the cell size was typically much larger than the skin depth of the current in the electrode. As such, the perfectly conducting electrode boundary condition was used in preference to the finite conductivity model. This treatment had the added benefit of simplifying the SCL emission particle creation algorithms, as will be discussed in section 3.9 [87].

Both the Quicksilver and LSP codes include models that improve on the stair-stepped
electrode approximation. The Quicksilver model allows a computational cell to be split along the diagonal, such that sloped electrode surfaces can be treated exactly [87]. LSP includes a sub-grid model for electrode cells of arbitrary shape. Here, the fraction of the cell volume filled by the electrode is calculated and used to correct the field solution. Due to the extra complication of implementing the interpolation and particle creation algorithms, as well as the more restrictive constraint on the Courant time step in the sub-grid electrode cells, we did not implement either of these models in our code. As such, we encountered a number of issues relating to the electrode stair-steps when running and initialising the convolute simulations. Firstly, we observed electric field enhancements at the electrode cell corners; in the SCL emission cells this lead to early breakdown and enhanced charge creation. The impact of this on the convolute simulation results will be considered in chapter 4. Additionally, extra care had to be taken to ensure that the stair-stepping gave a good approximation to the true vacuum impedance of the transmission line, which is a function of the a-k gap spacing.

3.4.3 Simulation Domain Boundary Conditions

To close the difference equations for the electric field, Eqn.(3.17-3.19), at open (i.e. not electrode) simulation domain boundaries, the magnetic field was defined in a single layer of ‘ghost cells’ and set by additional boundary conditions [62]. In the simulations of the convolute presented in the next chapter, we modelled a $1/24^{th}$ of the full $2\pi$ extent along the $\theta$-direction; at the domain boundaries along the $\theta$-direction, the symmetry of the convolute was modelled with reflective boundary conditions. Here, $B_\theta$ in the ghost cell was set equal to the value in the adjacent (in the $\theta$-direction) computational cells, whilst $B_r$ and $B_z$, were set equal to the negative of the values.

As discussed in section 3.4, to avoid the simulation time step becoming too small, the field solution below a minimum radius was transitioned to 2D cylindrical r-z coordinates, where symmetry along the $\theta$-axis was assumed. This had the added benefit of avoiding the issue of the arc-length going to zero at $r = 0$, negating the requirement for an additional boundary condition on the axis.

In the convolute simulations, open boundaries were present where the inner MITL connected to the load and the radial lines connected to the four level radial disk feed.
As will be described in the next section, both the load and radial lines were modelled as external circuits; as such the magnetic field in these ghost cells was set in the relevant circuit model.

### 3.5 Circuit Models

#### 3.5.1 Transmission Line Model

As described in chapter 1, the Z vacuum radial lines begin at the insulator stack at a radius of 1.6m. In order to remain close to uniform vacuum impedance, the a-k gap in these lines was reduced proportionally to the radius such that the electric field strength increases with reducing radius. The threshold for cathode plasma formation and subsequent SCL electron emission is $240 \text{kV cm}^{-1}$, this is expected to be exceeded for $r<1.3 \text{m}$ [13,31]. It was not practical to model both the convolute and radial lines out to this radius with the PIC model. Instead, a radial extent of 14.4cm, which included the inner MITL, DPHC and a small part of the radial lines, was included in the PIC domain; the remaining part of the vacuum radial lines were modelled with a transmission line circuit model. The water convolute bi-plate lines, intermediate stores and Marx banks, comprising the rest of the pulse forming circuit, were modelled as an equivalent voltage source used to drive the transmission line model [2,14,16].

The transmission lines comprising the circuit model were assumed to be 1D and lossless. The voltage and current waves in the lines were therefore described by the telegrapher equations, Eqn.(2.1) and Eqn.(2.2), derived from a simplified equivalent circuit model, as described in section 2.1 of chapter 2. Circuit codes such as Screamer [88] solve these equations directly to evolve the voltage and current wave through the transmission line circuit. Such a model was coupled to the Gorgon EM field solver by Jennings [2]; here, the telegrapher equations were solved implicitly for guaranteed stability. We implemented an alternate solution scheme in our model, similar to the Bertha [20] and TL [52] codes, which evolves the voltage waves in the lines with a set of algebraic, as opposed to differential, equations.

As discussed in section 2.1, the general solution to the 1D wave equation for the voltage in a lossless transmission line, Eqn.(2.4), is a sum of left to right (forward),
$V_1$, and right to left (backward), $V_2$, travelling waves. The circuit comprises a number of transmission line elements, each characterised by a vacuum impedance, $Z_0$, and a temporal length, $\tau$ [19], connected through a series of junctions. Consistent with the general solution, each line had two 1D arrays which stored values for the forward and backward travelling components of the voltage wave along the line. The circuit model was evolved with the EM field solver time step, $\Delta t$. As such, each element was split into $N_{\text{segments}} = \tau/\Delta t$, segments; the arrays storing the voltages along each element, $V_1$ and $V_2$, therefore had lengths of $N_{\text{segments}}$. In practice, the arrays were initialised with the maximum number of segments in the system and $N_{\text{segments}}$ was stored as an integer reference for each element [20].

To model the propagation of the voltage wave along the lines, at each time step the forward travelling components were shifted one segment to the right and the backward travelling components one segment to the left. The ends of the transmission lines were connected through junctions; here the reflection, Eqn.(2.5) and transmission, Eqn.(2.6), coefficients, defined in section 2.1 of the previous chapter, were applied to the component of the voltage leaving each end of the element, in order to set the voltages entering the elements connected through the junctions. Here, $Z_1$ and $Z_0$ are the impedances of the elements connected by the junction. Note that for $Z_0 = Z_1$, $R = 0$ and $T = 1$ and the junctions is perfectly transmissive. The model included junctions of up to three transmission line elements connected in either series or parallel, including resistive elements.

The effective voltage source used to model the machine from the insulator stack to the Marx banks, was included as an additional junction type. Here, the junction was connected to one end of the element and set the voltage entering the element; for the convolute simulations, the voltage was linearly interpolated from a file read list of times and voltages.

To model both the EM wave entering the PIC domain from the radial lines and the reflected component from the convolute to the radial lines, the circuit model was connected to the EM field solver at the edge of the simulation grid through a transmission boundary condition. The incoming (from the circuit to the simulation domain) and outgoing (from the simulation domain to the circuit) components of the voltage were calculated self consistently. Assuming the PIC grid was connected to the left hand side
of the circuit element, the incoming component, $V_{in}$, was simply equal to the value of $V_2$ leaving the element. The outgoing component, $V_{out}$, was calculated as follows; the total voltage, $V$ at the simulation domain boundary was first calculated from a numerical integration of the $z$-component of the electric field on the cell edges, $V = \int_{z_c}^{z_a} E_z dz$, averaged along the $\theta$-direction. Here, $z_c$ and $z_a$ were the axial positions of the cathode and electrode respectively. The outgoing voltage was then calculated as $V_{out} = V - V_{in}$; note that this computation was complicated by the fact that in order to enforce the Courant condition, $\Delta t c \neq \Delta r$, where $\Delta r$ is the spatial step along the radial direction. As such, the incoming component of the voltage, $V_{in}$ and the total voltage, $V$, were known at different times. To overcome this timing mismatch, the incoming voltage, which was known at later times as $\Delta t < \Delta r/c$, was stored. The value at the field solve time was then calculated via a linear interpolation of the stored values. A sum of the outgoing and incoming voltages was then used to set the electric field on the edge of the ghost-cell. The magnetic field in the ghost-cell at the new time (required to close the field equations) was then updated using the standard explicit solution of the induction equation, as described in section 3.4.

An example of the transmission boundary in action is shown in Figure 3.5. Here, a single element transmission line circuit was connected to a shorted section of parallel plate radial transmission line, modelled in 2D cylindrical r-z geometry. A short (less than the transit time of the lines) single period sine wave voltage pulse was applied to the start of the circuit model. Figure 3.5 shows a plot of the voltage measured at the circuit-PIC interface. Here, we see the voltage pulse passes from the circuit to the PIC domain, is reflected from the short in the radial line and travels back into the circuit transmission line. Numerical noise, due to the interpolation step described above, can be seen in the reflected component at $\sim$1.7ns; the amplitude of this noise was small compared to the peak voltage. In fact, the test voltage rise time was much faster than the convolute simulations, so was a good stress test of the interface.

### 3.5.2 Load model

The wire array Z-pinch load was modelled using the well-known 0D model [55]; here, the load is treated as a conducting cylinder of initial radius, $r_0$, length, $l$ and total mass,
Figure 3.5: Voltage trace at the circuit model-PIC interface for a single sine wave voltage pulse.

$m$, which is equal to the sum of the mass in each wire comprising the load.

The current delivered to the load by the accelerator, $I_{\text{load}}$, applies a magnetic pressure directed radially inward which drives the load to implode. The load is initialised at rest, $v_{\text{load}} = 0$; the current is related to the magnetic field on the surface of the load by $B_\theta = \mu_0 I_{\text{load}}/2\pi r(t)$, with the corresponding force, $F = -\mu_0 I_{\text{load}}^2/4\pi r(t)$, which was directed radially inwards, used to update the load velocity according to Eqn.(3.29) [55]. The velocity at the new time was then used to update the radius of the load, $r_{\text{load}}$, according to Eqn.(3.30) [16].

\begin{align*}
    v_{\text{load}}^{n+1} &= v_{\text{load}}^n + \Delta t \frac{F}{m} \quad (3.29) \\
    r_{\text{load}}^{n+1} &= r_{\text{load}}^n + \Delta t v_{\text{load}}^{n+1} \quad (3.30)
\end{align*}

As the load implodes, its inductance increases, generating a back electromotive force (emf) into the inner MITL and convolute. The radial position of the load and electrical response were evolved self-consistently using the following method [16,55].

The load voltage is given in Eqn.(3.31), with contributions from the changing load current and inductance.

\begin{equation}
    V_{\text{load}} = \frac{d}{dt}(L_{\text{load}}I_{\text{load}}) = L_{\text{load}}\frac{dI_{\text{load}}}{dt} + \frac{dL_{\text{load}}}{dt} I_{\text{load}} \quad (3.31)
\end{equation}
Treating the load at an instantaneous radius of \( r(t) \) and the anode at a fixed radius of \( r_{\text{return}} \), as a coaxially transmission line, the inductance of the load at this time, \( L_{\text{load}}(t) \), was calculated from Eqn.(3.32) [19].

\[
L_{\text{load}}(t) = \frac{l\mu_0}{2\pi} \ln \left( \frac{r_{\text{return}}}{r(t)} \right) \quad (3.32)
\]

The load current at the new time, \( I_{\text{load}}^{n+1} \), was calculated from a forward explicit difference of Eqn.(3.31) as in Eqn.(3.33). Here, the load voltage at the current time, \( V_{\text{load}}^n \), was calculated from an integral of the electric field at the domain boundary along the radial axis, averaged along the \( \theta \)-direction. Note, that we solved for \( I_{\text{load}} \) instead of \( V_{\text{load}} \) for stability purposes; the latter involved dividing the current by the time step, which was typically many orders of magnitude smaller than the current.

\[
I_{\text{load}}^{n+1} = I_{\text{load}}^n + \Delta t \left( \frac{I_{\text{load}}^{n+1}}{I_{\text{load}}^n} V_{\text{load}}^n - I_{\text{load}}^n \left( \frac{I_{\text{load}}^{n+1} - I_{\text{load}}^n}{I_{\text{load}}^{n+1}} \right) \right) \quad (3.33)
\]

The new load current was then used to set the \( \theta \)-component of the magnetic field in the ghost cell of the simulation grid, \( B_\theta = \mu_0 I_{\text{load}}^n / 2\pi r \), where \( r \) is the radial coordinate along the boundary.

### 3.6 Particle Push

The macroparticle velocities, \( \vec{u} \), and positions, \( \vec{x} \), are evolved in time via a central explicit difference of the relativistic Newton-Lorentz equation of motion, Eqn.(3.34) and Eqn.(3.35) [62].

\[
\frac{\vec{u}^{n+1/2} - \vec{u}^{n-1/2}}{\Delta t} = \frac{q}{m} \left( \vec{E}^n + \frac{(\vec{u}^{n-1/2} + \vec{u}^{n+1/2})}{2\gamma^n} \times \vec{B}^n \right) \quad (3.34)
\]

\[
\frac{\vec{x}^{n+1} - \vec{x}^n}{\Delta t} = \frac{\vec{u}^{n+1/2}}{\gamma^{n+1/2}} \quad (3.35)
\]

Here, \( q \) and \( m \) are the macroparticle charge and mass, \( n \), is the time index and \( \Delta t \), is the time step. To ensure second order accuracy in the time step, the macroparticle positions and velocities were leap frogged in time, with their values known half a time step apart [62]. Note that it is the charge to mass ratio, \( q/m \), that appears in the
equation of motion. Although each macroparticle represents many real particles, the macroparticle charge to mass ratio is the same as the real particle, such that it behaves identically to a single real particle.

An efficient implementation of Eqn.(3.34) is due to Boris [62]. In this scheme, the actions of the electric and magnetic fields are separated as in Eqn.(3.36-3.40).

\[
\vec{u}^- = \vec{u}^{n-1/2} + \frac{q\Delta t \vec{E}^n}{2m} \tag{3.36}
\]

\[
\vec{u}' = \vec{u}^- + \vec{u}^- \times \vec{t}^n \tag{3.37}
\]

\[
\vec{u}^+ = \vec{u}^- + \vec{u}' \times \frac{2\vec{t}^n}{1 + t^2} \tag{3.38}
\]

\[
\vec{u}^{n+1/2} = \vec{u}^+ + \frac{q\Delta t \vec{E}^n}{2m} \tag{3.39}
\]

\[
\vec{t}^n = \hat{B} \tan \left( \frac{q\Delta t B^n}{2\gamma^n m} \right) \tag{3.40}
\]

Here, \(|\vec{u}^-| = |\vec{u}^+|\), such that the only effect of the magnetic field is to rotate the velocity vector. This property allows the particle kinetic energy to be calculated simply at the full time step, \(n\), as

\[
E_{\text{kinetic}} = m \left( u_{\cdot}^{+} \right)^2 / \left( \gamma \left( u_{\cdot}^{+} \right) + 1 \right) \tag{62}
\]

The particle position is updated using the velocity at the new time, \(\vec{u}^{n+1/2}\); in 2D cylindrical \(r-z\) and 3D Cartesian this simply involves evaluating each component of Eqn.(3.35). In 3D cylindrical coordinates the scheme must be modified to account for the fact that the first two components of \(\vec{u}_r\), are directed along the radial and \(\theta\)-directions. Moving to a coordinate system where \(r^n\) lies along the \(x\)-axis the radial and \(\theta\)-directed components of the velocity are operated, Eqn.(3.41) and Eqn.(3.42), to form the dummy variables \(x'\) and \(y'\). The new radial coordinate is then \(x_r^{n+1} = \left( x'^2 + y'^2 \right)^{1/2}\) and the change in the angular coordinate, \(\alpha = \arctan \left( y' / x' \right)\), such that the new angular coordinate is given by \(x_\theta^{n+1} = x_\theta^n + \alpha\). The new z-coordinate is simply \(x_z^{n+1} = x_z^n + \Delta t u_z^{n+1/2} / \gamma^{n+1/2}\) [62].

\[
x' = x_r^n + \Delta t u_r^{n+1/2} / \gamma^{n+1/2} \tag{3.41}
\]
\[ y' = \Delta t \frac{\gamma^{n+1/2}}{\gamma^{n+1/2}} \] (3.42)

The velocity is then rotated to the new particle position through the angle \( \alpha \) according to \( \vec{u}_{n+1/2} \rightarrow (u_r\cos \alpha + u_\theta \sin \alpha, -u_r \sin \alpha + u_\theta \cos \alpha, u_z) \) [62]. This step is important to ensure that the velocity vector is consistent with the new position; if this step is skipped, an effective particle drift motion will be introduced.

The stability of this explicit scheme can be investigated in 1D, \( x \), by analysis of a particle undergoing simple harmonic motion (SHM) as in Eqn.(3.43-3.44), at an angular frequency of \( \omega_0 \) [63].

\[
\frac{d^2x}{dt^2} = -\omega_0^2 x
\] (3.43)

\[
\frac{x^{n+1/2} + x^{n-1/2} + 2x^n}{dt^2} = -\omega_0^2 x^n
\] (3.44)

Assuming solutions of the form \( x^n = A \exp(-i \omega t) \), the scheme is stable for \( \omega_0 \Delta t < 2 \) [62]. For plasma systems, this stability condition is linked to the electron plasma frequency, \( \omega_{pe} \Delta t < 2 \), limiting the maximum plasma density that can be modelled with a given time step [63].

The resolution of the electron cyclotron frequency, Eqn.(3.6), where \( B \) is the magnitude of the magnetic field at the macroparticle position, is an issue of accuracy and not stability [12, 70]. In the Boris scheme, \( |\vec{u}^-| = |\vec{u}^+| \), such that the magnetic field cannot drive an instability to heat the particles [63]. In a single time step, the particle angle is rotated by \( \theta = 2 \tan^{-1} \left( \frac{\omega_e \Delta t}{2} \right) \), giving the exact rotation for \( \omega_e \Delta t << 1 \). For \( \omega_e \Delta t >> 1 \), \( \theta \approx \pi - 4 \omega_e \Delta t \) and the particle reverses direction in each time step, giving a 'zig zag' trajectory [12]. For the convolute simulations, we require good resolution of the electron cyclotron motion to accurately reproduce the \( \vec{E} \times \vec{B} \) and other drift motions. Practical experience has shown that \( \omega_e dt = 1.9 \), which enforces at least three steps per cyclotron orbit, gave a good balance between orbit accuracy and run time efficiency.

### 3.6.1 Particle Tracking

After the positions were updated, the particles were tested to see if they had impacted an electrode or left an open simulation boundary. The old, \( \vec{x}^n \) and new,
\( \vec{x}^{n+1} \), particle positions were first transformed to Cartesian coordinates according to 
\( \vec{x}^{n/n+1} \rightarrow (x_n \cos \theta, x_n \sin \theta, x_z)^{n/n+1} \). Assuming a straight line trajectory (as is done in the current interpolation step, section 3.7.1), the line between the old and new positions was parameterised as 
\( \vec{x}^{n+1} = \vec{x}^n + t (\vec{x}^{n+1} - \vec{x}^n) \) [89]. The values of \( t \) at each cell crossing (if they existed) were then computed by equating the parameterised line with the appropriate expressions for the cell boundaries. The split path was then ordered by comparing the distance from \( \vec{x}^m \) to each crossing point. Note that care had to be taken due to the fact that the cell boundaries normal to the radial axis were curved in 3D cylindrical geometry; it was therefore possible for the particle to cross this boundary twice in a single time step.

Electrode impacts were identified by testing whether any of the segments were inside an electrode cell. Due to the electrode stair-stepping, it was possible for a particle to pass through an electrode during the time step, but still be in vacuum at the new time. It was decided that these cases would be treated like any other electrode impact, the particle position would be truncated to the location of the first electrode impact and after its current had been interpolated to the grid, the particle would be deleted from the active list.

At open simulation boundaries, the particle trajectory was truncated to the position the particle left the simulation domain, its current interpolated to the grid and the particle deleted from the active list. At the \( \theta \)-boundaries, reflective boundary conditions were applied. Here, the particle path was truncated at the position it crossed the boundary and the remainder of the path reflected back into the simulation domain; specifically, the \( \theta \)-component of the new position was updated as 
\( x_\theta^{n+1} \rightarrow \theta_{\text{boundary}} - (x_\theta^{n+1} - \theta_{\text{boundary}}) \). Additionally, the sign of the \( \theta \)-component of the velocity was reversed, \( u_\theta \rightarrow -u_\theta \).

Note that the path splitting information was stored for use in the current interpolation step, as will be described in section 3.7.1.

### 3.6.2 Particle Push Sub-cycling

The magnetic field strength is inversely proportional to the radial coordinate. To enforce the condition \( \omega_{ce} \Delta t < 2 \) for all the macroparticles, the largest magnetic field strength, corresponding to the minimum macroparticle radius must be used. It was inefficient
to push all the macroparticles with this time step as for example at peak current, the
magnetic field strength ranged from 14T at the feed input, to 200T at the load. Ad-
ditionally, as the current and therefore magnetic field strength increased, the cyclotron
time step reduced below the Courant and plasma frequency time scales; at peak cur-
rent $\Delta t_{\omega c} \sim (1/10) \Delta t_{\text{Courant}}$. It was therefore desirable to sub-cycle the particle push
within the field solution step. A stable method, developed by Pointon et al in [12], has
been incorporated into the Quicksilver [78] PIC code, for use in Z convolute charged
particle sheath simulations. Here, the particles were separated into $N_{\text{sub}}$ sub-cycling
groups, indexed with $s_n \in \{1, 2, \ldots, N_{\text{sub}}\}$, based on the EM field time step, $\Delta t_{\text{Courant}}$, 
Eqn.(3.45) [12].

$$\frac{qB(\vec{x}_n)}{m} \left( \frac{\Delta t_{\text{Courant}}}{s_n} \right) < \theta_{\text{max}}$$  

(3.45)

Here, $\theta_{\text{max}}$ was the maximum allowed rotation angle, which for $\omega_{ce}\Delta t = 2$ is $\frac{2}{3}\pi$.
The macroparticles in each subgroup were then pushed $s_n$ times using a time step of
$\Delta t_s = \Delta t_{\text{Courant}}/s_n$. At the end of each PIC cycle, particles were transferred between
sub-cycling groups and their velocity vectors corrected using a time step of $\Delta t_{\text{correction}} =$
$\Delta t_{s, old}/2 - \Delta t_{s, new}/2$, to maintain half a time step between the macroparticle position
and velocity. The efficiency of this scheme followed from the fact that the macroparticle
current interpolation step, which represents one of the largest computational overheads
in the PIC model, was still only carried out once per cycle at the field solution time [12].

A potential issue with the method, highlighted in [12], was the loss of second order
accuracy for $s_n > 1$, as the magnetic field at time step $n$ was used to advance the particle
through all the sub-cycle steps. However, for systems with slowly varying EM fields,
such as the convolute, the Quicksilver simulations with and without sub-cycling showed
no major differences [12].

We implemented a similarly particle push sub-cycling algorithm in our PIC code. To
avoid reordering the particle arrays, instead of separating the macroparticles into
sub-groups, each macroparticle was pushed up to the field solution time with its own
time step based on its cyclotron frequency. As was found in the Quicksilver simulations,
sub-cycling the particle push provided a large reduction in the run time for the Z DPHC
charged particle sheath simulations; the sub-cycling did however introduce noise into the

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electric field, but the sheath dynamics and electrical histories were in good agreement with simulations with no sub-cycling. These results will be discussed further in section 4.12 of the next chapter.

An attempt was made to apply the sub-cycling algorithm to the convolute plasma simulations. As will be discussed in section 4.12, this proved unsuccessful, as the sub-cycling resulted in numerical heating of the plasma electrons to unphysically high temperatures.

3.7 Interpolation

As outlined in section 3.3, the EM fields are updated and the macroparticle forces calculated, by interpolating the particle currents to the grid and the grid EM fields to the particles, respectively. A range of interpolation, or weighting, schemes are available for this purpose. These differ in their order and therefore level of complexity and computational overhead. As mentioned in section 3.1.2, the interpolation gives the macroparticles an effective finite size; the particle shape is determined by the interpolation scheme. This is defined as the charge seen by a stationary observer located at a grid node when a macroparticle passes at constant velocity. [62].

The simplest weighting scheme, nearest grid point (NGP), assigns the total particle charge to the closest grid node; this gives a step function in the charge density of the width of the grid cell, $\Delta x$, as the particle crosses a cell boundary [62]. This is typically not sufficient for accurate simulation [68]. As such, we implemented both a first and second order interpolation scheme in our code. As will be discussed below, both schemes are naturally charge and can be made to be energy conserving. However, the second order scheme, which maintains at least first order weighting in all directions, was used in the baseline DPHC and inner MITL simulations described in the next chapter.

3.7.1 Current Interpolation

As we did not solve Gauss’ law, Eqn.(3.12), explicitly in the electric field update, in order to ensure exact (to machine precision) charge conservation, the current interpolation scheme had to satisfy the charge continuity equation, Eqn.(3.16) [12, 62, 82, 90].
3.7.1.1 Linear Current Interpolation

A schematic of the current interpolation path is shown in Figure 3.6. For ease of description, we have limited the problem to 2D cylindrical r-z coordinates; the extension to 3D is simple.

As is shown in Figure 3.6, the charge densities were defined on the cell corners, whilst the current densities were defined on the cell edges. During a time step, the particle was assumed to follow a straight line trajectory between the old, \( \vec{x}^n \) and new, \( \vec{x}^{n+1} \), positions. In practice, the r- and z-components of the current were interpolated to the grid by following paths 1 and 2 shown in the Figure, where the particle moves parallel to each axis in turn, and then averaging. In 3D, there are six possible paths, which were again averaged to give the final current [87]. It can be shown that averaging the currents from motions parallel to the axes in this way, is equivalent to the current calculated by following the direct straight line trajectory [68].

Taking path 1, the particle first moved parallel to the z-axis. The two z-components of the current in the cell, \( j_{z,i+k+1/2} \) and \( j_{z,i+1,k+1/2} \), for this part of the motion, were calculated as follows; at the old position, \( \vec{x}^n \), the linear interpolation weights, \( \vec{w}^m_+ \) and \( \vec{w}^m_- \), were calculated according to Eqn.(3.46) and Eqn.(3.47), respectively. Here, \( \vec{X}_{i,k} \) is the position of the bottom left hand corner of the cell in Figure 3.6.

\[
\vec{w}^m_+ = \frac{\vec{x}^n - \vec{X}_{i,k}}{\Delta \vec{X}}
\]  

(3.46)
\[ \vec{w}_n^\beta = 1 - \vec{w}_\perp^n \]  

(3.47)

The particle charge, \( q_p \), was then linearly interpolated to the cell corners at \( i, k \) and \( i + 1, k \), according to \( Q_{i,k}^n = w_{r,n} w_{z,n} q_p \) and \( Q_{i+1,k}^n = w_{r,n} w_{z,n} q_p \), respectively. Moving along the z-axis, the particle charge was interpolated to grid from the position \( (x_{r}^n, x_{z}^{n+1}) \) according to \( Q_{i,k}^{n+1} = w_{r,n} w_{z,n+1} q_p \) and \( Q_{i+1,k}^{n+1} = w_{r,n} w_{z,n+1} q_p \); here, \( \vec{w}^{n+1} \) were the weights at the new z position, calculated as in Eqn.(3.46-3.47). The change in the grid charge between times \( t^n \) and \( t^{n+1} \), \( \Delta Q_{i,k} = Q_{i,k}^{n+1} - Q_{i,k}^n \) and \( \Delta Q_{i+1,k} = Q_{i+1,k}^{n+1} - Q_{i+1,k}^n \) was then equal to the charge that had flowed across the surfaces normal to the z-direction, at \( i, k + 1/2 \) and \( i + 1, k + 1/2 \). Dividing the \( \Delta Q \)'s by the area of these surfaces, gave \( \Delta t j^{n+1/2}_{z,i,k+1/2} \) and \( \Delta t j^{n+1/2}_{z,i,k+1/2} \). The current density could then be calculated by dividing these quantities by the time step, \( \Delta t \); in practice it was \( \Delta t J \) which was stored, as this appeared directly in the field equations. Avoiding dividing and then multiplying the current by the time step in this way, was found to significantly improve the numerics.

The second part of path 1 involved the motion parallel to the radial direction; the currents \( j^{n+1/2}_{r,i,k+1/2} \) and \( j^{n+1/2}_{r,i+1/2,k+1} \) were calculated in an equivalent manner to z-components as described above. For simplicity, the paths for particles that crossed a cell boundary during a time step, were split into segments within each cell and the current interpolated to the grid for the motion along each segment separately, following the above method [91]. As noted in section 3.6.1, the information about the path splitting was stored in the particle tracker step, after the position update, so did not have to be recalculated in the current interpolation algorithm.

### 3.7.1.2 Quadratic Spline Current Interpolation

In the linear scheme described in the previous section, in the directions parallel to the particle motion, the current was interpolated at 0th order i.e. to the NGP. To mitigate the numerical electron heating instability, this forces NGP interpolation of the electric field components in the parallel directions [62, 64, 68]. As will be discussed in section 3.7.3, this is not desirable for simulating the particle motions in the high-voltage Z transmission lines. In general, for charge conserving current interpolation, the order of the interpolation in the parallel direction is one less than in the perpendicular directions.
Figure 3.7: A schematic of the current interpolation path used in the quadratic spline scheme.

Therefore, to recover linear interpolation in the parallel directions, second order interpolation must be used in the perpendicular directions. To this end, we implemented a second order charge conserving interpolation scheme in the code, following [68], which was based on quadratic splines.

In vacuum cells, the current interpolation methodology was identical to the linear scheme. A schematic of the quadratic spline current interpolation path in 2D cylindrical r-z coordinates is shown in Figure 3.7 [68].

Again, the particle was assumed to follow a straight line between the old, \( \bar{x}^n \) and new, \( \bar{x}^{n+1} \) positions which was approximated by the two paths 1 and 2. In the linear interpolation scheme, the particle contributed charge to two grid positions along each axis; in the second order scheme, the particle contributes charge to six grid positions along each axis. As such, for each part of the motion, six components of the current were calculated at the grid positions \( X_{i-1,k-1/2}, X_{i,k-1/2}, X_{i+1,k-1/2} \) and \( X_{i-1,k+1/2}, X_{i,k+1/2}, X_{i+1,k+1/2} \). Considering path 1, the particle first moved parallel to the z-axis. At the old position, the particle charge \( q_p \) was interpolated to the six cell corners. Taking the bottom set of nodes, \( Q_{i-1,k-1} = w_{-z} w_{-x} q_p \), \( Q_{i,k-1} = w_{0x} w_{-z} q_p \) and \( Q_{i+1,k-1} = w_{-x} w_{-z} q_p \); \( Q_{i-1,k}, Q_{i-1,k} \) and \( Q_{i-1,k} \) are similarly constructed with \( w_{-z} \rightarrow w_{0z} \). The
quadratic spline weights, \( \vec{w}_{n \pm} \) and \( \vec{w}_{n 0} \), are given in Eqn.(3.48-3.49), where \( \vec{u}_{n \pm} \) and \( \vec{u}_{n} \) are defined in Eqn.(3.50-3.51). Here, \( \vec{X}_{i-1/2,k-1/2} \) is the position of the bottom left hand corner of the dashed cell in Figure 3.7 [68].

\[
\vec{w}_{n \pm} = \frac{1}{2} (\vec{u}_{n \pm})^2 \tag{3.48}
\]

\[
\vec{w}_{n 0} = 1 - \vec{w}_{n +} - \vec{w}_{n -} \tag{3.49}
\]

\[
\vec{u}_{n +} = \frac{x^n - \vec{X}_{i-1/2,k-1/2}}{\Delta \vec{X}} \tag{3.50}
\]

\[
\vec{u}_{n -} = 1 - \vec{u}_{n +} \tag{3.51}
\]

Moving the particle parallel to the z-axis, the particle charge was interpolated to the same six grid nodes, from the position \( (x^n_{r}, x^{n+1}_{z}) \), to give the \( Q_{n+1} \)’s. As in the linear scheme, the change in the charge at each node \( \Delta Q = Q^{n+1} - Q^n \), was then divided by the area of the cell face normal to the z-axis to form \( \Delta t_{jz} \). Current from motion along the second part of path 1, parallel to the r-axis, was calculated in an equivalent manner. The currents from the two (in 2D) and six (in 3D) possible paths were averaged to give the final currents used in the field update, which was again equivalent to the current calculated following the straight line trajectory [68].

For simplicity, the particle paths were again split over cell boundaries and the current from each segment interpolated separately. However, as can be seen in Figure 3.7, for the second order scheme, the particle path was defined within the cell with corners at the full grid cell centres. The particle paths were split over these half grid cells, in an equivalent manner to the full grid cells described in section 3.6.1. Note that this path splitting had to be done in addition to the particle tracker and as such represented an additional computational overhead of the second order interpolation scheme.

### 3.7.1.3 Modifications to the Current Interpolation at the Electrode Boundaries

In the linear scheme, as long as particles were not allowed to enter an electrode cell, they could only contribute current to the vacuum cells. In the second order scheme,
if the standard interpolation described above was used for particles within half a cell of an electrode surface, they would contribute current to the inside of the electrode. Following [68], this was avoided by smoothly transitioning the current interpolation to first order for particles within half a cell of an electrode surface (or open boundary). The scheme employed to achieve this, which will be described in 1D below, maintained exact charge conservation. This transition to linear interpolation was also beneficial in terms of the particle creation algorithms; here the SCL emission algorithms, which assume linear weighting, did not need to be modified [68]. This was good, as otherwise we would have to treat the whole emission surface at once; this is possible, but is a complicated procedure in 3D [87].

Consider the 1D geometry in Figure 3.8; below $X_i$ is electrode and the particle at position $x^n$ lies within half a cell of the electrode surface. For this particle, the current was interpolated to the grid as described above, but using modified weights, that were a mixture of first and second order, transitioning to first order on the electrode surface [68].

The standard second order weights are given in Eqn.(3.52-3.53), where the $u$’s are defined in Eqn.(3.54-3.55) [68].

\[
\begin{align*}
    w_{x\pm}^n &= \frac{1}{2} \left( u_{x\pm}^n \right)^2 \\
    w_{x0}^n &= 1 - w_{x-}^n - w_{x+}^n \\
    u_{x+}^n &= \frac{x^n - X_{i-1/2}}{\Delta X} \\
    u_{x-}^n &= 1 - u_{x+}^n
\end{align*}
\]
The fraction of the second order scheme, \( f_Q^n \), is a function of the particle height above the electrode surface as in Eqn.(3.56).

\[
f_Q^n = \frac{x^n - X_i}{X_{i+1/2} - X_i}
\]  

(3.56)

The second order weights, Eqn.(3.52), were then modified as in Eqn.(3.57-3.58). Here, the linear weights for the full grid nodes, \( v_{xp}^n \), are defined in Eqn.(3.59-3.60).

Note that the calculation of the central weight, Eqn.(3.53), was unmodified \[68\].

\[
w_{x-}^n = \frac{f_Q^n}{2} (u_{x-}^n)^2
\]  

(3.57)

\[
w_{x+}^n = \frac{f_Q^n}{2} (u_{x+}^n)^2 + (1 - f_Q^n) v_{x+}^n
\]  

(3.58)

\[
v_{x+}^n = \frac{x^n - X_i}{\Delta X}
\]  

(3.59)

\[
v_{x-}^n = 1 - v_{x+}^n
\]  

(3.60)

As the particle moves towards the surface, \( x^n = X_{i+1/2} \rightarrow X_i \), the fraction of the second order scheme, \( f_Q^n = 1 \rightarrow 0 \), such that the interpolation smoothly transitions from second to first order over half of the cell. Note that on the surface, \( x^n = X_i \), \( f_Q^n = 0 \) such that all of the charge was interpolated to the surface node at \( X_i \). Notice that in this scheme you will always get some charge interpolated inside the electrode, apart from when the particle is exactly on the surface; this was done to simplify the extension to 2 and 3D. This is an error of a few percent in the charge interpolated to the surface node, which only affects the SCL emission algorithm, which will be described in section 3.9.1 and was tolerable. The scheme can be made to transition to first order faster by increasing the power of \( f_Q^n \) in Eqn.(3.57-3.58) \[68\]; however, we found that the standard first order transition was sufficient.

In 2 and 3D, the implementation of the surface cell modification is quite involved. It is outlined in \[68\], but the general idea of transitioning to first order within half a cell of the surface is the same as in this 1D example. For convenience, the surface cells are split into seven types; within the interpolation algorithm an additional if statement to
test for vacuum or surface and then a case statement for each of the different surface
types, was added. As such, the computational overhead for each particle was higher
than the standard first order scheme.

3.7.2 Domain Current Boundary Conditions

The open domain boundaries at the transmission line and load circuit model connections,
were treated in the same manner as the electrodes i.e. within half a cell of the edge of
the simulation domain the interpolation was transitioned to first order; this prevented
current being interpolated outside of the domain, which would have given rise to charge
conservation errors.

The reflective boundary condition at the $\theta$-boundaries was treated as follows; in
the current interpolation, the boundary was treated as if it was not there and the
vacuum cell weights applied. As such, a layer of ‘ghost’ cells were defined on each
boundary, to which the current from particle motions within half a cell of the boundary
was interpolated. After the current interpolation, the current in the ghost cells was
mapped back into the simulation domain according to Eqn.(3.61-3.63), for the $r$-, $\theta$-
and $z$-components, respectively. Here, the $i$ and $k$ indices are run over the domain boundary,
i.e., $i \in \{0, 1, \ldots, N_r\}$ and $k \in \{0, 1, \ldots, N_z\}$, where $N_{r,\theta,z}$ were the number of cells along
each direction.

\[ j_{r,i,1,k} = j_{r,i,1,k} + j_{r,i,-1,k} \]
\[ j_{r,i,N_\theta,k} = j_{r,i,N_\theta,k} + j_{r,i,N_\theta+1,k} \]  (3.61)

\[ j_{\theta,i,1/2,k} = j_{\theta,i,1/2,k} - j_{\theta,i,-1/2,k} \]
\[ j_{\theta,i,N_\theta-1/2,k} = j_{\theta,i,N_\theta,k} - j_{\theta,i,N_\theta+1/2,k} \]  (3.62)

\[ j_{z,i,1,k} = j_{z,i,1,k} + j_{z,i,-1,k} \]
\[ j_{z,i,N_\theta,k} = j_{z,i,N_\theta,k} + j_{z,i,N_\theta+1,k} \]  (3.63)
Additionally, to model the mirror charges, the components $j_r$ and $j_z$, as well as $\rho$, which coincided with the domain boundary, were doubled.

### 3.7.3 Electromagnetic Field Interpolation

As discussed in section 3.1.2, in the convolute plasma simulations $\Delta x > 100\lambda_e$; to mitigate the electron heating instability and unphysical plasma electron temperatures, an energy conserving scheme was used to interpolate the electric field from the grid to the macroparticle positions. Here, the electric field components were interpolated directly from the staggered Yee-mesh, such that the position to which the current (which is a source term in the electric field update) and from which the electric field were interpolated were consistent; this is the EM equivalent of the well-known electrostatic energy conserving algorithm [64, 68]. As the magnetic field does not change the magnitude of the particle velocity, only its direction, the energy conservation was insensitive to the order of the magnetic field interpolation. For speed, we therefore linearly interpolated the magnetic field from cell corner averages. Note that to avoid halving the strength of the magnetic field on the electrode surface, only vacuum cells were included in this average.

#### 3.7.3.1 Linear Force Interpolation

Again considering 2D cylindrical r-z coordinates, the electric field components are defined on the cell edges, Figure 3.6, coincident with the particle current. For the first order energy conserving scheme, the field components in the tangential directions are linearly interpolated, whilst in the longitudinal direction NGP interpolation is used. For example, consider the particle at the new position, $\vec{x}^{n+1}$. The linear weights, $\vec{w}_{\pm}$, are given in Eqn.(3.46) and Eqn.(3.47), respectively. The r- and z-components of the electric field at the particle position, $E_{pr}$ and $E_{pz}$ are then formed according to Eqn.(3.64).

\[
E_{pr}^{n+1} = w_{z}^{n+1} E_{r,i+1/2,k}^{n+1} + w_{r}^{n+1} E_{r,i+1/2,k+1}^{n+1} - E_{r,i+1/2,k}^{n+1}/2 - E_{r,i+1/2,k+1}^{n+1}/2
\]

\[
E_{pz}^{n+1} = w_{r}^{n+1} E_{z,k+1/2}^{n+1} + w_{z}^{n+1} E_{z,i+1,k+1/2}^{n+1} - E_{z,k+1/2}^{n+1}/2 - E_{z,i+1,k+1/2}^{n+1}/2
\]

(3.64)

As discussed in the previous section, the magnetic field was first averaged to the cell
corners, coincident with \( Q \) in Figure 3.6. In 2D only \( B_\theta \) is non-zero and is interpolated to the particle position according to Eqn.(3.65). Here, \( w_{r/z} = w_{r/z-} \) and \( w_{r/z} = w_{r/z+} \).

\[
B_{\theta}^{n+1} = \sum_{\alpha=0}^{1} \sum_{\beta=0}^{1} w_{\alpha}^{n+1} w_{\beta}^{n+1} B_{av,\alpha+k,\beta}^{n+1}
\]  

(3.65)

The extension of this linear scheme to 3D is simple.

### 3.7.3.2 Quadratic Spline Force Interpolation

As discussed in section 2.6.2 of chapter 2, NGP interpolation of the electric field in the longitudinal directions is usually insufficient, especially in the convolute simulations where the high voltages give rise to large electric field gradients in the lines [18]. In the vacuum cells, the second order quadratic spline extension of the above described linear interpolation scheme was straight forward. Again, considering the 2D \( r-z \) cylindrical geometry in Figure 3.7 and the particle at the new position, \( \vec{x}^{n+1} \), the quadratic spline weights, \( \vec{w}_{\pm} \) and \( \vec{w}_0 \), were calculated according to Eqn.(3.48-3.49), where the half-grid linear weights, \( \vec{u}_{\pm} \) and \( \vec{u}_0 \), are given in Eqn.(3.50-3.51). Now, second order weighting was used for the tangential directions and linear weighting in the longitudinal direction as in Eqn.(3.66), where \( w_{r/z-1,0,+1} = w_{r/z-,0,+} \) [68]. Again, the extension to 3D is simple.

\[
E_{pr}^{n+1} = \sum_{\beta=1}^{+1} w_{\beta}^{n+1} \left( u_{r}^{n+1} E_{r,i-1/2,k+\beta} + u_{r}^{n+1} E_{i+1/2,k+\beta} \right)
\]

\[
E_{pz}^{n+1} = \sum_{\alpha=1}^{+1} w_{\alpha}^{n+1} \left( u_{z}^{n+1} E_{z,i+\alpha,k-1/2} + u_{z}^{n+1} E_{i+\alpha,k+1/2} \right)
\]

(3.66)

### 3.7.3.3 Modifications to the Force Interpolation at the Electrode Boundaries

As discussed in section 3.7.1.3, to avoid interpolating the particle charge inside the electrode, the second order scheme was smoothly transitioned to first order for particles within half a cell of an electrode surface. For the energy conserving electric field interpolation, the weighting was transitioned from second to first order along the tangential directions and from first to zeroth order along the longitudinal direction. For the latter,
Figure 3.9: A schematic of the quadratic spline electric field interpolation used at an electrode surface normal to the radial axis.

As an example, consider the 2D electrode geometry in Figure 3.9. Here the electrode is the shaded region and the particle position, \( \vec{x}^n \), is within half a cell of the surface. In this case, the z-component of the electric field is given by Eqn.(3.66), with the corrected weights given in Eqn.(3.57-3.58). For the radial component, which is normal to the electrode surface, the half grid weights, \( u_{r\pm} \), were also modified. Here, \( u_{r-} = 0 \) and \( u_{r+} = 1 \), consistent with the assumption that \( E_{r,i+1/2} \) is constant across the half-cell above the surface [68].

The extension to other electrode shapes and 3D was again more involved and is outlined in [68]; here, the same idea of transitioning the tangential weights to first order and the longitudinal weights to zeroth order, was employed. As with the current interpolation, the surface cells were split into six possible types such that the interpolation algorithm included an additional if and case statement compared to the linear scheme.

In [68], it was suggested that an additional modification to the interpolation of the electric field component normal to the electrode surface, in SCL emission cells, should be made. Here, to account for the fact that in the SCL limit, \( E_{normal} = 0 \) at the electrode...
surface, within half a cell of the surface the \( u' \)'s were multiplied by \( f_Q \) before forming the weights. In this way, the electric field interpolated to the particle tends to zero as the particle moves towards the surface [68]. In the convolute plasma simulations we found that this lead to non-satisfactory results, where in the surface cells, the electron temperature was found to rapidly increase, as in the electron heating instability. As such, this modification was not included in our simulations.

### 3.7.3.4 Domain Electric Field Boundary Conditions

For the electric field interpolation, we again treated the open domain boundaries as electrode surfaces, such that the interpolation transitioned to the lower order scheme within half a cell of the boundary.

At the reflective \( \theta \)-boundaries, we again applied the standard vacuum cell interpolation, with a layer of ghost cells defined behind the boundary. In the ghost cells, the \( r, \theta \) and \( z \)-components of the electric field were set as in Eqn.(3.67-3.69), respectively. Here, the \( i \) and \( k \) indices were run over the domain boundary, \( i \in \{0,1,\ldots,N_r\} \) and \( k \in \{0,1,\ldots,N_z\} \), where \( N_{r,\theta,z} \) were the number of cells along each direction.

\[
E_{r,i,-1,k} = E_{r,i,1,k} \\
E_{r,i,N_\theta+1,k} = E_{r,i,N_\theta,k}
\]

(3.67)

\[
E_{\theta,i,-1/2,k} = -E_{\theta,i,1/2,k} \\
E_{\theta,i,N_\theta,k} = -E_{\theta,i,N_\theta,k}
\]

(3.68)

\[
E_{z,i,-1,k} = E_{z,i,1,k} \\
E_{z,i,N_z+1,k} = E_{z,i,N_z,k}
\]

(3.69)

### 3.8 Coulomb Collisions

As discussed in section 3.1.3, calculating the particle interactions via a numerical grid means that for macroparticles with separations smaller than this grid length, the inter-
particle force is modified compared to the Coulomb force law; the force tends to zero for zero particle separation [62]. For the range of plasma densities and temperatures expected in the DPHC and inner MITL the effect of short range Coulomb interactions within a Debye sphere, must therefore be reintroduced.

As reviewed in [74], a range of methods to model Coulomb collisions in the weakly coupled plasma limit have been developed. Of these, binary models [75, 76], where the collisions are applied to pairs of macroparticles, are the most popular as it is easy to conserve energy and momentum, especially for variable weight particles [74].

We implemented the relativistic binary MC collision scheme described in [75]. This scheme is general in the sense that it makes no assumptions about the form of the distribution of the velocities of the colliding particles [75]. The model, which treats only elastic collisions, involves randomly pairing particles within a grid cell and applying a rotation to the velocity vectors in the centre of momentum frame (CM) based on the relative velocity and parameters of the plasma, calculated from an energy dependent collision cross-section [75]. This is a MC scheme in the sense that a particle could interact with all other particles in the cell and by randomly pairing the particles we are taking a statistical sample of the possible interactions [74].

The collision algorithm is described in detail in [75]. To speed up the pairing process, the macroparticles were first ordered according to the grid cell in which they lay. The particle pairing followed the method of Takizuka [76]; first, the ordering of the particle list within in each grid cell was randomised. For intra-species collisions, adjacent particles in the list were collided. If there were an odd number of particles, then the final three particles in the list formed a triplet, where each particle was collided with the other two with a factor of 0.5 applied to the collision angle [76].

For inter-species collisions, if the number of particles in each species was equal, then particles with the same index in each list were collided. If the number of particles in each species was different then the pairing was more complicated. Labelling the number of particles in species 1 and 2 as $N_1$ and $N_2$ where $N_1 > N_2$ then the particles were split into two groups labelled a and b according to Eqn.(3.70) and Eqn.(3.71) respectively. Here, $N_1/N_2 = i + r$ where $i$ is a positive integer and $0 < r < 1$ [76].
\[ N_{1,a} = (i + 1)rN_2 \]
\[ N_{2,a} = rN_2 \]  
(3.70)

\[ N_{1,b} = i(1 - r)N_2 \]
\[ N_{2,b} = (1 - r)N_2 \]  
(3.71)

Now, each particle of group 2a was collided with \( i + 1 \) particles from group 1a, whilst each particle in group 2b was collided with \( i \) particles from group 1b. In this way, every particle in species 2 is collided with a particle from species 1. If \( N_2 > N_1 \) then the 1 and 2 indexes are simply switched \[76\].

The collision of each pair of particles, labelled \( \alpha \) and \( \beta \) was treated as follows; the particle momenta, \( \vec{p}_\alpha \) and \( \vec{p}_\beta \), were first boosted to the centre of momentum (CM) frame, in which the sum of the particle momenta is zero, \( \vec{P}_\alpha + \vec{P}_\beta = 0 \). For easy calculation of the scattering angles, the momentum coordinate system was then rotated such that the momentum of one of the particles was directed along the z-axis \[75\].

The collision frequency for small angle scattering between species \( \alpha \) and \( \beta \), with charges \( Z_\alpha \) and \( Z_\beta \), is defined in the one-particle-at-rest (OPR) frame and given in Eqn.(3.72). Here, \( v_{cm,rel} \) and \( p_{cm,rel} \) are the relative velocity and momentum, \( n_{min} \) is the minimum of \( n_\alpha \) and \( n_\beta \) \[75\] and \( ln\Lambda \) is the Coulomb logarithm as defined in \[73\].

\[ \nu_{\alpha\beta} = \frac{Z_\alpha^2 Z_\beta^2 e^4 n_{min} ln\Lambda}{8\pi\epsilon_0^2 p_{cm,rel}^2 v_{cm,rel}^2} \]  
(3.72)

The scattering angle, \( \theta \), was calculated according to Eqn.(3.73), where \( \hat{N} (\sigma) \) represents the operation of choosing a random number from a Gaussian distribution with a standard deviation of \( \sigma \). Here, \( \tau_{coll} \) was the simulation time that had elapsed between calls of the collision routine e.g. if the routine was called every time step then \( \tau_{coll} = \Delta t \) \[75\].

\[ \tan (\theta) = \hat{N} (\nu_{\alpha\beta} \tau_{coll}) \]  
(3.73)
The scattering angle in the CM frame, $\theta_{cm}$, is related to the angle in the OPR frame, $\theta$, by Eqn.(3.74). Here, $\beta_{cm}$ and $\gamma_{cm}$ are the reduced velocity and Lorentz factor of the CM system; $\beta$ is the unknown reduced velocity after scattering in the OPR frame, so was simply replaced with the initial velocity. This was justified if the energy transfer rate in the collision was small [75].

$$\tan\theta_{cm} = \frac{\sin\theta}{\gamma_{cm}(\cos\theta - \beta_{cm}/\beta)} \quad (3.74)$$

Throughout the collision the magnitude of the momentum is constant, $||\vec{P}_a|| = ||\vec{P}_\beta|| = |\vec{P}_a| = |\vec{P}_\beta| = P$, where primed variables represent the post collision values, but its direction is altered according to Eqn.(3.75). Here the azimuthal angle, $\phi_{cm}$, was chosen randomly between 0 and $2\pi$ radians [75].

$$(0, 0, P) \rightarrow (P\sin\theta_{cm}\cos\phi_{cm}, P\sin\theta_{cm}\sin\phi_{cm}, P\cos\theta_{cm}) \quad (3.75)$$

The momentum change in the CM frame, $\Delta\vec{P}$, was now obtained by rotating the right hand side of Eqn.(3.75) back to the original CM frame and subtracting the initial momentum vector, such that the particle momenta after the collision in the CM are given by Eqn.(3.76) [75].

$$\vec{P}_a = \vec{P}_a + \Delta\vec{P}$$
$$\vec{P}_\beta = \vec{P}_\beta - \Delta\vec{P} \quad (3.76)$$

Finally, the momenta in Eqn.(3.76) were boosted back into the lab frame [75].

Each macroparticle typically represents many, $> 10^9$, physical particles; the collision algorithm calculates the binary interaction of two particles with the physical masses. As such, in the creation algorithm we found it necessary to ensure that each macroparticle represented an integer number of physical particles. If this was not enforced then energy conservation errors of up to 0.5% per collision were observed.

As described above, the collision algorithm assumes that the macroparticles in each pair have equal weights. Due to the nature of the particle creation algorithms, this was not guaranteed to be true. For collisions between two particles with different weights, it was not possible to conserve both momentum and energy simultaneously in each
collision. A simple scheme which conserves neither of these properties is the rejection method [92]. Here, the momentum of the macroparticle with the larger weight of the two is updated after the collision with a finite probability based on the relative weights. This scheme conserves momentum and energy only on average over many collisions and is only recommended for simulations with over 100 particles per cell [75].

For collisions between particles with unequal weights, labelled by $w_\alpha$ and $w_\beta$, we chose to enforce exact energy conservation. Assuming, $w_\alpha > w_\beta$ the idea here was to partially scatter the larger weight particle according to Eqn.(3.77) and Eqn.(3.78). Here $P_\alpha = w_\beta/w_\alpha$ and $\vec{p}/E_{\text{scattered}}$ and $\vec{p}/E_{\text{before}}$ are the post and pre-scattering momentum/energy of particle $\alpha$ where $\vec{p}_{\text{scattered}}$ was calculated as above assuming equal weights [75].

\[
\vec{p}_{\text{corrected}} = P_\alpha \vec{p}_{\text{scattered}} + (1 - P_\alpha) \vec{p}_{\text{before}} \tag{3.77}
\]

\[
E_{\text{corrected}} = P_\alpha E_{\text{scattered}} + (1 - P_\alpha) E_{\text{before}} \tag{3.78}
\]

Now, $\vec{p}_{\text{corrected}}$ is not consistent with $E_{\text{corrected}}$. This condition is enforced at the expense of momentum conservation in individual interactions by adding a new perpendicular component of momentum as in Eqn.(3.79) [75].

\[
\vec{p}_{\text{final}} = \vec{p}_{\text{corrected}} + \Delta \vec{p}_{\alpha\perp} \tag{3.79}
\]

The magnitude of $\Delta \vec{p}_{\alpha\perp}$ was obtained by equating the energy in Eqn.(3.78) with the energy calculated from $\vec{p}_{\text{final}}$; the resulting non-linear equation was solved using a Newton-Raphson root finding algorithm [93]. As with the rejection method, although momentum was not conserved in individual collisions, it was conserved on average over many collisions [75].

To form the Coulomb logarithm, $\ln A$, in the collision frequency, Eqn.(3.72), an estimate of the plasma electron and ion temperature was required. This was defined in each computational cell by Eqn.(3.80), where $\vec{v}$ are in individual macroparticle velocities in the cell and $\vec{V}_i = \langle \vec{v} \rangle_i$ is the mean velocity of the cell [72]. Here the index $i$ refers to the electron and ion species with mass $m_i$. Note that for a Maxwellian distribution of velocities, $\vec{V}_i = 0$, such that Eqn.(3.80) gives the standard result, $\langle \vec{v}^2 \rangle /2 = (3/2) T$. 

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\[ T_i = \frac{m_i}{3} \left\langle \left( \vec{v} - \vec{V}_i \right)^2 \right\rangle \]  

(3.80)

The collision algorithm represented one of the largest computational overheads of each cycle. This came from a combination of first sorting then pairing the particles and the large number of floating point operations required to update the velocities of each pair of particles. However, as was discussed in section 3.1.3, for the DPHC plasma the various interaction times of interest were typically greater than the time step. As such, the algorithm was not called every time step; the \( \tau_{\text{coll}} \) parameter in Eqn.(3.73) was therefore set to the simulation time that had elapsed between calls to the collision algorithm. To avoid single large scattering events, as suggested in [75] and [76], \( \nu \) was limited to 1/50. In practice, we found that ensuring the collision algorithm was called at least ten times for the shortest interaction time of interest was sufficient. For the fully ionised proton plasma simulated in the DPHC, this was the electron-ion collision time defined in Eqn.(3.7).

A number of tests of the collision algorithm were carried out. Here, the particle motion and Lorentz force were neglected, such that the particle velocities were only updated due to the collisions. To test the intra-species collisions, we loaded the electron and ion macroparticles on a shell in velocity space; after a collisional relaxation time, the particle velocities were binned and compared to the expected Maxwellian distribution, where good agreement was found in all cases. Additionally, the scaling of the relaxation time with the plasma density and temperature was found to follow the Spitzer relation [71].

Next, the inter-species collisions were tested by loading the electron and ion macroparticles in Maxwellian distributions, using the method described below in section 3.9.3, but at different temperatures. The electron-ion thermalisation time was then compared to the Spitzer result [71], where again good agreement was found in all cases.

The electron-ion collisional momentum exchange was tested by applying a constant electric field along the z-axis. The steady state current was then compared to that expected from the Spitzer resistivity [71], where again good agreement was found.

Physically, in a plasma, the short range Coulomb interactions are important on the scale of the Debye length [71, 72]. We have already stated that the spatial resolutions
used in the DPHC simulations gave $\Delta x > 100\lambda_e$. However, in [75], it was found that as long as the grid resolved the density and temperature gradient, it was not crucial to resolve the Debye length, for accuracy.

3.9 Particle Creation

The convolute simulations were initialised with no particles. As discussed in chapter 2, the electric field stress on the cathode electrodes in the vacuum section of $Z$ is sufficient to form a plasma via neutral contaminant molecule desorption and ionisation. The plasma acts as a zero work function surface from which electrons are emitted into the a-k gap. Where the magnetic field strength is not sufficient to insulate the electrons, they impact the anode, heating the electrode material and driving the thermal desorption and ionisation of neutral contaminants to form plasma on the anode [21]. The anode plasma acts as a zero work function surface for ion emission into the a-k gap. Models for these various particle creation mechanisms were included in the code.

In the cathode electrode emission cells, SCL electron emission and plasma creation began when the normal component of the electric field strength exceeded $240\text{kVcm}^{-1}$, which is the expected threshold for neutral desorption and ionisation [16]. As will be discussed below, the creation algorithms were applied at the cell corners. As such, this test was applied to the normal components of the electric field on the cell edges above the emission node. In the anode emission cells, ion SCL emission began when the surface temperature exceeded 700K, where the heating mechanism was bombardment by electrons emitted from the cathode plasma. This is the threshold where thermal desorption dominates stimulated processes [21]. The electrode temperature was defined at the cell centres; the temperature was therefore first averaged to the cell corners before the test was applied. Note that only electrode cells were included in this average.

3.9.1 Space-Charge-Limited Emission

The simplest treatment of the cathode and anode electrode plasmas is to assume that they are formed, but remain tightly bound to the electrode surface; in this case SCL emission of electrons and ions is allowed directly from the cathode or anode electrode
A schematic of a SCL emission cell in 2D cylindrical r-z coordinates.

Figure 3.10: A schematic of a SCL emission cell in 2D cylindrical r-z coordinates.

surface, respectively. This is a common approximation used for simulating a large range of pulsed power systems.

A schematic of a SCL emission cell is shown in Figure 3.10. Here, we have restricted the problem to 2D cylindrical r-z coordinates to simplify the explanation; the extension to 3D is simple. In the SCL approximation we create sufficient new charge, $Q_s$, in the emission cell to force the normal component of the electric field to be zero. The new charge, $Q_s$, is calculated by applying Gauss’s law over the surface, $S$ of the emission cell as in Eqn.(3.81) [87]. Here, the electric field components are defined on the cell edges and $Q$ is the macroparticle charge from the current time step which has been interpolated to the cell corner (this was stored in the current interpolation step and therefore did not have to be recalculated).

$$Q_s = \int_S \vec{E} \cdot d\vec{S} - Q$$ (3.81)

Taking $S$ to be the square highlighted by the dashed lines in Figure 3.10, the integral in Eqn.(3.81), is replaced by the sum in Eqn.(3.82). Here, $A$ are the areas of the emission cell faces. The second expression follows from the perfect conductor electrode boundary conditions, where the components of the electric field parallel to the electrode surface are set to zero.
The charge, $Q_s$, was split between a number of new macroparticles. For both the first and second order interpolation schemes, within the first half cell of the emission surface, the interpolation was linear. If the particles were created throughout the emission cell, defined by $i + 1/2$ to $i + 3/2$ along $r$ and $k + 1/2$ to $k + 3/2$ along $z$, then they would contribute charge to other emission cells. In order to set the particle weights, such that the correct charge was created in all the emission cells, a set of linear equations taking the whole emission surface into account would need to be solved. In 3D this step is particularly complicated; as such the particle positions were initialised along a line normal to the surface, such that they only contributed charge to a single emission cell [87]. For example, in Figure 3.10, the particles were created along the diagonal line bisecting the quarter cell, defined by $i + 1$ to $i + 3/2$ along $r$, and $k + 1$ to $k + 3/2$ along $z$. The initial particle positions along this line were randomised and the weights adjusted accordingly to ensure the interpolated charge gave $Q_s$ at the surface node. To avoid losing particles to the electrode within a time step, they were created above the surface. Due to this, the particles contributed charge to the vacuum cells; to enforce charge conservation the particles were in fact created on the surface node and moved up to their initial positions. The current from this motion, which was interpolated to the grid as described above, then ensured that charge was conserved in the vacuum cells [87].

To model the fact the SCL particles are in fact being emitted from the electrode plasma, a random velocity, set by a user defined temperature, could be applied to the initial particle velocity [94]. Here, the temperature set the magnitude of the velocity according to $v_{th} = (3k_BT/m)^{1/2}$ and the direction was set by choosing two angles at random in velocity space. In the convolute simulations a temperature of $T = 0.1\text{eV}$ was used.
3.9.2 Electrode Heating by Electron Impact

When an electron impacts an electrode surface it will travel a short distance into the material and exchange energy with the atoms via collisional processes, causing the material to be heated [22, 94]. The stopping power, \(dE/dx\), gives a measure of the energy deposited in the material per unit length. Combined with the specific heat capacity of the material, \(c_p\) and an estimate for the stopping length, \(\Delta x\), the temperature rise, \(\Delta T\), can be calculated as in Eqn.(3.83) [94]. Here, \(\rho\) is the material mass density, \(\Delta V\) is the volume of the surface cell and \(q_p\) is the charge of the macroparticle.

\[
\Delta T = \frac{dE}{dx} \frac{\Delta x}{c_p \rho \Delta V} q_p e \tag{3.83}
\]

The stopping power is a function of the incident electron kinetic energy. We used a tabulated Bethe stopping power for Iron (the convolute and inner MITL electrodes are stainless steel) taken from the free online NIST database [95]. Here, the final particle kinetic energy was used to linearly interpolate from the table. The stopping path length was calculated from the incident angle of the particle with the electrode surface, \(\theta\) as \(\Delta x = d/cos\theta\) [22, 94]. Here, \(\theta\) was defined relative to the surface normal and \(d\) is the depth the particle reached in the material. This was typically taken to be equal to the cell length; the stopping length was limited to the maximum range of the electron, which was again a function of the incident kinetic energy and interpolated from the same look up table as the stopping power.

The temperature increase from each macroparticle impact was added to a running total in the grid cell in which the particle impacted the electrode; as such thermal conduction in the electrode was neglected, which is expected to be a good approximation for the duration of the \(\sim 100\text{ns} \) Z current pulse [94]. The factor \(q_p/e\) in Eqn.(3.83), accounts for the fact that each macroparticle represents more than one physical particle.

3.9.3 Cathode Plasma Creation Model

In section 2.2 of chapter 2, the Shefer model of a cathode plasma in a 1D high-voltage gap [27], was reviewed. Here, the gap of length \(L\), was separated into three regions; a weakly ionised source layer \((0 < x < x_0)\), a source free fully ionised plasma layer
(x_0 < x \leq \bar{x}) and a vacuum gap (\bar{x} < x < L) containing SCL electron flow\ [27].

To inject a plasma from the cathode in the DPHC and inner MITL simulations, we followed the method in [94] and assumed that the neutral source layer was much smaller than the cell size \( (x_0 << \Delta x) \). As the source layer was not resolved explicitly, a fully ionised plasma was instead loaded into the first vacuum cell next to an electrode emission surface by creating pairs of electron and ion macroparticles at a user defined rate of \( \nu_{\text{desorp}} \). Here, \( \nu_{\text{desorp}} \) was defined in units of monolayers per nanosecond, mlns\(^{-1}\), where 1ml=10\(^{15}\)cm\(^{-2}\). The number of physical neutral particles desorbed into each cell was given by Eqn.(3.84), where \( A_{\text{cell}} \) is the surface area of the cell in square centimetres and \( \tau_{\text{desorp}} \) is the time elapsed since the creation algorithm was last called in nanoseconds. Note that if the algorithm was called every time step then \( \tau_{\text{desorp}} = \Delta t \), where \( \Delta t \) is the simulation time step. The plasma creation began once the strength of the normal component of the electric field exceeded 240kVcm\(^{-1}\); this is the expected threshold for neutral contaminant desorption and ionisation [21].

\[
N_{\text{physical}} = \nu_{\text{desorp}} A_{\text{cell}} \tau_{\text{desorp}}
\]

(3.84)

The neutral particles were assumed to instantaneously ionise, such that for singly ionised ions, \( N_{\text{physical}} \) was equal to the number of physical electron and ion pairs to create. These were described by a smaller number of macroparticles, \( N_{\text{macro}} \), such that the weight of the electron and ion macroparticle in each pair was given by \( w = N_{\text{physical}} / N_{\text{macro}} \).

Assuming LTE, the initial macroparticle velocities were sampled from a Maxwellian distribution with a temperature, \( T \). In early simulations we used the rejection method to sample the total velocity Maxwellian distribution [62]. The initial direction of the velocity vector was then set by randomly sampling two angles in spherical coordinates in velocity space, before transforming to 3D Cartesian coordinates. This scheme proved to be relatively slow, so was replaced by a Box-Muller scheme to sample separate Gaussian distributions along each axis in velocity space [93].

Taking two independent random numbers, \( R_1 \) and \( R_2 \), in the interval \([0, 1]\), we can define two new independent random variables, \( Z_1 \) and \( Z_2 \), Eqn.(3.85), which are distributed according to a normal distribution, Eqn.(3.86). Here, \( \mu \) and \( \sigma \), are the mean
and standard deviation of the distribution \[93]\.

\[
Z_1 = \mu + \sigma \sqrt{-2 \ln R_1} \cos (2\pi R_2) \\
Z_2 = \mu + \sigma \sqrt{-2 \ln R_1} \sin (2\pi R_2)
\]  

(3.85)

\[
f(x, \mu, \sigma^2) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{x-\mu}{\sigma}\right)^2}
\]  

(3.86)

For a Maxwellian, \(\mu = 0\) and \(\sigma = \sqrt{k_b T/m}\), where \(m\) is the mass of the particle species \[94\]. For each pair of particles we require three \(Z\)'s (one for each velocity component); as such we generated four values of \(R\) and \(Z\) for each pair of particles. As will be discussed further in section 4.4 in the next chapter, in order to conserve charge and prevent the formation of unphysical electric fields in the source cell, the initial magnitude of the electron and ion macroparticle velocities in each pair were equal; here the ion mass was used to calculate the standard deviation of the distribution. In this way the electrons were loaded with an effective temperature of \((m_e/m_i) T \sim 5.45 \times 10^{-4} T\).

Loading equal weight macroparticles using this method was used in preference to uniformly sampling Eqn.(3.86), by for example using a Sobol sequence of random numbers \[96\]. As a relatively small number of macroparticles, < 5, were created in each emission cell, each time the algorithm was called, the latter method gave rise to particles with a large range in their weights.

In order to establish the plasma in the emission cell, the macroparticle pairs were loaded throughout the cell. In the same way as the SCL emission algorithm, to avoid initially contributing charge to adjacent source cells, the particles were loaded along the line normal to the surface. The initial height above the surface was chosen randomly for each pair of particles. The random initial velocities would ensure that the particles filled the emission cell.

In the Shefer model, current was returned to the cathode by the ions \[27\]. As was found in \[94\], to avoid the formation of an unphysical sheath in the source cell in our simulations, this current had to be supplemented by SCL electron emission directly from the electrode surface. To be consistent with the plasma creation, these electrons were loaded at the same temperature, i.e. \(\sim (m_e/m_i) T_i\).
As will be presented in the next chapter, the above described cathode plasma creation model was sufficient to load a fully ionised plasma into the vacuum cell next to the electrode surface, from which a SCL electron sheath could self-consistently form.

### 3.10 Time Step Management

In order to efficiently resolve the various time scales of interest, such as the plasma and cyclotron frequencies, the time step could be dynamically varied. This will be discussed in detail for the specific case of the convolute plasma simulations in section 4.5 of the next chapter. In fact, a variable time step was necessary to practically resolve the electron cyclotron frequency, which varied by approximately a factor of ten during the current pulse. The general method was to first test the plasma parameters; if the shortest time scale was smaller than the current time step, then the current time step was reduced. This reduction was carried out in integer divisions of the initial time step; this was done in preference to reducing the step by smaller increments to avoid having to re-centre the magnetic field and particle velocities in time with the electric field and particle positions respectively, too frequently. The re-centring, which ensured second order accuracy in time was maintained, was achieved by evolving the magnetic field using the standard EM field solver and the particle velocities with the Boris push, using a time step of $\Delta t_{\text{old}}/2 - \Delta t_{\text{new}}/2$ starting from the values at the old time, before the actual field update and particle push were applied.

### 3.11 Simulation Diagnostics

In Z experiments, the pulsed power operation is diagnosed by a range of current and voltage measurements taken at various points within the pulse forming and vacuum sections of the machine. We included a range of electrical diagnostics in the code which could be compared directly to the experimental measurements. These diagnostics, which involved integrals of the electric and magnetic field, were calculated during run time as we typically wanted temporal resolutions of $\sim 0.1\text{ns}$, which was too short a time scale on which to write out all of the field data for post processing. As these integrals could
cover multiple domains and to avoid global communications during run time, they were written out from each domain separately and combined in post-processing.

The voltage across an a-k gap was calculated from a line integral of the electric field, Eqn.(3.87), where the integral was approximated by the sum over the edge centred electric field components, $E_i$, multiplied by the cell length, $\Delta x_i$, in the integration direction. For simplicity, this integration was limited to directions parallel to an axis.

$$V = \int \vec{E} \cdot d\vec{l} = \sum_i E_i \Delta x_i$$  \hspace{1cm} (3.87)

The current was calculated from a line integral of the magnetic field using the integral form of Ampere’s law, as in Eqn.(3.88). Again for simplicity, the integral was defined such that each part of the integration path, $l$, was parallel to an axis direction. For example, to obtain the convolute current, which is measured by a B-dot in the anode electrode at a radius of $\sim 6$cm, we integrated the $\theta$-component of the magnetic field, $B_i = B_{\theta,i}$ along the $\theta$-direction, using the arc-length of a cell, $\Delta l_i = r \Delta \theta$ over the total number of cells in this direction, $N_i = N_\theta$. Here, $r$ was the radius of the cell centre closest to the diagnostic (coincident with the face centred magnetic field components) and $\Delta \theta$ was the cell size along the $\theta$-axis. Assuming symmetry along the $\theta$-direction, the result was then multiplied by $2\pi/N_\theta \Delta \theta$, to give the total current that would be measured in experiment. Typically we required an estimate of the bound current in the cathode or anode electrode. In these cases the integration was carried out using the value of the magnetic field in the vacuum cell next to the electrode cell (half a cell away from the electrode surface).

$$I = \frac{1}{\mu_0} \oint \vec{B} \cdot d\vec{l} = \frac{1}{\mu_0} \sum_i B_i \Delta l_i$$  \hspace{1cm} (3.88)

The current in the anode posts of the convolute was calculated using an integration path that followed the curve of the grid at two radii bounding the post and was closed along the radial axis at two values of $\theta$ which again bounded the post. In this way, the integration was always parallel to an axis.

The electron flow current, $I_e$, was diagnosed using two methods. Firstly, a plane could be defined, over which the normal component of the vacuum electron current density, $\vec{j}_p$, could be integrated as in Eqn.(3.89). Here, the surface integral was ap-
proximated by a sum over the areas of the cell faces lying in the plane. This method of calculation was found to be quite noisy; as an alternative, the electron flow current could be calculated from a difference of the bound currents in the anode and cathode electrodes, \( I_e = I_a - I_c \), where the bound currents were calculated from Eqn.(3.88), as described above.

\[
I_e = \int_S \vec{j}_p \cdot d\vec{S} = \sum_A \vec{j}_p \Delta \vec{A} \tag{3.89}
\]

In addition to the electrical diagnostics, the grid data such as the electron and ion density and electric and magnetic fields, were written out and visualised with the freely available ParaView software [96]. The grid data was typically output every 2ns during the simulation. Note that the temperature calculated in the collision algorithm by Eqn.(3.80), could also be output as a grid diagnostic.

To monitor the simulation performance, an energy accounting diagnostic was included. This will be described in detail in section 4.13 of the next chapter; this diagnostic output a running sum of the EM field, load, particle and circuit energy, as well as the error in the total energy. This was written on the time scale of the electrical diagnostics, \( \sim 0.1 \text{ns} \). Similarly, diagnostics to check charge conservation by calculating Gauss’ law on the cell corners and the condition \( \vec{\nabla} \cdot \vec{B} = 0 \), were also included. The grid values, to give a spatial map of the errors, as well as the peak error, could also be output.

### 3.12 Parallelisation and Load Balancing

As discussed in section 3.1.1, the model equations were exclusively explicitly differenced. To offset the tighter stability constraints placed on the spatial and temporal steps, the code was parallelised using domain decomposition; here, the simulation grid was split into cubes, with each cube residing on its own processor. The MPI library of message passing subroutines was used to transfer information between the domains (processors). This method was used in preference to splitting the particle arrays over multiple processors for two reasons; firstly, for 3D simulations the domain was relatively large, such that globally communicating the whole grid every time step in order to obtain the source terms for the EM field solution and the force interpolation was inefficient. Secondly, the
binary collision algorithm discussed in section 3.8, involved pairing particles that resided in the same simulation cell; this was simpler with domain decomposition as the particles within in a cell were guaranteed to be in the same domain i.e. on the same processor.

For each domain, the EM field solution proceeded as described in section 3.4. For multiple processor runs, a layer of ghost cells was defined around each domain which stored the magnetic field from the corresponding cells on the adjacent domains. These fields were passed at each time step, after the field update and acted as boundary conditions to close the equations for the electric field update at the next time step. For the particle force calculation, this information was also used to spatially average the magnetic field to the cell corners. For the quadratic spline electric field interpolation, where a particle within half a cell of the domain boundary could sample the electric field on the adjacent domain, the electric field was also passed and stored in the ghost-cells after the field update.

For both linear and quadratic spline interpolation, the macroparticle charge and current on the domain boundary, which was common to adjacent domains, had to be communicated. To avoid double counting in this sum, the result for the pass in one direction was stored in a dummy array and then added to the final result, after the pass in the opposite direction. With quadratic spline interpolation, particles within half a cell of the domain boundary could also contribute charge and current to the adjacent domain. These components were initially interpolated to the ghost-cells on the local domain, before being communicated to the adjacent domains. In this way, the source terms used in the field solution on each domain were consistent with the global particle distribution.

As well as EM field and macroparticle source information, the macroparticles themselves could cross a simulation domain. After the particle push step, this was tested for in the particle tracker, section 3.6.1, and the particle index stored in a separate array. Before the current interpolation, these particles were passed to the new domains. As we did not know how many particles would be passed in each time step, we first communicated this information, such that the passing array memory could be allocated and the minimum information sent in the actually communication. This method was found to be significantly more efficient than a single communication of larger, nearly empty arrays. In practice the particle pass involved creating a new particle on the target do-
main with the parameters on the current domain and then removing the particle on the current domain from the active particle list. For simplicity, passes to diagonal domains were handled by a series of passes to adjacent domains along each axis. As such, for 3D simulations, the particle passing routines were called three times along each axis.

In terms of particle load balancing, the convolute simulations were quite challenging. As the simulations were initialised with no particles, we did not know a priori what the particle distribution would be, making it difficult to split the domains in a way to spread the particle load evenly. For simplicity, we therefore split the domains uniformly along each axis. This choice had a number of negative implications; firstly, due to the relatively large volume of the electrodes in the convolute compared to the vacuum gaps, we could have a large number of processors sitting inside the electrode, essentially doing nothing. Secondly, the nature of the cathode plasma, where the highest plasma density and therefore largest number of simulation particles, was on the electrode surface, meant that we typically had many particles spread over a few processes. As such, it would be beneficial to allow the simulation to be split into a number of smaller grids, which could be fitted to the electrode geometry more efficiently. The coding for the domain communications would be significantly more complicated and as such this was left as a future extension of the code.

### 3.13 Adaptive Particle Management

The LSP Z DPHC convolute plasma simulations employed an algorithm to dynamically and conservatively control the number of macroparticles in each cell [15, 16]. The algorithm was based on [97] and involved replacing $N$ old particles with $M$ new particles in a cell, where $M$ could be either smaller or larger than $N$. In this way, the computational overhead in dense cells could be reduced by reducing the number of macroparticles, whilst the statistics could be improved in lower density cells by increasing the number of macroparticles. The new particle weights were calculated from the solution of a system of linear equations to ensure the interpolated grid charge and momentum were conserved. To enforce energy conservation, a random component of momentum was added to each new particle which was scaled to conserve the total kinetic energy. As such, the momentum was not conserved exactly, however as the extra components of
momentum were added randomly, it would be conserved statistically over multiple calls to the algorithm [97].

To form the system of linear equations to solve for the new particle weights required a linear interpolation scheme. As such this method was not compatible with the second order quadratic spline interpolation employed in our code. However, we did test the applicability of this method of population control to our convolute plasma simulations, by reverting to first order interpolation, as described in section 3.7.1.1 and 3.7.3.1.

In 3D, the new particle weights and momentum were calculated by solving a system of eight linear equations (one for each corner of the cell). This was achieved numerically using Gauss-Jordan elimination [93]. The random components of the momentum added to the particles to conserve energy, were sampled from a Gaussian distribution and in the relativistic case, the scaling parameter was obtained via a numerical solution of the resulting non-linear energy equation, using a Newton-Raphson root finding algorithm [93].

To define the system of linear equations for the new particle weights and momentum, the new particle positions had to be defined [97]. For tests cases, where the old particles were distributed uniformly throughout the cell, it was sufficient to randomly place the new particles within the cell. However, for real convolute simulations, were the old particle distribution was more complicated, this scheme was not sufficient and the algorithm would fail to reduce the number of particles in the cell over 90% of the time. The success rate could be improved by defining a sub-grid within the cell on which the old particle charge was binned and used to place the new particles to better approximate the distribution. However, at best the routine reduced the number of particles only 60% of the time. In addition, the success of the model was very sensitive to the ratio of the new to old particle number, where we found the model failed regularly for $M/N < 0.8$.

As such, we found that the total number of simulation particles was not significantly reduced in our convolute simulations using this method.

### 3.14 Chapter Summary

The PIC method is a particle based MC solution of the collisionless Valsov equation; Coulomb collisions can be included consistent with the FP collision integral using a
range of supplementary algorithms. The simulation macroparticles are pushed with the relativistic Newton-Lorentz equation of motion. Interactions through self-consistently generated and externally applied EM fields are calculated on a numerical grid via a solution of Maxwell’s equations with the interpolated macroparticle current as a source term; the fields are interpolated to the particles to apply the Lorentz force [62].

In this chapter, the PIC model used to simulate the plasma and charged particle sheaths formed in the Z radial lines, DPHC and inner MITL, was developed. The collisionless PIC model was applicable to modelling the charged particle sheath with a density of between $10^{12-13}\text{cm}^{-3}$ expected from SCL emission, as long range interactions dominate short range Coulomb interactions here. The cathode plasma density was expected to range between $10^{13-16}\text{cm}^{-3}$, with temperatures of between 1 and 10eV. A plasma is said to be collisionless if $\omega_{pe}\tau_{ei} > 1$, where $\omega_{pe}$ is the electron plasma frequency and $\tau_{ei}$ is the electron-ion collision time [62]. At 1eV, $\omega_{pe}\tau_{ei} \sim 700-16$ and therefore Coulomb collisions in the convolute plasma were expected to have an important effect on the particle distribution function and transport. As such, Coulomb collisions were modelled as binary interactions between randomly paired particles within a simulation cell; the velocity vectors were rotated using an energy dependent collision frequency, which made no assumptions about the distribution of the particle velocities [75].

In this density and temperature range, the plasma Debye length is $\text{<10}\mu\text{m}$ and was at least one hundred times smaller than the simulation grid cell size. For simplicity and to allow easier parallelisation by domain decomposition, the model differential equations were exclusive explicitly finite differenced. To mitigate the numerical electron heating instability in this case, the electric field was interpolated directly from the staggered mesh to the macroparticle positions. For improved accuracy, a quadratic spline interpolation scheme was implemented [68].

The simulation time step was determined by resolving the electron cyclotron frequency; this was necessary to accurately model the electron drift motions in the crossed electric and magnetic fields and therefore to accurately simulate the sheath dynamics in the MITL, discussed in section 2.3 of chapter 2.

Particles could be injected into the simulation using either SCL emission directly from the electrode surface or injecting pairs of electron and ion macroparticles to load a fully ionised plasma next to the electrode. With circuit models of the load and radial
lines driving the convolute, self-consistently coupled to the EM field solver through
transmission boundary conditions, the PIC model could be used to model the evolution
and dynamics of the cathode plasma and charged particle sheaths in the Z DPHC
and inner MITL during the current discharge. Results from these simulations will be
presented in the next chapter.

The PIC model described in this chapter also formed the basis of the hybrid PIC-
MHD code that will be described in chapter 5 and will be extended to include an inertial
two-fluid description of the plasma in chapter 6.
Particle in Cell Simulation

Results

In this chapter, results from PIC simulations of the Z DPHC and inner MITL using the code described in chapter 3, will be presented. Here, the goal was to reproduce the multi-mega ampere current losses measured in the convolute and inferred from simulation to be occurring within the inner MITL [2,3]. This was successfully achieved using a phenomenological cathode plasma creation model, with the convolute driven by a representative circuit model and source voltage of the vacuum radial lines and pulse forming circuit. Our simulations will also be compared to published results from the LSP [15, 16] and Quicksilver [12,14,18] PIC codes, where in general good agreement regarding the plasma and sheath evolution and dynamics, was found.

4.1 Electrode Geometry

In this study we have exclusively modelled the pre-refurbishment convolute electrode geometry shown in Figure 1.2 in chapter 1. During the refurbishment, where the theoretical peak current was raised from approximately 20 to 26MA, the overall electrode geometry did not alter dramatically [15]; the a-k gaps were increased to accommodate the higher voltages associated with the increase in peak current and the load height was
raised to improve diagnostic access, resulting in more acute slopes in the feed lines [18]. Although larger percentage current losses have been measured post-refurbishment [2,17], we expect that our results regarding the charged particle sheath and plasma dynamics in the pre-refurbishment geometry will carry over to the refurbished convolute. One of the main reasons for focusing on Z, instead of ZR, was access to a relevant circuit model of the PF circuit. This was relatively simply on Z as the water lines were connected directly to the insulator stack, but was complicated on ZR due to changes made in the connection [2].

The standard convolute consists of two levels of 12 posts equally spaced around the axis [16]. To model the full 24 post convolute in 3D is practically impossible at any reasonable spatial resolution. Instead, we took advantage of the systems periodicity and modelled a single level of posts. Here, the natural choice was cylindrical coordinates \((r, \theta, z)\). Early simulations modelled a \(\pi/6\) extent along the \(\theta\)-direction i.e. the full posts and holes with either periodic or reflective EM field and macroparticle boundary conditions applied at the \(\theta\)-domain boundaries. Equivalent simulation results were found for a \(\pi/12\) extent along the \(\theta\)-direction, where the domain bisected the posts and holes and reflective boundary conditions were applied at the \(\theta\)-boundaries. This choice of geometry halved the computational domain size and therefore simulation run time and was adopted for all subsequent simulations. For reference, the Quicksilver simulations used a \(\pi/12\) extent [14, 18], whereas the LSP simulations used the larger \(\pi/6\) extent [15,16].

The approximate electrode geometry used in the PIC simulations is shown in Figure 4.1. As discussed in chapter 1, power is fed into the convolute from the four radial disk lines at the levels labelled A-D. For clarity, these labels will be used throughout the remaining text. To minimise electrode stair stepping, the level A and B electrodes were set at zero degrees to the horizontal; in reality these electrodes were at angles of 8.1 and 9.1 degrees, respectively [14,16]. The level C and D electrodes are conical; here the stair stepping is clearly visible. To avoid spurious reflections of electromagnetic waves at the simulation domain boundary, where the connections to the circuit model were made, the final 1cm of each line was purely radial. Experience has shown that this length, which is approximately equal to the a-k gap spacing of 1.15cm in the level C and D lines (the a-k gap measured normal to the electrode surface is 1cm), was sufficient for
Figure 4.1: Simulated DPHC electrode geometry, with the positions of the four levels of radial disk feeds, labelled A-D, and load, labelled. This purpose. For simplicity, the holes in the cathode electrodes were modelled with straight edges; in reality these edges are curved, as shown in Figure 1.2, but the precise shape could not be reproduced accurately from our 2D drawings. Attempts to obtain 3D engineering drawings from SNL, giving the exact electrode geometry, were unsuccessful. The effect of this approximation was to enhance the simulated electric field strength at these corners, a feature that will be discussed further in section 4.3.1.

4.2 Circuit Models

To minimise the size of the PIC domain, the radial feed lines were modelled as a series of ideal transmission line elements, as shown in Figure 4.2 [16]. The four levels of the radial feed were modelled with separate circuits, with vacuum impedances and lengths to approximate the physical electrode geometry. The element lengths and impedances were chosen to cover a radial extent beginning at the edge of the PIC domain, at a radius of 14.4cm and ending at the insulator stack, at a radius of 1.6m. Specifically, the shorter elements at the start and end of the circuit modelled the lines just after the insulator stack and the transition to a fixed 1cm a-k gap spacing close to the convolute,
The longer section of line in each circuit modelled the main part of the radial lines, which have nearly uniform vacuum impedance due to a reducing a-k gap spacing with radius [12]. The electrical pulse generated in the Marx banks and water lines was modelled with the equivalent voltage shown in Figure 4.3; this was generated by matching a detailed transmission line circuit model of the entire accelerator to typical experimental electrical histories [16]. The impedance of this voltage source was set equal to the line that it was driving and was therefore perfectly transmissive to the component of the voltage wave travelling away from the simulation domain.

As described in section 3.5.1 of the previous chapter, the transmission line circuits were connected to the PIC simulation domain through transmission boundaries across the a-k gaps of the level A-D feeds. Here, the impedance of the circuit element connected...
to the PIC grid was set equal to the vacuum impedance of the radial line at this radius (14.4 cm). The boundary allowed for a single transverse electromagnetic (TEM) mode comprising the z-component of the electric field and the $\theta$-component of the magnetic field, where the wave was assumed to be uniform along the $\theta$-direction. This was necessitated by the 1D nature of the transmission lines used in the circuit model, where the spatial axis was taken along the radial coordinate. As discussed in chapter 1, $\mathbb{Z}$ is comprised of 36 identical modules which are individually switched. For the fast Z-pinch loads considered in this study, each module is simultaneously switched, so we would expect the EM wave from each module to reach the insulator stack simultaneously. In reality, the switching exhibits some jitter, but this is minimised by laser triggering to give timing differences of only a few nanoseconds [9]. We therefore expect the assumption of a uniform drive to be a good one. In the simulations, we found that the $r$- and $\theta$-components of the electric field were at least two orders of magnitude smaller than the z-component at the transmission boundary. Additionally, the z-component of the electric field was found to be uniform to within a few percent along the $\theta$-direction, at radial positions several centimetres away from the boundary. A situation where this assumption would break down, is for experiments which require pulse shaping, such as isentropic compression [8]. Here, shaping of the current pulse is achieved by non-simultaneous switching of the pulse forming modules. In this case, modelling only a fraction of the convolute would also be inaccurate.

As discussed in section 3.5.2, the wire array Z-pinch load was modelled as a conducting cylinder of total mass $m$, initial radius $r_0$, return can radius $r_{\text{return}}$ and length $l$ using the 0D implosion model [55]. As in the LSP simulations [16], we modelled a large diameter aluminium wire-array Z-pinch load with $r_0 = 2\text{cm}$, $l = 2\text{cm}$, $m = 4.09\text{mg}$ and $r_{\text{return}} = 2.4\text{cm}$, which was consistent with the voltage source shown in Figure 4.3. The minimum grid length and maximum magnetic field strength both occurred at the minimum feed radius of 2 cm, such that the Courant and cyclotron limits on the simulation time step were both determined by the inner MITL cathode radius; the cyclotron frequency is proportional to the magnetic field strength, where the peak field occurred at this minimum radius. As such, these large diameter loads were less stressing on the model than the compact arrays considered in [2], where $r_0 = 1\text{cm}$. Although the experimentally measured loss currents are typically larger for compact arrays, losses of up to
∼10% have been measured for large diameter arrays [2, 16, 17], such that current loss within the convolute is still a large effect for the loads considered in this study.

### 4.3 Electromagnetic Simulations

In order to test the circuit and load models discussed above and their coupling to the simulation grid, the convolute model was initially run without any macroparticles. Uniform grid cell sizes of 1mm were used along the r- and z-axes and $\pi/12/20$ radians along the $\theta$-axis. This spacing was chosen to give an arc-length of approximately 1mm at the position of the anode posts at a radius of 8cm. Note that these relative coarse spatial resolutions, which gave four cells across the smallest a-k gap in the inner MITL, were used for consistency with the cathode plasma simulations, which will be described below. The total domain dimensions were 14.4cm x $\pi/12$ radians x 16.8 cm. The initial time step was set to 50% of the Courant limit given in Eqn.(3.26) in section 3.4 of the previous chapter, where the smallest cell length was calculated at a minimum radius of 1.9cm. As discussed in section 3.4, below this radius the field solution transitioned to 2D cylindrical r-z coordinates to avoid prohibitively small time steps required for a stable solution.

The load radius and inductance as a function of time, as predicted by the 0D implosion model, are shown in Figure 4.4. Up to 60ns the load remained close to its initial radius, after which time the load imploded over 70ns and stagnated at a radius of 0.2cm, set by the user defined 10:1 convergence ratio.

The simulated convolute current and voltage as a function of time are plotted in
Figure 4.5. Note that we have adopted the nomenclature of [2], where we call the current measured at the position of the B-dot monitors located in the anode at the start of the inner MITL at a radius of approximately 6cm, the convolute current, as opposed to the load current, which will be reserved for the current at the actual load, which is typically not measured directly in experiment. The current measured within the radial lines is simply referred to as the MITL current. Note that both the convolute and MITL currents are measured in experiment.

The simulated convolute current peaked at approximately 19MA at 110ns, before dropping to 14MA due to the rapid increase in the load inductance over the final 20ns of the implosion, as shown in Figure 4.4. Although the magnitude of this current dip was consistent with experiment, the peak convolute voltage of 6MV, which was calculated from a line integral of the z-component of the electric field across the a-k gap at the start of the inner MITL at a radius of approximately 6cm, was approximately twice the experimentally inferred voltage [2].

As shown in Figure 4.4, the 0D model predicts that the load was constantly accelerating during the implosion. This is in contrast to wire array experiments on Z and other pulsed-power facilities, which have shown that the arrays implode with nearly constant velocity [56, 57]. It is the corresponding rapid increase in the OD load inductance that gave rise to the rapid increase in the simulated voltage ($\propto dL/dt$) between 110 and 130ns and the over prediction of the voltage at stagnation shown in Figure 4.5. The peak convolute voltage at stagnation, could be reduced by terminating the implosion at a smaller convergence ratio, however the magnitude of the current drop was then
similarly reduced.

The 0D model is used extensively in Z circuit modelling, as well as the published LSP [15,16] and Quicksilver [14,18] convolute simulations. As simulated voltage histories were not plotted, it is not clear whether similar discrepancies between the simulated and experimental voltages were also found in these PIC simulations; however, the LSP paper does state that the experimental voltages were reproduced in the text [15], but without the traces, it is not clear exactly what level of agreement was achieved.

Ultimately, we would like to couple our PIC convolute simulations to a detailed 3D MHD model of the wire array Z-pinch load. As discussed in section 2.6, in [2] and [3], an experimentally inferred convolute voltage was used to drive such a Z-pinch model through a transmission line circuit model of the inner MITL. In these studies both the current and voltage, as well as the implosion diagnostics such as the radiated X-ray power and radiography, were consistently matched for a range of Z shots [2, 3]. However, for simplicity whilst developing the convolute model and for consistency with published convolute simulation results [14–16,18], we have used the 0D load model in all the simulations discussed in this chapter. Assuming the electron emission is SCL, we expect to over predict the sheath current at the end of the implosion where the 0D model over predicts the line voltages [29]. This point will be considered further when we discuss the sheath and plasma simulation results below.

It is important to note that in order to reproduce the inductive drop in the convolute current, the PIC simulation had to be driven with a circuit model. Simulations using a fixed current source showed no drop in the current during the implosion, as the boundary was effectively infinitely resistive and could not transmit the back emf generated as the load imploded.

4.3.1 Magnetic and Electric Field Topology

As discussed in chapter 1 and 2, a defining feature of the Z DPHC operation are the regions of zero magnetic field, known as magnetic nulls, formed by the current addition path. Slices of the magnitude of the magnetic field at 0 (through the middle of the anode posts) and 15 (mid-way between the anode posts) degrees, taken from the simulation at 100ns are shown in Figure 4.6. The magnitude of the field, in Tesla, has been calculated.
Figure 4.6: Slices of the magnitude of the magnetic field strength in Tesla, plotted on a log scale taken through the anode posts at 0 degrees and between the anode posts at 15 degrees. The positions of the four magnetic nulls have been labelled.

at the cell corners where the staggered field components were spatially averaged to these positions. Additionally, the data has been plotted on a log scale in order to highlight the magnetic nulls. In total, four distinct nulls can be identified; in the 0 degree slice on the upstream side (right hand side, away from the load) of the top (1) and bottom (2) anode posts, in the 15 degree slice between the level B cathode and anode (3) and across the entire $\theta$-extent in the central axis region (4).

Equivalent plots of the $\theta$-component of the magnetic field at 0 and 15 degrees are shown in Figure 4.7. Here, it can be seen that the (1-3) nulls correspond to regions where the polarity of the magnetic field changes and are a unavoidable consequence of the way the current is added in the convolute. The central null (4) occurs as no bound current flows on the axis.

As shown in Figure 4.1, we included a conductive region with a radius of 2cm between the bottom of the inner MITL cathode and the lower simulation domain boundary, which was not present in the real convolute. This was included to act as a physical barrier to stop the macroparticles dropping below the minimum radius of 1.9cm used to set the Courant time step limit. To model the fact that this region was under vacuum in reality, it was given a finite, but small conductivity. The magnitude of this conductivity was chosen such that the skin depth was larger than the size of the region and the simulated
Figure 4.7: Slices of the $\theta$ component of the magnetic field in Tesla, taken through the anode posts at 0 degrees and between the anode posts at 15 degrees.

Figure 4.8: Slices of the electric field magnitude in Vm$^{-1}$ taken through the anode posts at 0 degrees and between the anode posts at 15 degrees at 100ns.

position of the central null was therefore not modified. Like the rest of the electrode, the thin conductor with a height of 2mm, along the bottom of the simulation domain, was assumed to be a perfect conductor and was included to both avoid open boundaries for the macroparticles and model the ground plate of the machine.

Slices of the simulated magnitude of the electric field in Vm$^{-1}$, at 0 and 15 degrees at 100ns are shown in Figure 4.8. Here, the magnitude of the field has been calculated at the cell corners by spatially averaging the staggered field components to these positions. The effect of the electrode stair stepping approximation is clearly visible in these plots. The electric field strength is enhanced at the corners of electrode cells at the edge of the cathode holes and along the level C and D conical feeds, with field strengths of between $1.5 \rightarrow 2$ times higher than in the lines. In the simulations including SCL electron emission or plasma injection from the cathode electrode, we found emission first
occurred in cells with a field enhancement. However, once the sheath or plasma was established, the cathode was shielded from the line electric field and the enhancements were less pronounced. Note that the electric field was zero in cells bounded by two or more electrode surfaces as the field components parallel to the electrode surface were set to zero, assuming perfect conduction.

4.4 Cathode Plasma Creation Model

As described in section 3.9.3, we used a phenomenological model similar to those employed in the LSP [16] and Quicksilver [18] convolute simulations, to model the formation of a fully ionised Hydrogen plasma on the cathode electrode surfaces. As discussed in chapter 2, physically, the plasma is formed via ionisation of neutral contaminants that are desorbed from the electrode surface, where the cathode plasma is comprised of a partially ionised source layer next to the electrode and a fully ionised plasma which expands into the a-k gap. Using the expressions from the Shefer [27] model described in section 2.2.1, for typical line parameters in Z, the thickness of the source layer at the end of the current pulse was estimated to be $\sim 10\mu m$, which is much smaller than the simulation grid length. As such, we did not model the neutral layer explicitly. Instead, we injected a fully ionised plasma into the first vacuum cell next the electrode by loading pairs of electron and proton macroparticles at a defined desorption rate with randomised positions.

As discussed in section 2.2 of chapter 2, Z is estimated to have up to 100 monolayers of neutral contaminants absorbed on its electrode surfaces, included Hydrogen, Carbon and Oxygen. We have focussed solely on Hydrogen as it is both the most abundant element in the inventory and the least massive, so therefore most mobile. In addition, as discussed in chapter 2, recent optical spectroscopic measurements of the downstream a-k gaps of the ZR anode posts have observed a predominantly Hydrogen plasma expanding from the cathode into the gap [17, 59]. As will be discussed below, relatively low plasma desorption rates were required to match the experimental level of current loss [16]; as such we did not expect to deplete the neutral contaminant inventory during the current pulse. We therefore allowed plasma creation throughout the whole of the simulated current pulse.
To maintain charge conservation and avoid the formation of unphysical electric fields in the plasma source cells, we found it necessary to create the electron and ion macroparticles of each pair at the same spatial position, with equal weights (but opposite charges) and equal velocities. As discussed in section 3.9.3 in the previous chapter, the magnitude of the initial velocity was set by randomly sampling a Maxwell-Boltzmann distribution at a specified temperature using the Box-Muller scheme [93]. In our baseline simulations, a temperature of $T = 3$eV was used, consistent with typical cathode plasma measurements [16, 17, 21, 27]. In practice, it was the ion velocity distribution that was sampled and the electron macroparticles loaded at this velocity. As such, the electrons were loaded with an effectively lower temperature of $(m_e/m_i) T \sim 1.8 \times 10^{-3}$eV, where $m_e$ and $m_i$ are the electron and proton masses. In practice, we found that the electron population was quickly heated up to the ion temperature, $T$; as will be discussed below, we believe that this was mainly due to numerical heating, as the electron-ion collisional energy exchange rate was relatively long for the convolute plasma parameters.

At the plasma-vacuum interface, the plasma acts as a zero work function surface from which a SCL electron current is injected into the vacuum [27]. To model this emission process at early times, when the plasma had not yet fully established, SCL electron emission was allowed directly from the cathode electrode once the strength of the normal component of the electric field had exceeded the electrode breakdown threshold of $240\text{KVcm}^{-1}$ [16]. In the Quicksilver model, plasma injection was delayed until several nanoseconds after SCL electron emission had started. This was done with the goal of reducing the normal component of the electric field and avoiding an initial excessive loss of plasma ions to the cathode electrode and therefore to allow the plasma to become established [18]. This is in contrast to the LSP model, where we believe that the plasma creation began at the same time as SCL emission [16]. In our baseline simulations, plasma injection began at the same time as SCL electron emission. However, as will be discussed below, in order to match the early time measured current loss, a delay in the plasma creation had to be introduced. In order for the plasma to establish, it was found necessary to load the electron and ion macroparticle pairs throughout the first vacuum cell with initial positions chosen at random heights above the emission surface; with randomised velocities, the particles subsequently filled the cell. By loading plasma across the length of the entire first vacuum cell we effectively assumed that the
plasma had had time to expand and fill this volume. In experiment, cathode plasmas have been measured with expansion velocities between 1 and 10cmµs⁻¹ [16, 17, 27]. At the spatial resolution of our simulations, a plasma expanding at 3cmµs⁻¹, would take 33 ns to cross the 1mm cell, which is a significant fraction of the 100ns pulse length. This was the physical justification used for the plasma creation delay model that will be considered further in section 4.9.

In the cathode plasma model presented in [27], which was reviewed in section 2.2.1 of chapter 2, an electron current was drawn from the plasma surface, \( J_{e0} \), given approximately by the Child-Langmuir expression, Eqn.(4.1), where \( V \) is the gap potential, \( d \) the gap spacing and \( m \) and \( Z \) are the emission particle mass and charge [23].

\[
J_{CL} = \frac{4e_0}{9} \sqrt{\frac{2Ze}{m} \frac{V^{3/2}}{d^2}} \quad (4.1)
\]

In steady state, this current is returned to the cathode by the ions through a thin sheath region \( 0 < x < x_n \). Assuming that the temperature in the sheath is given by the potential drop, \( V_n \), the sheath thickness, \( x_n \) can be estimated from the effective Debye length, Eqn.(4.2) [94].

\[
x_n = \left( \frac{e_0V_n}{n_ee} \right)^{1/2} \quad (4.2)
\]

The ion current follows the Child-Langmuir expression as in Eqn.(4.3), where \( d = x_n \) was substituted into Eqn.(4.1) with \( m = m_i \) and we are assuming \( Z = 1 \) [94].

\[
J_i = J_{e0} = \frac{4}{9} \sqrt{\frac{2}{m_i} e^{3/2} n_e V_n^{1/2}} \quad (4.3)
\]

We estimated the sheath potential, \( V_n \), expected in the convolute from Eqn.(4.3) by substituting typical values for \( V \) and \( d \) in Eqn.(4.1), with \( m = m_e \) to give \( J_{e0} \) and rearranging. At early times in the current discharge \( V_n \sim 0.5kV \), which from Eqn.(4.2) gives a corresponding sheath thickness of \( x_n \sim 5\mu m \). As \( x_n \ll \Delta x \) in the simulations at these times, we found that the ion macroparticles could not provide all of the return current. Following [94], to avoid the formation of an unphysical sheath between the plasma and cathode electrode, this deficit was supplemented by allowing SCL electron emission from the electrode surface in the plasma injection cells after plasma creation had begun. Here, the magnitude of the potential drop in the cell next to the electrode
had to increase in order to supply this electron current; this can be estimated from
Eqn.(4.1) with $d = \Delta x$ and $m = m_e$ and gave $\sim 50$ kV for the convolute parameters.
This was approximately one hundred times larger than the potential estimate for the
case where the ions alone returned the plasma current. An issue highlighted in [94],
was therefore excessive heating of the plasma electrons through the thermalisation of
energy gained from acceleration through this larger potential. This could be mitigated
by improving the spatial resolution to resolve $x_n$ [94]; however, in practice we found that
although the electron macroparticles were heated, their temperature did not significantly
exceed that of the ions. At later times in the convolute current discharge, the electron
current drawn from the plasma had increased such that the estimates for $V_n$ and $x_n$ had
also increased and the sheath was therefore better resolved by the simulation grid.

In the simulations presented below, the plasma was injected at a constant rate in all
emission cells for all time. However, there is experimental and theoretical evidence that
the cathode plasma creation rate is in fact dependent on the plasma current [27,98]. We
included such a current dependent injection rate, using a scheme inspired by the Shefer
model [27] which was reviewed in chapter 2. To source the plasma, a target electron
density was calculated from Eqn.(2.12), in section 2.2 of chapter 2, taken from the
numerical model used in [27]. This function was dependent on the normal component of
the macroparticle current at the electrode surface (the interpolated grid current in the
simulation) and an electron impact ionisation cross-section. The latter was taken from
the free online NIST database [95] and integrated over a Maxwellian velocity distribution
to give $\langle \sigma v \rangle_i$. The target density calculated from Eqn.(2.12), was then compared to the
number density at the electrode surface in the simulation and any positive difference
was added by creating pairs of electron and ion macroparticles, as in the standard
creation model. However, we found that this model gave unsatisfactory results; due
to positive feedback from the plasma current, the effective desorption rate typically
exceeded 1 mlns$^{-1}$. This rate was $\sim 130$ times higher than the fixed desorption rate
used in the baseline simulations. As such, the plasma density peaked at $10^{18}$ cm$^{-3}$
with a simulated current loss significantly larger than experiment. This high effective
desorption rate could be reduced by using a time average of the particle current in
Eqn.(2.12), however this was not sufficient to mitigate the over prediction of the current
loss. In the baseline simulations, we therefore followed the method of [16] and used a
fixed desorption rate which was tuned to match the experimental current loss. Note that the Quicksilver simulations used a different method; the plasma injection rate was varied to maintain a specified target density in the first vacuum cell next to the electrode. This was done mainly to control the peak density and therefore electron plasma frequency used to set the simulation time step [18].

To accurately capture the Z post-hole electrode geometry, the convolute must be simulated in 3D. We expect plasma to be formed on both the convolute and inner MITL cathode electrodes and ideally would have modelled plasma formation in both of these regions simultaneously. However, with practical spatial grid resolutions in the convolute, the inner MITL was relatively poorly resolved, with as little as four computational cells across the smallest a-k gap. Simulations where particles were sourced within the inner MITL showed large oscillations in the load voltage and perturbed the fields in the convolute. We therefore did not source charged particles below a radius of 5cm within the inner MITL. The inner MITL electrode is axially symmetric, so assuming the voltage wave from the convolute is similarly symmetric, the inner MITL was well approximated by 2D r-z cylindrical coordinates. We therefore carried out separate, higher resolution 2D simulations of the inner MITL, which will be described in section 4.14.2.

In the LSP simulations [15], the cathode plasma appeared to be sourced only on the inner edges of the cathode holes. In our simulations, plasma was sourced over the entire cathode electrode between \( r =5 \) and 12.5cm, which included part of the radial lines and the central null. This seemed consistent, as the electric field strength was found to exceeded the electrode breakdown threshold of 240kVcm\(^{-1}\) over the entire emission region.

### 4.4.1 SCL Ion Emission

The anode plasma formed via ionisation of neutral contaminants desorbed from the electrode by a combination of stimulated and thermal desorption driven by electron bombardment [21], was not modelled explicitly. Instead, the anode plasma expansion velocity was assumed to be small, such that it remained tightly bound to the anode electrode for the duration of the current pulse. As the anode plasma expansion is driven by the plasma ions, it will typically evolve on a slower time scale, compared to the
cathode plasma. As such, this seemed a valid assumption. It was also assumed, that the plasma was dense enough to provide a SCL current of protons. As such, SCL proton emission was allowed directly from the anode electrode once the electrode surface had been heated above a threshold of 700K by electrons emitted from the cathode plasma impacting the anode [15, 16]. As discussed in chapter 2, this is the threshold for the formation of the plasma via ionisation of thermally desorbed neutral contaminants, which at this temperature dominates the stimulated process [16, 21].

4.5 Time step, cell size and population control

As discussed in section 3.1.2, the shortest time scale in the convolute simulations was set by the electron cyclotron frequency, $\omega_{ce}$, where to accurately model the gyro-orbits and drift motions, the time step needed to enforce $\omega_{ce}\Delta t < 2$. At peak current this time step was approximately ten times smaller than the Courant limit. In order for the simulations to be tractable, the time step was allowed to vary dynamically. The time step was initially set to $\Delta t_{init} = 0.5\Delta t_{Courant}$. At the beginning of each cycle, the maximum electron macroparticle cyclotron frequency was found and used to compute a minimum cyclotron time step according to $\Delta t_c = 1.9/\omega_{ce,max}$. To maintain second order accuracy in the field solution and particle push, each time the global time step was reduced, the magnetic field and particle velocities were re-centred in time accordingly. To avoid carrying out this correction at the start of every cycle, the simulation time step was set to integer divisions of the initial time step, $\Delta t = \Delta t_{init}/N$, where $N = ceiling(\Delta t/\Delta t_c)$ and $ceiling(f)$ returned the largest integer of the floating point variable $f$. The global time step was then only decreased when $N$ increased by one from the previous cycle.

As discussed in the previous section, due to the poor spatial resolution, no particle creation was allowed within the inner MITL. As such, the simulated plasma density remained relatively low for the majority of the simulation, below a radius of 5cm. We found that the macroparticle push could be safely sub-cycled for particles within this radius, which significantly reduced the overall run time, as the highest magnetic field strengths and therefore electron cyclotron frequencies occurred within the inner MITL. At later times, the plasma density below 5cm was seen to increase as plasma created in the convolute was transported into the inner MITL; at this point in the simulation the
particle push sub-cycling was terminated to avoid excessive numerical electron heating and macroparticles at all radii were included in the global time step calculation.

To avoid creating many small weight macroparticles which had little effect on the simulation, the plasma and SCL creation algorithms were called approximately every ten time steps and enforced a minimum macroparticle weight. This threshold was resolution dependent and set to $10^{-12}$C in the baseline convolute simulations; if the charge to be created was less than this threshold, then no new particles were created in the cell at this time.

In the convolute simulations, the particle number density ranged between $\sim 10^{12}$ cm$^{-3}$ in the sheath and $>10^{15}$ cm$^{-3}$ in the densest plasma regions. As the sheath was formed from particles emitted by the plasma, in order to maintain good particle statistics in the sheath, the plasma macroparticles had to be loaded with relatively small weights. This is a common issue for PIC simulations of particle distributions with large density gradients [62, 63]. In order to maintain good particle statistics i.e. at least 40 particles per cell, a maximum macroparticle charge was enforced. This was again resolution dependent and set to $10^{-11}$C for the baseline convolute simulations; if the charge to be created was larger than this threshold, then it was split between a number of macroparticles with this maximum weight. With these population control measures, the total number of macroparticles in the plasma simulations peaked at approximately 15 million.

The spatial resolution used in the plasma simulations was driven by the desire to maintain good particle statistics. To achieve the same number of macroparticles per cell at higher spatial resolutions, the total number of macroparticles must be increased. For example, if we halved the cell size along each axis, the cell volume would be reduced by a factor of eight in 3D and the average particle weight should be reduced by the same amount, increasing the total number of particles by eight times. We found that it was not practical to track this number of macroparticles whilst resolving the electron cyclotron frequency, with the available computing resource; as such we compromised with a coarser spatial mesh.

The LSP simulations employed a charge and energy conserving macroparticle coalescence algorithm that was described in section 3.13 of the previous chapter, in order to control the number of particles per cell in the plasma regions [16]. This algorithm depends on a linear interpolation scheme and as such could not be used in our simula-
tions which employed second order quadratic spline interpolation [97]. In any case, as discussed in this section, we had limited success applying this algorithm to our convolute simulations using linear interpolation.

4.6 Simulated Current Loss

As discussed in section 4.4, the plasma desorption rate and initial temperature were free parameters in the cathode plasma creation model. Our baseline simulations used a desorption rate of $0.0075 \text{mln s}^{-1}$ and an initial temperature of $3 \text{eV}$ to set the velocities of the pairs of electron and ion macroparticles. For these parameters, the simulated MITL and convolute currents are plotted as a function of time in Figure 4.9 (solid lines); the MITL current was calculated by summing the currents upstream (away from the load) of the convolute in the four level radial disk feed at a common radius of 70 cm (consistent with the location of the real B-dots) [2]. Note that this position was within the transmission line circuit model. Here, the current was calculated from the forward, $V_1$, and backward, $V_2$, travelling components of the voltage wave according to $I = (V_1 - V_2) / Z$, where $Z$ was the impedance of the transmission line element [20]. To allow direct comparison, the MITL current was translated in time to account for the delay introduced by the EM wave propagating between the positions of the MITL and convolute current measurements.

The simulated current loss, calculated as the difference between the MITL and convolute current, is also plotted in Figure 4.9 (solid line); this peaked at $\sim 2 \text{MA}$, or $\sim 10\%$ of the MITL current at peak current (120 ns) and was consistent with peak experimental losses measured in large diameter wire array experiments on Z [2, 16]. The predicted current loss above $\sim 10 \text{MA}$ was consistent with the equivalent LSP simulations [16]. However, at earlier times ($<10 \text{MA}$) our results predicted a loss of up to 1 MA, which was larger than both the LSP result [16] and typical experimental measurements [2, 17]. For example, consider the experimental current traces plotted in Figure 1.3 in chapter 1. Here we see that the loss is actually reducing up to 12 MA, before increasing to its peak at peak current. Although this result was for a compact wire array Z-pinch load, it is typical of wire array experiments on Z [2, 16, 17]. As discussed in section 2.6.1 of chapter 2, in [2], the initial current loss was attributed to an electron flow current loss,
which reduced as the current increased, due to improving magnetic insulation in the radial lines, whilst the loss at peak current was parameterised by an electrode plasma expansion [2]. Similarly, the LSP current loss prediction, which was estimated by comparing the simulated convolute currents for cases with a cathode plasma and where only SCL electron emission from the cathode was allowed, showed that the loss including the cathode plasma was almost identical to the electron flow current loss only results below ∼10MA [16].

Simulations of the convolute including only SCL electron emission directly from the cathode electrode will be discussed in section 4.6.2, in terms of understanding the current loss mechanism. The MITL, convolute and current loss (difference) from this simulation (dashed lines) are compared to the case with cathode plasma injection in Figure 4.9. Firstly, we note that the MITL current is larger in the plasma simulation, peaking at ∼20.5MA compared to ∼19.5MA in the SCL emission case; this was due to the lower current delivered to the 0D load in the plasma case delaying the implosion. Considering the convolute currents, up to 35ns, corresponding to a time when the cathode plasma had yet to be fully established, they agreed well. However, after this time, the convolute current in the plasma case was lower, predicting a higher current loss. As will be
discussed in section 4.6.2, after \( \sim 45\text{ns} \) the MITL and convolute currents in the SCL emission only case converged. This behaviour was consistent with the early time LSP [16] and Quicksilver [14] results and experiment [2], suggesting that the loss was due to an electron flow current loss at this time. However, in Figure 4.9, we see that the SCL emission does not reproduce the 10% current loss at peak current, which was achieved in the simulation including a cathode plasma explicitly. As such, the experimental result was bounded by our cathode plasma and SCL emission only simulations.

Considering that our SCL emission only result was closer to that expected from experiment [2] and the LSP [16] prediction, the early time current loss in the plasma simulation could be reduced by delaying the start of the cathode plasma injection relative to SCL electron emission. This will be investigated in section 4.9, where the delay was justified by considering the finite plasma expansion velocity into the source cell. In unpublished Quicksilver plasma simulations of the DPHC [58], a similarly high level of current loss (\( \sim 1\text{MA} \)) at early times in the current pulse, was found. These simulations used the same energy conserving quadratic spline interpolation scheme [18, 68], as was used in our simulations. In contrast, the LSP simulations used a 'Cloud-in-Cell' interpolation scheme; although the effective particle size covers two computational cells, the weighting function is first order [16, 94]. As such, the sensitivity of the early time current loss to the order of the electric field interpolation will also be considered in section 4.10.

The simulated convolute voltages with and without cathode plasma injection are compared in Figure 4.10. With plasma, the peaks in the simulated voltage at 50 and 90\text{ns} are approximately 10\% lower, consistent with a delayed implosion due to the slower

Figure 4.10: A comparison of the simulated convolute voltages with and without particles.
rise of the load current. The voltage from the SCL emission only simulations was close
to the result with no particles; this delayed implosion and lower voltage was responsible
for the higher peak MITL current found in the plasma simulation and shown in Figure
4.9. Similarly, the rate of voltage increase during the load implosion after 100ns was
reduced, peaking at approximately 2.2 compared to 3MV at 120ns. After 120ns, the
voltage in the plasma simulations was seen to oscillate by approximately ±20%. These
oscillations were linked to the electron macroparticle dynamics during the rapid increase
in the line voltage during the implosion and could be damped by further refining the
simulation time step, significantly increasing the simulation run time through the final
part of the implosion and stagnation. As such, our results have been terminated at
120ns; this is a limitation of the model as accurate prediction of the current during
and after stagnation, is required to accurately reproduce the energetics of the X-ray
emission [2, 3]. For example, in [3] it was predicted that approximately 50% of the
radiated energy was sourced from the local inductance at stagnation.

### 4.6.1 Current Loss Mechanism

The baseline simulation proceeded as follows: SCL electron emission and plasma creation
was established across the entire cathode emission region by 20ns. By 40ns a plasma of
density $\sim 10^{15}\text{cm}^{-3}$ had established on the cathode surface as shown in slices of the ion,
Figure 4.11, and electron, Figure 4.12, densities taken at 0 (through the anode posts)
and 15 degrees (between the anode posts). Here, the particle number densities are in
Figure 4.12: Slices of the simulated electron density in m$^{-3}$ on a logarithmic scale, taken at 0 (through the anode posts) and 15 (between the anode posts) degrees at 40ns.

Figure 4.13: Slices of the magnitude of the electric field strength in Vm$^{-1}$, at 0 (through the anode posts) and 15 (between the anode posts) degrees at 40ns.

units of m$^{-3}$, plotted on a logarithmic scale. Note that these units will be maintained throughout the remainder of this chapter.

Electrons emitted from the surface of the plasma formed a lower density, $\sim 10^{12}$ cm$^{-3}$, sheath which extended across the a-k gap. The magnitude of the electric field at this time is plotted in Figure 4.13. Comparing this to the case with no particles, Figure 4.8, we found that including particles, the effective position of the cathode moved towards the anode electrode; this was consistent with the position of the centroid of the electron sheath charge density, as predicted from the MITL theory outlined in section 2.3 of chapter 2. In line with this effective reduction of the a-k gap, the electric field strength was increased by several times.

Slices of the magnetic field strength at 40ns are plotted on a log scale in Figure 4.14:
Figure 4.14: Slices of the magnitude of the magnetic field strength in Tesla, plotted on a logarithmic scale at 0 (through the anode posts) and 15 (between the anode posts) degrees at 40ns.

the topology is identical to the case with no particles, Figure 4.6, where the difference in magnitude is due to the higher current at the later time of 100ns. As shown in Figure 4.11, in the radial lines at radii above 10cm, the Larmor radii of the electrons was smaller than the a-k gap, such that the magnetic field strength was sufficient to insulate the electrons in the sheath; the trajectories here consisted of a counter-clockwise Larmor orbit about the predominantly minus $\theta$-directed magnetic field and an $\vec{E} \times \vec{B}$ drift in the direction of power flow towards the load, associated with the electric field of the line. Considering the slice of the electron density at 0 degrees in Figure 4.12, at the positions of the (1) and (2) magnetic nulls, the magnetic insulation was lost such that the electrons in the sheath could cross the a-k gap and impact the upstream sides of the anode posts, shunting current from the inner MITL and load. Similarly, as can be seen in the 15 degree slice, Figure 4.12, insulation was lost at the positions of the (3) and central (4) magnetic nulls. Further losses of electrons to the anode electrode were observed on the downstream sides (left hand side, towards the load) of the anode posts. Here, the electron sheath was comprised of electrons emitted from the cathode plasma at radii below 6cm, as well as electrons emitted upstream which had been transported around the anode posts by their drift motions.

Slices of the electron density taken at the later time of 100ns are shown in Figure 4.15. Here we see the plasma evolution on the downstream side of the anode posts, the details of which will be discussed below. Focussing on the electron sheath, we found similar structure to the slices taken at 40ns; specifically, the magnetic insulation of the
sheath in the radial lines was lost at the magnetic nulls and on the downstream side of the posts, in the convolute. As such, the electron sheath continued to shunt current away from the inner MITL and load, throughout the current pulse via a loss of electrons to the anode at the locations described above.

A diagnostic of this electron deposition on the anode was given by the anode surface temperature, shown in Figure 4.16, where the upstream (left) and downstream (right) sides of the anode posts are shown. As described in section 3.9.2 of the previous chapter, the anode temperature increase was a function of the impacting electron kinetic energy, angle of incidence and material specific heat capacity. Note that the stainless steel anode was initialised at approximately room temperature (300K). The temperature increase due to deposition on the upstream side of the anode posts was consistent with the positions of the (1) and (2) magnetic nulls. Similarly the deposition on the level B anode was consistent with the position of the (3) magnetic null. On the downstream side of the posts, an equivalent temperature rise was found at the height of the (1) and (2) magnetic nulls. A smaller, but significant (>400K) temperature rise was also found on the level D anode where the bottom post is attached, consistent with the central (4) magnetic null.

The loss of electrons from the sheath to the convolute anode electrode shunted current away from the inner MITL and accounted for the simulated current loss shown in the current histories in Figure 4.9. Note that the regions of maximum anode heating shown in Figure 4.16, were consistent with the locations of post shot physical damage.
Figure 4.16: Anode surface temperature in Kelvin, looking at the up-stream (left) and downstream (right) sides of the posts.

observed on the convolute hardware [16].

4.6.2 SCL Electron Emission Simulations

A comparison of the simulations including cathode plasma, with simulations where only SCL electron emission was allowed from the cathode electrode, aided in understanding the role of the cathode plasma in the current loss. These simulations used the same spatial mesh and time step management as discussed in section 4.5. Note that here we were assuming that plasma was formed on the cathode electrode surface that was dense enough to supply a SCL electron current, but that its expansion was slow, such that it remained tightly bound to the cathode electrode for the duration of the current pulse. As such, SCL electron emission was allowed directly from the cathode once the normal component of the electric field exceeded a strength of 240kVcm\(^{-1}\), which is the expected threshold for cathode plasma formation [21]. This is the same approximation that was made in the Quicksilver [14, 18] and LSP [16] electron flow current loss simulations, which were reviewed in section 2.6.2 of chapter 2. Note that this assumption of negligible plasma expansion is also used extensively within the pulsed power community to model a range of diode and MITL systems.

A comparison of the MITL and convolute currents for the SCL electron emission only simulation has already been shown as the dashed curves in Figure 4.9. Here, there was an early time current loss occurring between 25 and 45ns. However, between 45
and 95ns the current loss was negligible, before increasing up to its peak value of just under 0.5MA at peak current. Overall, the level of current loss was significantly lower than was found in the plasma simulations, as was discussed in section 4.6. Note that in these simulations, the MITL current peaks at 19 compared to 21MA in the plasma simulations, as the faster increase in the load current lead to an earlier implosion.

Slices of the electron density at 80ns are shown in Figure 4.17. Here we see that the electron sheath structure was similar to the plasma case; specifically, an unstable electron sheath was formed, which was magnetically insulated in the radial lines, but the insulation was lost at the positions of the magnetic nulls and electrons were lost to the anode at the nulls and on the downstream sides of the posts, shunting current away from the inner MITL; this was the mechanism for the early and late time current loss shown in the current histories in Figure 4.9 (dashed lines).

A comparison of the electron flow currents measured upstream (r=10cm) and downstream (r=5cm) of the convolute taken from the SCL electron emission simulation is shown in Figure 4.18. Here, the electron flow current was calculated from the difference between the bound anode and cathode currents, $I_e = I_a - I_c$, where the bound current was calculated from a line integral of the $\theta$-component of the magnetic field at the centre of the first vacuum cell next to the electrode, as discussed in section 3.11 of the previous chapter. The upstream curve is the sum of the currents in the level A-D radial lines and therefore equals the total electron flow current entering the convolute. Note that
for clarity both curves have been smoothed by temporally averaging over 2ns; due to an instability in the electron sheath which will be discussed in section 4.8, electron vortices were formed that resulted in approximately 50% oscillations in the electron current as they passed through the fixed current diagnostic planes. This level of oscillation was consistent with LSP [31] and Quicksilver [13] simulations of the electron sheath in the Z radial lines.

In Figure 4.18, we found a peak in the electron flow current at 35ns of 400kA, consistent with the early time current loss seen in Figure 4.9 (dashed lines). At this time, the downstream electron current was approximately 10kA, from which we can conclude that the majority of the electron current entering the convolute was subsequently lost within the convolute through electron losses to the anode electrode at the magnetic nulls and on the downstream side of the posts.

After 40ns, the upstream electron current reduced, consistent with the increasing bound current and therefore magnetic field in the radial lines, improving the magnetic insulation and re-trapping current in the cathode; this mechanism was discussed in section 2.5 of chapter 2. Up to 80ns, the lines operated in the strongly insulated limit ($I_a >> I_e$). As such, between 40 and 80ns, even though the majority of the electron flow current entering the convolute was still being lost, the current loss between these times, shown in Figure 4.9 (dashed lines), was reduced as the electron flow current entering the convolute was smaller. This result was consistent with the coupled circuit and MHD load simulation results and measured current losses, presented in [2].

Between 80 and 120ns the upstream electron flow current entering the convolute,
increased to its peak of just under 1MA, consistent with the increase in the current loss shown in Figure 4.9 (dashed lines). This increase, was due to the increasing line voltage, Figure 4.10, as the load imploded; considering the strongly insulated limit, $I_e << I_a$ of the Mendel pressure balance theory [29] discussed in section 2.4.3 of chapter 2, it can be shown that the electron flow current scales with the square of the line voltage, $I_e(r) \sim V^2 r^2 / I_a d(r)^2$ [31]. The increasing voltage was also responsible for the increase in the downstream electron flow current at these times, due to enhanced emission from the downstream cathode.

A diagnostic of the relative contributions of the electron flow current losses to the total current loss, was given by the electron charge deposition rate on the anode electrode. This was binned over the upstream and downstream sides of the top and bottom anode posts and is plotted in Figure 4.19. As can be seen, the traces are consistent with the early and late time losses shown in Figure 4.9 (dashed lines), as well as the electron flow current measurements in Figure 4.18. The early time loss between 20 and 50ns, was dominated by electrons lost to the bottom anode post, where the peak loss on the upstream was approximately twice that on the downstream side of the post; the upstream loss was due to electrons crossing the a-k gap at the position of the (2) magnetic null, whilst the downstream loss was due to a combination of electrons emitted upstream being transported around the anode post by their drift motions and electrons emitted from the downstream cathode. After 40ns, there was a reduction in the charge deposition rate, consistent with the reduced electron flow current entering the convolute as shown in Figure 4.18. After 80ns, the charge deposition rate began to rise to its peak at the end of the simulation. This late time loss was dominated by electron deposition on the downstream side of the top anode post and was consistent with the enhanced electron flow current from the cathode electrode on the downstream side of the anode posts due to the increasing line voltage as the load imploded.

As in the cathode plasma simulations, SCL proton emission from the anode electrode was also allowed where the anode temperature exceeded 700K, due to heating by electron bombardment. The anode temperature profile was qualitatively similar to the plasma simulation result, shown in Figure 4.16, but both the magnitude and spatial extent were smaller, consistent with the reduced level of electron deposition in the anode. However, Figure 4.16 is sufficient to infer the locations from which SCL proton emission occurred.
The proton Larmor radii were typically comparable to, or larger than, the a-k gap and as such, the anode protons were found to propagate across the a-k gap and impact the cathode electrode. The presence of the positive space charge at the cathode emission surface acted to enhance the SCL electron current drawn from the cathode [12, 14, 16]. The convolute current differed by a $\sim 2\%$ in simulations where the SCL proton emission was turned off. Physically, ions impacting the cathode electrode can lead to stimulated desorption of electrons [94]. This mechanism has been found to enhance the electron flow current in certain MITL systems, but was not included in our simulations as the protons only impacted the cathode at locations where the electron emission was already SCL.

From the SCL emission only results in Figure 4.9, we see that including only SCL electron and proton emission in the simulations, was not sufficient to reproduce the experimentally observed level of current loss around peak current. As discussed in section 2.6 of chapter 2, this result was consistent with equivalent LSP [16] and Quicksilver [14, 18] simulations, as well as results from circuit models including only the electron flow current loss [2, 52, 53]. It should be noted that in our simulations, emission was only allowed within a radius of 12.5cm. In reality, electron emission is expected to occur within a radius of 1.3m in the radial lines [13, 31]; as such there is the possibility that our simulations under predicted the electron current entering the convolute and therefore the magnitude of the current loss. However, as described in section 2.6.2 of chapter 2, including a more realistic prediction of the electron flow current entering the convolute.
from the radial lines in the Quicksilver simulations, was not sufficient to match the measured current loss at peak current with only SCL electron emission from the cathode electrode [14,18].

Considering that our simulations including a cathode plasma reproduced the measured current loss at peak current as shown in Figure 4.9, this suggests that the plasma evolution in the convolute is responsible for the measured current loss at this time. This conclusion is consistent with the LSP simulation results [15,16], as well the coupled circuit-MHD simulations [2]. Although in the latter the late time current loss was parameterised by plasma from the anode shorting the a-k gap at the position of one of the magnetic nulls, the conclusion that including the dynamics of the electrode plasma was required to match the measured current loss at peak current, is consistent. The role of the cathode plasma dynamics, in the simulated current loss, will be discussed in the next section.

4.7 Role of the Cathode Plasma in the Current Loss

A plot of the electron charge loss rate to the anode electrode, for the simulation including a cathode plasma, is shown in Figure 4.20; here, the same binning of the anode posts was used as in the SCL emission only simulation. Overall, the charge loss rate was higher in the plasma simulation, consistent with the higher current loss compared to the SCL emission case, as shown in Figure 4.9. The relative contributions of the various regions to the total loss rate were also different.

Considering the electron loss to the top anode post, between 25 and 60ns the loss rate showed similar behaviour to the SCL emission simulations; specifically, a rise to an early time peak followed by a drop, consistent with improving magnetic insulation in the upstream electron sheath in the level A and B radial lines reducing the electron flow current entering the top part of the convolute. However, the relative magnitudes of the upstream and downstream losses were reversed, with the peak in the downstream loss around three times the upstream value. After 60ns, both loss rates to the upstream and downstream sides of the top anode post remained relatively constant up to peak current.
Now focussing on the electron loss to the bottom anode post, we found that the charge deposition on the downstream side was dominant after 45ns. In fact, this represented the largest fraction of the overall loss rate, peaking between 60 and 85ns and was several times higher than the loss rate to the top post for the majority of the current pulse.

A clear feature of the SCL emission results, Figure 4.19, was the increasing loss rate at late time; this was related to the increase in the electron flow current, due to the increasing line voltage during the load implosion. Due to the slower current rise time in the baseline plasma simulation, the load imploded later such that the line voltage at 120ns was lower as shown Figure 4.10; the SCL emission result was closer to that of the simulation with no particles. The baseline plasma simulation was terminated during the implosion, such that the line voltage would continue to increase if the simulation was continued. Consistent with the late time behaviour of the SCL emission simulations, we would therefore expect the electron flow current and subsequently current loss within the convolute, to continue increasing with the increasing line voltage during the implosion and up to stagnation.
4.7.1 Plasma Evolution and Dynamics

As shown in Figure 4.11, by 40ns in the baseline simulation, a plasma of density $\sim 10^{15}\text{cm}^{-3}$ had established across the entire cathode emission region. The higher current loss found in the plasma compared to the SCL emission simulations was a result of this cathode plasma penetrating the post-hole gaps within the convolute, reducing the effective a-k gap and subsequently increasing the level of electron loss to the anode posts. This penetration is shown clearly in slices of the ion density taken at the later times of 70 and 90ns, Figure 4.21 and Figure 4.22, respectively. Here we see the plasma on the inner edge of the cathode on the upstream side of the top post had penetrated into the (1) magnetic null. Similarly, plasma had penetrated into the post-hole gaps on the downstream side of the anode posts; this was especially true on the downstream side of the bottom post.

At 90ns, the edge of the plasma at a density of approximately $5\times10^{13}\text{cm}^{-3}$, was acting as a zero-work function SCL electron emission surface, such that the cathode had effectively moved closer to the anode electrode. On the downstream sides of the anode posts, the plasma penetration had reduced the effective a-k gap from 1cm to $\sim 2\text{mm}$. This is clearly shown in slices of the electric field strength at this time plotted in Figure 4.23. Comparing this plot with the ion density, Figure 4.22, on the downstream side of the posts the cathode plasma within the region defined by a density of $\sim 5\times10^{13}\text{cm}^{-3}$, shielded the cathode electrode from the line electric field.

Figure 4.21: Slices of the simulated ion density in units of m$^{-3}$ on a logarithmic scale, taken at 0 (through the anode posts) and 15 (between the anode posts) degrees at 70ns.
Figure 4.22: Slices of the simulated ion density in units of m$^{-3}$ on a logarithmic scale, taken at 0 (through the anode posts) and 15 (between the anode posts) degrees at 90ns.

Figure 4.23: Slices of the simulated magnitude of the electric field strength in units of Vm$^{-1}$, taken at 0 (through the anode posts) and 15 (between the anode posts) degrees at 90ns.

As discussed in the previous section, the electron loss rate was highest on the downstream side of the bottom anode post in the plasma simulation. This was consistent with the evolution of the plasma described above, where the effective a-k gap was reduced by the plasma penetrating the a-k gap, enhancing the number of electrons that could cross from the plasma to the anode post here. Slices of the electron density at 90ns from the baseline plasma and SCL electron emission only simulations are compared in Figure 4.24. On the downstream side of the anode posts, we found that the electron density in the effective a-k gap identified above, was approximately an order of magnitude higher in the plasma compared to the SCL emission simulation. The Child-Langmuir result for the SCL electron current drawn across a 1D gap at a voltage of $V$ and with an a-k gapping spacing of $d$, scales as $j_e \propto V^{3/2}/d^2$ [23]. Similarly, the electron flow current in the
Figure 4.24: A comparison of the simulated electron density in units of m$^{-3}$ on a logarithmic scale, taken at 0 (through the anode posts) and 15 (between the anode posts) degrees at 90ns from the baseline plasma (left) and SCL emission (right) simulations.

strongly insulated limit of the Mendel pressure balance theory scales as $I_e \propto V^2/d^2$ [31]. The higher electron density in the plasma simulation was consistent with a higher SCL electron current being drawn from the plasma, due to a reduction in the effect a-k gap spacing and an increase in the strength of the electric field across the gap. In addition, the area of the plasma emission surface was larger than the cathode electrode, further increasing the electron current; on the upstream side of the bottom anode post, this lead to the electron sheath filling a larger volume of the post-hole gap, in the plasma compared to SCL emission simulation, as shown in Figure 4.24. Note that an enhanced current loss to the downstream side of the bottom anode post, due to cathode plasma penetration into the a-k gap, was consistent with the LSP simulations [16], reviewed in section 2.6.2 of chapter 2.

Focussing on the top post, slices of the electron and ion density normal to the z-axis at a height of 12cm (through the middle of the level B and C cathode) at 90ns, are shown in Figure 4.25. Here we found that the plasma with a density of $\sim 10^{15}$cm$^{-3}$ covered the entire inner edge of the cathode hole. The plasma penetrating into the post-hole gap on the downstream side of the anode post, shown in Figure 4.22, can be seen to extend around the inner edge of the cathode to a radius of 7cm in these slices. As such, it was concluded that the plasma penetration into a-k gap on the downstream side of the top anode post, was partly due to plasma drifting along magnetic field lines connecting the cathode holes upstream of this region and collecting downstream of the post. This was
Figure 4.25: Slices of the simulated electron and ion densities in units of $m^{-3}$ on a logarithmic scale, taken normal to the $z$-axis, through the middle of the level B and C cathode, at a height of 12cm.

Figure 4.26: Traces of the magnetic field lines in the cathode post-holes at 90ns showing the field lines collecting on the downstream side of the anode posts.

also observed in slices of the ion density taken through the bottom post hole and was again consistent with the plasma evolution found in the LSP simulations [16].

These dynamics were consistent with traces of the magnetic field lines in the cathode post-holes shown in Figure 4.26 at 90ns. Here we see that the field lines sourced on the upstream cathode, collected on the downstream sides of the anode posts, consistent with the locations of the plasma penetration into the a-k gap on the downstream side of the anode posts, as shown in the slices of the ion density taken in the 0 degree plane at this time in Figure 4.22.

Considering the ion density at 70ns, Figure 4.21, at a radius of around 6cm and
heights between 4 and 7.8cm, a plasma of density $\sim 10^{14}$cm$^{-3}$ had expanding into the central null, from the downstream cathode at the bottom post, towards the level D anode. Between 70 and 90ns, part of this plasma was transported in the positive $z$-direction, consistent with the direction of the $\vec{J} \times \vec{B}$ force, both enhancing the plasma penetration on the downstream side of the bottom anode post and eventually filling the downstream side of the top anode post with a plasma of density $\sim 5 \times 10^{13}$cm$^{-3}$, as shown in Figure 4.22. As will be described in section 4.7.3, similar plasma dynamics at later times in the current pulse were also observed. This evolution was also partly responsible for the plasma penetration into the a-k gaps on the downstream sides of the posts and as such the enhanced electron current loss compared to the SCL emission only simulation.

Again considering the ion density at 70ns, Figure 4.21, on the upstream side of the top anode post, the plasma penetrated into the a-k gap across the (1) magnetic null; this reduced the effective a-k gap and therefore increased the SCL electron current drawn from the plasma which was subsequently lost to the anode post. This was consistent with the enhanced charge deposition rate to the upstream sides of the posts, found in Figure 4.20, compared to the simulation with only SCL electron emission. Considering the plasma density at the later times of 90ns, Figure 4.22 and 100ns, Figure 4.15, we found that in the 0 degree plane (through the anode posts), the penetration of this plasma was reduced from approximately half of the a-k gap at 70ns to a quarter of the gap at 100ns. Taking slices of the density normal to the $z$-direction through the top cathode post-hole, this was found to be due to the 'finger' of plasma in the magnetic null, being transported along the $\theta$-direction, enhancing the plasma penetration around the upstream inner edge of the cathode post hole.

A common feature of the convolute plasma simulations was the formation of a low density, $\sim 10^{12}$cm$^{-3}$, ion sheath filling a large part of the a-k gap. Considering the ion density at 40ns in Figure 4.11, the ions in this sheath were sourced from the denser cathode plasma (SCL proton emission from the anode electrode had not started by this time). Comparing this with a plot of the electric field strength at the same time, Figure 4.13, the edge of the low density ion region was consistent with the effective position of the cathode due to the electron sheath formed by electrons emitted from the cathode plasma. As can be seen in the plots of the ion density at 70ns, Figure 4.11, and 90ns, Figure 4.22, this low density sheath persisted and was supplemented by SCL emitted
protons from the regions of the anode electrode where the surface temperature had exceeded 700K. As discussed in section 4.6.2, the presence of positive space-charge on the cathode due to SCL emission of protons from the anode electrode enhanced the SCL electron current drawn and gave an enhancement to the simulated current loss in the SCL emission simulation. In a similar way, we expect that the protons emitted from both the cathode plasma surface and anode electrode further enhanced the SCL electron current drawn from the cathode plasma in the plasma simulations. As discussed in section 2.5.1 of chapter 2, this mechanism was considered in 2D LSP simulations of the Z radial lines, as a way to enhance the SCL electron current entering the convolute from the radial lines. Here, the cathode plasma was not modelled explicitly, but the SCL emission algorithm was modified on the cathode to allow the creation of positive ion space-charge if the field was reversed. Here, the field reversal mechanism was the formation of vortices in the unstable electron sheath [31].

4.7.2 Magnetic Field Topology

The electron flow current was on the order of 100kA, compared to several mega-amperes bound in the electrodes; as such, in these regions, the magnetic field was dominated by the bound current. The simulated plasma density and temperature were used to calculate the electron-ion collision time, $\tau_{ei}$, defined in Eqn.(3.7) in section 3.1.3 of the previous chapter [72]. Combined with the electron cyclotron frequency, $\omega_{ce}$, the magnetisation, $\omega_{ce}\tau_{ei}$ was estimated to range between approximately 40 and 1000 within the densest part of the cathode plasma.

Slices of the magnetic field strength at 90ns from the baseline plasma simulation are shown in Figure 4.27. Comparing this to the simulation with no particles, Figure 4.6, we see that the magnetic field topologies in both the sheath and plasma regions are almost identical to the simulation with no particles. As noted in section 4.6.1, this was also true at the earlier time of 40ns. Within the sheath regions this is explained by the higher bound current dominating the current in the sheath. In the plasma regions, the high magnetisation is consistent with Hall like transport of the magnetic field into the plasma [16,56], which was self-consistently captured in the PIC model.

From Figure 4.27, we also found that the plasma did not significantly alter the
positions of the magnetic nulls discussed in section 4.3.1. In terms of the magnetic field confining the cathode plasma, considering the ion density at 90ns, Figure 4.22, we found that the plasma on the level B cathode at the position of the (3) magnetic null was eroded.

4.7.3 Late Time Plasma Dynamics

As discussed earlier in this section, between 70 and 90ns, plasma which had penetrated the central null from the downstream cathode was transported, consistent with the direction of the $\vec{J} \times \vec{B}$ force, into the a-k gap on the downstream side of the anode posts, enhancing the plasma penetration here. At later times, the plasma in the central null was found to short the a-k gap on the downstream side of the bottom anode post, leading to POS like behaviour, where the a-k gap was reopened here and plasma was transported into downstream side of the top anode post and inner MITL.

A time sequence of the ion density in the downstream side of the anode posts taken between 102 and 110ns at 2ns intervals and at 120ns, are shown in Figure 4.28. Focussing on the downstream side of the bottom anode post between 102 and 104ns the high density plasma, $\sim 10^{15}$ cm$^{-3}$, in the central null shorted the a-k gap, connecting with the anode post at a height of approximately 6cm. The current drawn through the resulting plasma short, $\vec{J}$, was directed along the negative radial direction; the magnetic field, $\vec{B}$, was directed along the negative $\theta$-direction, with the $\vec{J} \times \vec{B}$ force directed in the positive $z$-direction. As such, between 104 and 110ns, the plasma short moved upwards.
along the downstream side of the posts, opening the a-k gap at the bottom post and increasing the plasma density on the downstream side of the top anode post. By 120ns, the plasma density within the inner MITL was increased, due to plasma continuing to be transported in the positive z-direction along the downstream side of the posts.

The current loss between 104 and 120ns was still high, even though the effective a-k gap on the downstream side of the bottom anode post had increased. Specifically, in Figure 4.20, we found that the electron loss rate to the downstream side of the bottom anode post was still dominant between these times. An explanation for this follows from considering the voltage traces in Figure 4.10. Here, we found that the voltage was increasing at this time; the SCL electron current drawn from the plasma was proportional to $V^{3/2}/d$, such that the increase in the effective a-k gap spacing, $d$, was offset by the increase in the line voltage, $V$.

### 4.8 Electron Sheath Instability

As mentioned in section 4.6.2 in relation to smoothing the electron flow current traces, the electron sheaths in both the plasma and SCL emission simulations, formed electron vortices as a result of the diocotron instability [13,31]. The structure and dynamics of electron vortices was discussed in section 2.5.1 of chapter 2. As an example of their formation in the convolute plasma simulations, consider the electron density at 70ns in the level A and B radial lines, shown in Figure 4.29. In the 0 degree slice, the electron vortices, comprising a relatively dense core surrounded by a lower density region, can be
Figure 4.29: Slices of the simulated electron density in m⁻³ on a logarithmic scale, taken at 0 (through the anode posts) and 15 (between the anode posts) degrees at 70ns.

seen at a radius of approximately 11cm. The Larmor radii of the electrons were <10µm; as such, the electron orbits in a vortex consisted of a counter clockwise $\vec{E} \times \vec{B}$ drift about the centre of the vortex, due to the electric field associated with negative vortex space charge (which was directed towards the centre of the vortex) and a global $\vec{E} \times \vec{B}$ drift in the negative radial direction, associated with the line electric field, such that the whole vortex structure drifted downstream towards the load. Comparing the density slices at 0 and 15 degrees in Figure 4.29 we found that the electron vortex structures in the radial lines extended along the entire $\theta$-extent.

As discussed in section 2.5.1 of chapter 2, as the instability was driven by the interaction of waves on two free surfaces, the electron sheath was vulnerable to the diocotron instability if it lifted away from either the cathode electrode, or the cathode plasma surface in the case of the plasma simulations. The radial lines in the convolute have a non-uniform vacuum impedance, which increases with decreasing radius according to $Z(r) = 60d(r)/r$. Here, $d(r)$ is the a-k gap spacing at a radius of $r$. As the electrons drifted to smaller radius, the electron sheath tried to maintain pressure balance (constant flow impedance) by expanding into the gap, thereby reducing the effective a-k spacing. In the process, the electron sheath was susceptible to the diocotron instability, resulting in the formation of the vortices [13,31].

The vortices were found to affect the electron sheath evolution in a number of ways. On the upstream side of a vortex, the electric field associated with the electron space-charge attracted electrons from the component of the sheath bound to the cathode
plasma surface, which 'wrapped around' the counter-clockwise rotating vortex. On the downstream side of the vortex, the electric field on the cathode electrode or cathode plasma surface was reversed, which was an efficient electron re-trapping mechanism. Additionally, this field reversal could be partly responsible for the low density ion sheath drawn from the cathode plasma. As discussed in section 2.5.1 of chapter 2 and section 4.7.1 of this chapter, this was considered as a mechanism for enhanced SCL electron emission in the Z radial lines in [31] and was also observed in our 2D simulations of the inner MITL, which will be described in section 4.14.2.

As stated above, the vortices were formed in the radial lines and the whole structure drifted into the convolute due to the $\vec{E} \times \vec{B}$ drift associated with the line electric field. Here, they were found to interact with the electron sheath in a non-trivial way. Comparing the plots of the electron density at the various times during the simulated current pulse, it was clear that no steady state was established.

The counter-clockwise drift of the electrons in the vortex generated a current which opposed the magnetic field associated with the bound current and as such, they were diamagnetic. As discussed in section 4.7.2, due to the small electron flow compared to bound current, the magnetic field was dominated by the bound current, such that the vortex current had little effect on the simulated magnetic field strength.

### 4.9 Varying the Plasma Parameters in the Creation Model

As discussed in section 4.4, the free parameters of the cathode plasma creation model were the desorption (injection) rate and temperature (used to set the initial velocities) of the pairs of electron and proton macroparticles. In the LSP study, the current loss at peak current was found to be a strong function of the plasma desorption rate, Eqn.(4.4), where $D$ is the desorption rate in mlns$^{-1}$ [16]. Our baseline simulations used a desorption rate of 0.0075mlns$^{-1}$ and gave a peak current loss of $\sim$2.1MA at 120ns, compared to 1.7MA calculated from Eqn.(4.4).

$$I_{loss} (MA) \approx 8.96 + 1.48\ln(D)$$ (4.4)
Due to the long run times of the plasma simulations, where over one month of wall-clock time was required to reach 120ns (this time was even longer when queuing times in the batch system were included), we did not carry out a similar sensitivity study of our model to the plasma creation rate. We did however carry out a limited study of the sensitivity of the model to the initial temperature. At the baseline desorption rate of 0.0075mlns\(^{-1}\), varying the temperature between 1 and 10eV (the typical range of cathode plasma temperatures measured in experiment [21,27]) was found to give a less than one percent change in the simulated current loss. This insensitivity was believed to be a result of the large discrepancy between the ion kinetic and the electric potential, energy in the a-k gap, coupled with the relatively coarse spatial mesh [18]. This point will be considered further in section 4.11, in relation to the effect of the order of the electric field interpolation on the plasma evolution.

In the baseline simulations, cathode plasma creation was started when the normal component of the electric field exceeded 240kVcm\(^{-1}\), consistent with the threshold for the ionisation of desorbed neutral contaminants. As discussed in section 4.4, in order to establish a plasma within the first vacuum cell, the electron and proton pairs were loaded throughout the computational cell; we were therefore setting the initial plasma layer thickness to be the same as the grid cell of length of \(\sim1\text{mm}\). However, at a typical experimentally measured cathode plasma expansion velocity of 3cm\(\mu\text{s}^{-1}\) [17,21,27], the plasma would take \(\sim33\text{ns}\) to cross this distance, which is a significant fraction of the 100ns current rise time. The baseline plasma simulation was therefore repeated with a 30ns delay applied to the plasma creation model; SCL electron emission began on the cathode electrode when the electric field strength exceeded the usual threshold of 240kVcm\(^{-1}\), where the assumption was that a plasma dense enough to supply this current had formed, but had remained tightly bound to the cathode electrode; 30ns after the start of SCL emission, electron and proton pairs were loaded in to the cell as before.

The MITL and convolute currents and their difference, are compared to the baseline simulation in Figure 4.30. Here we see that up to approximately 80ns the current loss was reduced as expected by delaying the plasma formation. However, after this time, both the MITL and convolute currents converged with the baseline simulation results. This agreement was consistent with the formation of similar distribution of plasma within
Figure 4.30: A comparison of the simulated MITL and convolute currents from the baseline and 30ns creation delay plasma simulations.

As discussed in section 4.6, our baseline plasma simulation showed a larger divergence in the convolute and MITL currents (i.e. current loss) at early times (<10MA) compared to the equivalent LSP [16] and typical experimental results [2, 17]. As discussed in section 4.6, these results were in fact in better agreement with the SCL emission only simulations. The currents from the delayed plasma simulation (dashed line) are compared to the case with SCL emission only (solid line) in Figure 4.31. Comparing the current loss predictions (blue lines) we see that they agree closely up to 45ns. As such, the delay model agreed more closely with the measured current loss at early times. After 45ns, the current loss predicted by the delay model increased up to the baseline plasma simulation result. As such, the later time current loss could also be captured by the delay model.

An expansion velocity of $3\text{cm}\mu\text{s}^{-1}$ is at the higher end of measured values, which are typically closer to $2\text{cm}\mu\text{s}^{-1}$ [17]. As such, there was scope to delay the start of the plasma injection for longer, assuming a lower expansion velocity. As such, the delay could be used as an additional free parameter of the plasma creation model to fit the experimental data. In terms of comparing to the LSP simulation results [16], it was not ascertained whether the LSP creation model introduced a similar delay. However, we reiterate that unpublished Quicksilver simulations [58], including a cathode plasma using the creation model described in [18], which introduced only a few nanosecond delay between the start of SCL emission and plasma creation, where consistent with our baseline simulations in that they predicted a similarly high early time (<10MA) current.
loss of up to $\sim 1\text{MA}$.

As discussed in section 2.2.1, the Z electrodes are estimated to be contaminated with over 100 monolayers of neutral molecules, including a range of hydrocarbons, $C_nH_m$, $H_2$, water, $H_2O$, $CO$ and $CO_2$ [21]. As well as Hydrogen, we see that both Carbon and Oxygen form a large part of the available inventory. However, as discussed in section 2.2.1 of chapter 2, due to their lower mass, protons are expected to dominate the a-k gap closure. This is also consistent with the recent experiments on ZR which used optical spectroscopy to measure a Hydrogen cathode plasma with a peak density of approximately $10^{18}\text{cm}^{-3}$, expanding across the a-k gap on the downstream side of the anode posts [17, 59]. As such, we did not consider the effect of including other cathode plasma ion species, on the simulated current loss.

### 4.10 Sensitivity to the Simulation Grid Cell Size

To give tractable run times, the baseline plasma simulations used a relatively coarse spatial mesh of $\sim 1\text{mm}$; note that this was comparable to the equivalent LSP simulations [16]. As such, a number of the plasma length scales were not well resolved. In section 4.4, we considered the thickness of the sheath, $x_n$, through which the plasma current is returned to the cathode. At early times in the convolute current discharge, $x_n \sim 5\mu\text{m}$ and therefore $x_n << \Delta x$. As such, the return current was supplemented by SCL electron emission from the electrode surface [94], where the potential drop in-
creased by approximately a factor of one hundred to supply the electron current. We have already noted that this resulted in some, but not excessive heating of the electron macroparticles. Additionally, at later times in the current discharge, the plasma current increased, giving a corresponding increase in $x_n$, such that the sheath was better resolved at these times. As such, we concluded that it was not vital to resolve the sheath in the convolute simulations. Note that a similar conclusion was drawn in [94] with regard to simulations of high voltage electron diodes.

The range of Coulomb interactions within the plasma is given by the Debye length [71]. In the convolute simulations, $\Delta x > 100\lambda_e$ and as such the Coulomb collision algorithm collided particles over length scales significantly longer than the Debye length. However, tests of the binary collision algorithm, on which we based the model in our code, found that resolving the Debye length was not crucial, as long as the plasma density and temperature gradients of interest were resolved [75].

In the strongly insulated limit, $I_e << I_a$, of the Mendel pressure balance theory [29], described in section 2.4.3 of chapter 2, the thickness of the electron sheath, $d_s$, was predicted to be inversely proportional to the square of the bound anode current as in Eqn.(4.5). Here, $V$ is the voltage, $r$ is the radial coordinate and $d(r)$ is the a-k gap spacing [31].

$$d_s = \frac{142Vr^2}{I_a^2d(r)} \quad (4.5)$$

Taking the electrical parameters at a radius of 12cm in the level A radial feed from the DPHC plasma simulation, Eqn.(4.5) predicts that the electron sheath thickness will be smaller than the grid cell size of 1mm from 60ns and onwards in the current pulse. Considering the electron density slices at 70ns, Figure 4.29, we found that the part of the sheath bound to the cathode plasma was in fact resolved with only a single cell. This is also true for the sheath formed next to the anode in the inner MITL below a radius of $\sim$6cm. However, in the other parts of the convolute we were helped by the non-uniform vacuum impedance, which acted to broaden the sheath and the diocotron instability, which broke the sheath into vortices which, as is shown in Figure 4.29 and 4.15, we found to have a diameter of at least half of the a-k gap. As such, the electron sheath covered several cells in these regions.
As discussed in section 3.7.3.2 in chapter 3, in the energy conserving force interpolation scheme, to be consistent with the current interpolation, the order of the electric field interpolation in the parallel direction was an order lower than in the normal directions; this corresponded to linear weighting for the baseline plasma simulations, which used second order quadratic spline interpolation [68]. Due to the relatively low convolute plasma ion temperature, there was a large discrepancy between the ion thermal kinetic energy, of order 10eV, and electric potential energy in the a-k gap, of order 1MeV, at the edge of the cathode plasma. This issue was studied using a 1D electrostatic version of the Quicksilver PIC code [18]. Here, a plasma was injected next to the cathode electrode, with an applied voltage of \( \sim 1\text{MV} \) across the gap and allowed to expand. It was found that the plasma expansion velocity was a strong function of the grid cell length. Within the plasma cells, the electric field was screened; if the cell size was too large, ions emitted from the edge of the plasma were quickly accelerated back into the plasma by the large electric field present in the gap. In this way, increasing the cell size would slow and eventually halt the plasma expansion. Additionally, for sufficiently low resolutions, the plasma expansion was driven by a numerical instability, rather than an ambipolar diffusion process [18]. We repeated this study with a 1D, 3-velocity (3v) electrostatic version of our PIC code; a plot of the ion phase space \((x, v_x)\), is shown in Figure 4.32. Here, we observed a clear transport barrier for the cathode plasma ions, which coincided with the cell boundary at \( x=200\mu\text{m} \).

**Figure 4.32:** The ion phase space \((x, v_x)\) taken from a 1D3v electrostatic simulation of a cathode plasma expanding into a vacuum a-k gap.
In [18], a sub 100µm cell size was required to mitigate this issue, which occurred using both linear and quadratic spline interpolation. Obviously, this was significantly smaller than the 1mm cell sizes used in the 3D baseline plasma simulations; assuming linear scaling, reducing the cell size to 100µm would require a 20,000 times (10^3 times the number of spatial cells with 20 times more time steps) increase in the required computer resource, which is obviously not practical!

Considering the slices of the ion density between 40 and 90ns, Figure 4.11 and Figure 4.22, the most notable region that exhibited minimal plasma penetration was in the level A and B radial feeds. Here, the higher density plasma was confined to a single cell (remembering the charge density interpolation is over multiple cells) for most of the current pulse. As mentioned in the previous section, the plasma evolution and subsequently, the predicted current loss, were found to be relatively insensitive to varying the initial macroparticle temperature between 1 and 10eV. In the convolute simulations, the bound current generated strong magnetic fields; at 10eV, the Larmor radius was of the order of 60µm in the level A and B radial lines. As such, it is not obvious how applicable the conclusions from the electrostatic study are to the electromagnetic case. Further work is therefore required to determine if the plasma transport was affected by the spatial resolution.

At later times we also found that the plasma was eroded in the conical radial feeds. For example, consider the slices of the ion density at 90ns, Figure 4.22. In the 0 degree slice the plasma had been eroded in the level C line between a radius of 11 and 12cm. We believe that this was associated with electrode stair stepping. Note that the plasma was not eroded at the same positions in the 15 degree slices.

With the above considerations, it was important to try and assess the impact of the grid cell size on the simulated current loss. However, carrying out a thorough convergence study was not possible; assuming linear scaling, halving the grid cell length required a sixteen times increase in the computational resource. As such, we only ran the plasma simulations with 500µm resolution along the r- and z-axes and π/12/40 radians along the θ-axis for a small part of the current pulse. The simulated convolute currents are compared to the 1mm resolution baseline simulations in Figure 4.33.

Here, we have also plotted results from control simulations where the grid spacing was kept at 1mm, but the time step was halved and the particle weights reduced by a
Figure 4.33: A comparison of the simulated MITL and convolute currents from the baseline simulation with simulations where the time step was halved (dt/2), the spatial step was halved along the three axis (dx/2) and the number of macroparticles was increased by eight times (8Np).

factor of eight; in the 500µm simulations the Courant limit forced the time step to be halved over the baseline case and the number of particles was increased by eight to keep the same number of particles per cell on average.

From Figure 4.33, we found that the 500µm simulation gave a slightly higher convolute current (slightly lower loss current) up to the end of the simulation at 37ns. Reducing the time step appeared to have no effect on the baseline convolute current. However, reducing the particle weights in the baseline simulation gave an almost identical result to the 500µm simulation, where the particle weights were reduced by the same factor. As such, we concluded that the difference between the 500µm and 1mm resolution simulations, came from the improved particle statistics and not the improved spatial resolution.

From the results in Figure 4.33, we can also conclude that these refinements to the spatial, temporal and particle statistics had little effect on the over prediction of the early time current loss (<10MA), that was highlighted in section 4.6. This gives further credence to the plasma injection delay model, which was considered in the previous section, as a means to match the measured current loss at early times.

Running the 500µm simulations to peak current and refining the grid cell size further, was not practical with the available computing resource; as such, we believe the issue of convergence with the cell size, would be better addressed with a series of smaller scale simulations, which are left as further work.
4.11 Quadratic Versus Linear Interpolation

As discussed in the previous section, the energy conserving electric field interpolation forced an order lower interpolation in the longitudinal compared to the transverse directions [68]; second order quadratic spline interpolation was chosen for the baseline simulations to give first order weighting in the longitudinal directions. To investigate the sensitivity of the model to the order of the interpolation scheme, the DPHC plasma simulation was rerun with the energy conserving linear interpolation scheme described in section 3.7 of the previous chapter; now NGP interpolation was used in the longitudinal directions, giving rise to a piecewise electric field interpolation [68]. The simulated MITL and convolute currents are compared to the baseline plasma simulation in Figure 4.34.

Here, we found that linear interpolation reduced the current loss prediction by a factor of two at 55ns and was consistent with the convolute plasma penetrating a smaller fraction of the a-k gap on the downstream side of the anode posts. This reduced plasma penetration was consistent with the discussion in the previous section, regarding the discrepancy of the ion thermal and electric potential energies at the edge of the plasma. With NGP interpolation, when an ion left the screened plasma cell it instantaneously felt the full electric field in the gap [18].

The LSP DPHC simulations used a different energy conserving interpolation scheme to our baseline model; as for the quadratic spline scheme, each macroparticle had an
effective size of two computational cells along each direction, however the interpolation function was linear, as opposed to quadratic [15,16]. As discussed in section 4.6, although the current loss at peak current predicted by our baseline simulations, was consistent with LSP simulation [16] and experimental [2,17] results, our early time (<10MA) loss was significantly larger. The LSP and measured current losses at this time, were in fact closer to simulations where only SCL emission was allowed. Considering Figure 4.34, up to 50ns, the current loss was reduced from ~1MA to ~0.5MA with linear compared to quadratic spline interpolation. However, the linear interpolation result was still larger than the SCL emission result, which predicted the current loss to reduce to effectively zero after ~45ns. As such, the order of the interpolation scheme alone could not account for the over prediction of the early time current loss in our simulations. Again, this gives further credence to the delay model, described in section 4.9, as a means to match the measured current loss at early times.

However, considering the large impact that the choice of interpolation scheme had on the magnitude of the predicted current loss, as shown in Figure 4.34, the differences between the quadratic spline [18] and the LSP interpolation schemes, should be considered when making comparisons between the codes. Again, we note that the unpublished Quicksilver results [58], which were in qualitative agreement with our simulations, used the same energy conserving quadratic spline interpolation scheme [18,68].

### 4.12 Resolving the Electron Larmor Orbits

As discussed in section 4.5, the simulation time step was set by the requirement to resolve the electron cyclotron orbits, as in Eqn.(4.6). As the magnetic field strength increased with the rising current, it was necessary to keep reducing the time step to enforce Eqn.(4.6). Coupled with the relatively large number of macroparticles required to resolve the high density gradients between the plasma and sheath, this gave rise to the long run times discussed above.

\[
\omega_{ce} \Delta t < 2
\]  

As the magnetic field only rotates the particle velocity vector, the condition in
Eqn.(4.6) is one of accuracy and not stability [12]. Could we therefore reduce the simulation run time by simply not resolving the electron Larmor orbits? The condition in Eqn.(4.6), enforced at least three time steps per cyclotron orbit; less than this resulted in aliasing, giving rise to incorrect drift motions [12, 62]. Accurately reproducing the drift motions was important for the electron sheath dynamics in the crossed electric and magnetic fields, where not enforcing Eqn.(4.6), gave rise to electron drifts in the positive radial direction! Additionally, in section 4.7.2, the simulated plasma magnetisation was estimated to be between 40 and 1000; resolving the individual electron cyclotron orbits was therefore necessary to accurately model the plasma transport properties [56]. We therefore conclude that satisfying Eqn.(4.6) was a requirement for accurate simulation.

As discussed in section 3.6.2 of chapter 3, the Quicksilver SCL electron and ion emission simulations of the convolute, sub-cycled the particle push under the EM field solution. Here, the run time was significantly reduced, as the current interpolation, which represents one of the largest computational overheads, was done only once per EM field solution time step; it was stated that the results of their simulations with and without sub-cycling were equivalent [12].

We reran our equivalent SCL emission only simulations, which were described in section 4.6.2, with a similar sub-cycling scheme. As discussed in section 3.6.2, we chose to push each particle with its own time step up to the EM field solution time, in place of reordering the particles into a number broader sub-groups. In our case, the particle push sub-cycle time step was set by $\omega_{ce}\Delta t = 1.8$.

Slices of the simulated electron density for the cases with and without sub-cycling are compared at 84ns, at 0 and 15 degrees, in Figure 4.35 and 4.36, respectively. Plots of the magnitude of the electric field strength at the same time in the simulations are shown in Figure 4.37 and 4.38, respectively.

From Figure 4.37 and 4.38, we found that the sub-cycling introduced additional structure into the electric field; the simulations without sub-cycling had significantly smoother fields. However, comparing the electron densities in Figure 4.35 and 4.36, this appeared to have little effect on the distribution of electrons in the sheath. Note that the sheath instabilities made direct comparison difficult; however we found that the general structures were equivalent. As such, we found the simulated current traces to be almost identical between the cases with and without sub-cycling, consistent with
Figure 4.35: A comparison of the electron density in m\(^{-3}\) on a logarithmic scale, at 84ns taken at 0 degrees (through the anode posts) with (left) and without (right) particle push sub-cycling.

Figure 4.36: A comparison of the electron density in m\(^{-3}\) on a logarithmic scale, at 84ns taken at 15 degrees (between the anode posts) with (left) and without (right) particle push sub-cycling.

the statements made in the Quicksilver study [12].

Applying the particle push sub-cycling to the plasma simulations, the total run time of the baseline simulation could be reduced from approximately one month to less than two days! However, unlike in the SCL emission case discussed above, we found significant differences in the plasma dynamics between the simulations with and without sub-cycling. With sub-cycling, the predicted current loss was reduced over the entire pulse, with a \(<5\%\) loss at peak current compared to 10\% without sub-cycling. These differences were tracked to significantly higher electron temperatures in the simulations with sub-cycling, resulting from the electron heating instability numerically heating the electron population; this was diagnosed by large errors in the simulation energy conservation, the calculation of which will be described in the next section.
Figure 4.37: A comparison of the electric field strength in Vm⁻¹, at 84ns taken at 0 degrees (through the anode posts) with (left) and without (right) particle push sub-cycling.

Figure 4.38: A comparison of the electric field strength in Vm⁻¹, at 84ns taken at 15 degrees (between the anode posts) with (left) and without (right) particle push sub-cycling.

In the simulations without sub-cycling, this instability was mitigated by using energy conserving interpolation for the electric field [68]. The same interpolation scheme was used in the sub-cycled simulations; however, the sub-cycling was found to reintroduce the imbalance in the change in the particle kinetic and electric potential energy over a time step, such that the plasma electrons were numerically heated. Comparing the total electron macroparticle energies, we found that the sub-cycled result was many orders of magnitude higher than the baseline simulation. The cathode plasma was subsequently eroded, such that the high density plasma responsible for the enhanced electron loss to the anode was not established.

Attempts were made to stabilise the sub-cycled plasma simulations, firstly by staggering the times at which the electric field was interpolated to the particles and secondly
by limiting the number of sub-cycle steps by also dynamically reducing the field solution time step. However, in all cases, numerical electron heating was found to substantially alter the plasma dynamics.

Although not valid over the whole domain, as discussed in section 4.5, sub-cycling the particle push for particles only within the inner MITL was found to be stable for a large part of the current pulse. This was due to the fact that at as no particles were created within the inner MITL itself, the plasma density remained relatively low here. However, by 90ns, plasma transported from the convolute had filled the inner MITL such that the sub-cycling was truncated just before this time. As the highest magnetic field strengths and therefore cyclotron frequencies occurred within the inner MITL, sub-cycling up to this time represented a significant saving in the simulation run time.

Even if the stability of sub-cycling particle push in the plasma simulations could be fixed, for example by using an implicit solution, we have not addressed the issue of whether it would be accurate. For large magnetisations, the electrons decouple from the ions, such that the magnetic field is effectively frozen into the electron fluid. As such, only changes in the electron density that satisfy this condition will be allowed [56]. It is therefore not clear whether sub-cycling the particle push under the EM field solution would be accurate in this case. In chapters 5 and 6, we will investigate methods to reduce the computational overhead by treating part of the plasma with either an MHD fluid or an inertial two-fluid description. For the former, the cyclotron frequency did not have to be resolved within the plasma region, however for accuracy finite Larmor radius effects, such as the Hall current, had to be included [60, 69]. For the latter, the field solution proceeded in the same way as the PIC model and as such, the cyclotron frequency still had to be resolved for accuracy; this was however offset by pushing a smaller number of macroparticles, as will be discussed in this chapter.

4.13 Plasma Simulation Performance

As discussed in section 3.1.2 of chapter 3, the spatial resolution of $\sim 1$mm used in the baseline plasma simulations was over one hundred times the plasma Debye length. To avoid the numerical electron instability heating the plasma to an unphysical, high temperature, an energy conserving electric field interpolation scheme was used; the stag-
gered electric field components on the Yee-mesh [83] were interpolated directly to the macroparticles in place of averaged nodal quantities [68].

To test the effectiveness of this scheme, a global energy diagnostic was calculated during the simulations. The total energy in the system, $E_{\text{total}}$, was tracked with a running sum of the energy entering and leaving the PIC domain, through the four transmission boundaries at the level A-D radial lines. At each time step, the voltage and current of the forward and backward travelling components of the waves, at the boundary were, used to calculate a power $P_{1,2} = I_{1,2}V_{1,2}$ where $t$ is the time in the simulation and 1 and 2 refer to the forward and backward travelling components of the wave, respectively. The energy entering and leaving the PIC domain in a time step $\Delta t$, was then $\Delta E_{\text{in}} = \Delta t P_2$ and $\Delta E_{\text{out}} = \Delta t P_1$, respectively. The initial kinetic energy of particles created in the SCL emission and plasma creation algorithms were also added to $E_{\text{total}}$ and the final kinetic energies of particles lost through impacting an electrode or open simulation domain boundary, were subtracted.

In the simulation, this total energy was split between the EM fields, particles and load. The energy density in the EM field, split between the electric and magnetic field, was calculated by first averaging the staggered electric and magnetic field components to the cell nodes and then calculating the sum of Eqn. (4.7) [19] over the grid.

$$U = \frac{1}{2} \left( \epsilon_0 E^2 + \frac{B^2}{\mu_0} \right)$$

(4.7)

The load energy was split between the kinetic energy of the imploding shell, $K_{\text{load}} = \frac{1}{2} m_{\text{load}} u_{\text{load}}^2$ and the energy stored by the load inductance, $E_{\text{inductance}} = \frac{1}{2} L_{\text{load}} I_{\text{load}}^2$, in the magnetic field between the load and return can (the energy stored in the capacitance was much smaller and therefore neglected). The kinetic energy of each macroparticle was calculated as $K_p = m_p u_p^2 / (\gamma + 1)$, after the first half-acceleration in the Boris push step to ensure proper time centring [62]. These were summed and added to the EM and load energies to give a second estimate of the total energy in the PIC domain, $E_{\text{sum}}$.

The sum, $E_{\text{sum}}$, should be equal to the total energy in the system, $E_{\text{total}}$ such that the difference, $\Delta E_{\text{error}} = E_{\text{total}} - E_{\text{sum}}$ gave a measure of the energy conservation error. By 120ns in the baseline plasma simulation the error was found to be approximately 2% of the total energy, demonstrating the effectiveness of the energy conserving interpolation.
in mitigating the numerical electron heating instability. The equivalent LSP simulations quoted an energy conservation error of 10% [16]; however it should be noted that the LSP simulations were run to a later time in the current pulse.

As discussed in section 3.4, the electric and magnetic fields were calculated from Ampere’s and Faraday’s laws. To ensure the resulting electric field enforced Gauss’ law, the macroparticle current interpolation step enforced the continuity equation calculated at the cell nodes (the charge density is a nodal quantity whilst the currents are defined on the cell edges). As discussed in section 3.7.1.2 of chapter 3, this was complicated at the electrode surfaces due to the use of second order quadratic spline interpolation.

To ensure that the electric field did in fact enforce Gauss’ law and charge was being conserved, the quantity given in Eqn.(4.8), was evaluated at the cell nodes (ρ was defined at the cell corners and $\vec{E}$ on the cell edges) at various times during the simulation. Here, $\vec{E}$ is the electric field vector and $\rho$ the interpolated macroparticle charge density [68].

$$\frac{max \left( \epsilon_0 \nabla \vec{E} - \rho \right)}{max \left( \rho \right)}$$  \hspace{1cm} (4.8)

By 120ns in the baseline plasma simulations, this quantity had reached a maximum of approximately $10^{-11}$, consistent with charge being conserved to the precision of the machine round-off. In section 4.4, we described the requirement to load the electron and ion macroparticles with equal velocities, in the plasma creation model. If the electron and ions were loaded with different initial velocities, consistent with their different thermal velocities, in the cathode plasma creation model, then Eqn.(4.8) was found to quickly exceed 0.1; electric fields generated from the effective space-charge were found to significantly disrupt the plasma. This was the reason that the electrons were loaded at the ion velocity, in which case the charge conservation was at the level of machine round-off.
4.14 Current Loss within the Inner MITL

4.14.1 3D DPHC-Inner MITL Simulation Results

As reviewed in section 2.6.1 of chapter 2, in [2] and [3], 3D MHD (Gorgon) simulations of wire array Z-pinch experiments, driven with a detailed circuit model of Z, were matched to a range of experimental diagnostics. To fit the data, an undiagnosed multi-mega ampere current loss, in addition to the measured convolute loss, had to be introduced within the inner MITL. As the nature of the loss was unknown, it was represented by an electron flow loss in parallel with the load, within the inner MITL circuit; the effective resistance of this element was then scaled to match the simulated implosion diagnostics to experiment [2]. The magnitude of the inner MITL loss was found to be dependent on the electrode geometry; the right angled bend configuration used in our DPHC simulations was found to give the largest losses. As such, in later experiments the inner MITL geometry was modified; the inferred inner MITL loss was reduced with a conical electrode shape, which gave a smoother transition between the convolute and load impedance [3].

The inner MITL began at a radius of 6cm and as shown in Figure 4.1, consisted of a purely radial line which transitioned into a purely cylindrical line through a right angled bend. The a-k gap spacing of the radial section was 6mm, reducing to 4mm in the cylindrical part. With a cell size of 1mm this gave a relative poor resolution of six and four cells across the a-k gaps, respectively. As such no particle creation was allowed within the inner MITL in the baseline plasma simulations, as discussed in section 4.4. However, particles were transported into it from the convolute. Considering the electron density at 70ns in the plasma simulation, Figure 4.29, we found that an electron sheath was formed close to the anode electrode with a density comparable to the sheath within the radial lines and convolute. Electrons in this sheath were transported into the cylindrical section around the right angled bend and remained close to the anode; closer to the cathode the sheath density was lower and at the corner an electron vortex was formed, which persisted for much of current pulse. At 70ns, the ion density in the inner MITL was relatively low, as shown in Figure 4.21.

From 70ns onwards we found that plasma from the downstream side of the convolute
was transported into the inner MITL; comparing the ion density slices at 0 and 15 degrees, we found that this was true over the whole $\theta$-extent. Below a radius of $\sim$7cm (the edge of the anode post) in the level A line, the plasma filled the gap into the inner MITL. At 90ns, Figure 4.22, the radial section of the inner MITL was filled with a plasma with a density of close to $10^{15}\text{cm}^{-3}$, comparable with the densest part of the plasma in the convolute. By 120ns, the plasma density had increased and filled almost the entire inner MITL. This was consistent with plasma transported by the short on the downstream side of the bottom anode post, starting at 104ns, reaching the inner MITL, as discussed in section 4.7.3.

The presence of the electron sheath and plasma within the inner MITL resulted in the loss of electrons to the anode electrode in the radial section. This was again diagnosed by the anode surface temperature increase, which is plotted in Figure 4.39. Here we found that electrons were deposited across the entire radial part of the inner MITL anode electrode and heated it to temperatures comparable with the electron loss regions on the anode posts, as shown in Figure 4.16. This result was consistent Quicksilver simulations, which included only SCL electron emission from the cathode electrode [14,18].

The convolute and load currents, as well as their difference, from the baseline plasma simulation, are plotted in Figure 4.40. As was found within the convolute, electrons impacting the anode in the inner MITL shunted current away from the load and represented an additional current loss path in parallel with the load. Up to approximately 103ns, no
significant current loss was observed. After this time, the loss began to increase, peaking at around 120kA at peak current. This was significantly lower than the multi-mega ampere current losses at peak current inferred in [2, 3], however these results were for compact Tungsten wire array experiments; as discussed previously, we modelled a large diameter Aluminium array. In [2], the current loss was parameterised by an electron flow current loss resistance in the circuit model. The peak in the current loss in our simulations coincided with the higher density plasma filling the inner MITL. Considering the electric field at this time, it was confined to the electron sheath next to the anode electrode, consistent with the centroid of the electron sheath charge acting as an effective cathode. As such, the electron losses to the anode were driven by the electron sheath. However, due to the relatively poor spatial resolution here, the accuracy of this result should be addressed. To this end we carried out a separate series of higher resolution 2D simulations of the inner MITL, which will be presented in the next section.

4.14.2 2D Inner MITL Simulation Results

In our baseline DPHC plasma simulations discussed above, particle creation below a radius of 5cm within the inner MITL, was not allowed due to the relatively poor spatial resolutions here. However, as described in the previous section, electron macroparticles created within the radial lines and convolute were transported into the inner MITL, such that throughout the majority of the current pulse an electron sheath was present next to the anode electrode. At later times, ions from the convolute were also transported.
into the inner MITL; by 120ns, the inner MITL was filled with plasma at a density comparable to the highest density within the convolute. Comparing the load and convolute currents we found a 120kA current loss within the inner MITL at peak current.

As the inner MITL was only resolved with six and four cells across the radial and coaxial a-k gaps in the 3D convolute simulations respectively, we carried out a series of higher resolution simulations of the inner MITL in 2D r-z cylindrical coordinates. In experiment, the inner MITL electrode is cylindrically symmetric, such that a 2D representation is sufficient. In the 3D convolute simulations, we also found that the voltage measured across the a-k gap, below a radius of 6cm, varied by less than 1% along the $\theta$-direction. As such, the assumption of a uniform voltage drive was also consistent with a 2D representation.

The 2D simulations modelled the same right angled bend inner MITL configuration as was used in the 3D convolute simulations. The wire array load was again approximated by the 0D implosion model discussed in section 4.2; the load parameters were set assuming the same large diameter, aluminium array, with $r_0=2\text{cm}$, $l=2\text{cm}$ and $m=4.09\text{mg}$. The inner MITL begins at a radius of $5.4\text{cm}$; the simulation domain was extended to a radius of $6.4\text{cm}$, such that it included a small part of the convolute lines. This was done to prevent spurious reflections from the impedance transition at $r=5.4\text{cm}$, where the a-k gap reduces from $1\text{cm}$ in the convolute to $6\text{mm}$ in the radial section of the inner MITL. Again, the extra $1\text{cm}$ of line, which was equal to the a-k gap spacing at the domain boundary, was sufficient for this task. The inner MITL was driven with a transmission line representation of the simple Thevenin equivalent circuit shown in Figure 2.4 in section 2.6.1 of chapter 2, as shown in Figure 4.41, which models the convolute and radial lines out to the insulator stack. The effective voltage source used to drive the model is plotted in Figure 4.42; this was derived from a more complete circuit model, including the PF circuit [2]. The voltage was scaled to match the peak convolute current measured at the start of the inner MITL.

As described in section 2.6.1 of chapter 2, the current loss within the convolute was modelled as a parallel electron flow current loss in the Thevenin equivalent circuit. This was included as a variable resistor in parallel with the load. For simplicity the loss resistance defined in Eqn.(2.32), was calculated using a fixed flow impedance, $Z_f$, of $0.25\Omega$ [2]. This was sufficient to give a representative current drive for the inner MITL.
simulations, as we were not concerned with detailed comparisons to specific experimental shots. As for the 3D convolute simulations, the transmission line circuit was connected to the PIC domain through a transmission boundary condition. The impedance of the transmission line circuit element connected to the PIC domain, was matched to the vacuum impedance of the simulation domain using $Z_0 \sim \frac{60}{d/r}$, were $r=6.4\text{cm}$ and $d=1\text{cm}$.

For the 2D simulations, spatial resolutions of $\Delta r=\Delta z=200\mu\text{m}$ and an initial time step of $\Delta t_{\text{init}} = 0.5\Delta t_{\text{Courant}}$ were used. The global time step was dynamically reduced in order to enforce $\omega_{ce}\Delta t=1.9$ for all the electron macroparticles. Note that we did not employ any sub-cycling in the particle push step. Assuming symmetry along the $\theta$-direction, meant that only the $\theta$-component of the magnetic and $r$- and $z$-components of the electric field were non-zero. The macroparticle velocities along the $\theta$-direction were also zero, such that each macroparticle represented a square-torus of charge [62].

Initially assuming that plasma was formed on the cathode electrode, but remained tightly bound during the current pulse, SCL electron emission was allowed directly from the cathode electrode surface. This began once the strength of the normal component of
Figure 4.43: A comparison of the simulated currents at the load for the case with no particle creation and SCL electron emission directly from the cathode electrode.

The electric field exceeded 240kVcm\(^{-1}\). The simulated load current is compared against the case with no particle creation in Figure 4.43. Here we found that the current histories at the load were almost identical, demonstrating that the inclusion of SCL electron emission gave rise to a minimal current loss in the particle simulation.

The electron sheath dynamics were similar to those seen in the radial lines of the 3D convolute simulations; specifically the formation of an unstable sheath, resulting in electron vortices, due to the non-uniform vacuum impedance of the line [13, 31]. The simulated electron density between 40 and 54ns, at 2ns intervals, is plotted in Figure 4.44. Here, we can see the simulated electrode geometry for the right-angled bend inner MITL. The inner radius of the cathode at 2cm is consistent with the initial radius of the Z-pinch load. The a-k gap of the coaxial part of the line was 4mm; the open boundary at a height of 2.4cm was connected to the 0D load model. The a-k gap in the radial part of the line above a radius of 5.4cm was 1cm, consistent with the convolute electrode geometry. Below 5.4cm, this was transitioned to an a-k gap spacing of 6mm.

In Figure 4.44 at 40ns, we found that the electron sheath in the radial part of the inner MITL consisted of two parts; a bound part above the cathode electrode and electron vortices at a radius of \(\sim 4.5\)cm, which extended over half way into the a-k gap [13, 31]. The vortices consisted of a denser central region with a density of \(\sim 10^{14}\)cm\(^{-3}\).
Figure 4.44: A time sequence of the simulated electron density in m$^{-3}$ on a logarithmic scale, in the inner MITL for 40 to 54ns. Note that the earliest time is at the top left; time increases working down and then starting at the top right, working down again.

surrounded by a lower density region with a density of $\sim10^{12-13}$cm$^{-3}$. Considering the time sequence, the vortices were seeded on the curved part of the cathode at a radius of $\sim5.2$cm; this region represented a vacuum impedance transition from the 1cm to 6mm a-k gap spacing. The Larmor radii of the electrons were less than 50\(\mu\)m; the drifts of the electrons in the vortices consisted of a counter clockwise $\vec{E} \times \vec{B}$ drift about the centre of the vortex due to the electric field associated with the electron space-charge and an $\vec{E} \times \vec{B}$ drift in the negative radial direction, due to the line electric field. The latter resulted in the entire vortex structure propagating towards the load as shown in Figure 4.44. As the vortices drifted towards the load we found that their size increased; this was due to two processes. Firstly, the electrons from the bound part of the sheath were drawn into the vortex on the upstream side and wrapped around like a ribbon. Secondly, multiple smaller vortices were found to merge into a single larger vortex. For example between 40 and 42ns, at a radius of 4.7cm and 46 and 48ns, at a radius of 4.4cm, and 50 to 54ns at a radius of 4.2cm, we found that multiple denser regions of the sheath, merged
into one larger vortex. These larger structures then propagated down the line, moving away from the cathode towards the anode, at the start of the right angle bend and propagated along the coaxial anode to the load boundary. At the bend, the line electric field was reducing, whilst the magnetic field was increasing, such that the $\vec{E} \times \vec{B}$ drift velocity was reduced and the electrons moved towards the anode. As the bound current increased during the pulse, the propagation speed of the vortex structures toward the load was found to reduce. This was due to the increasing strength of the magnetic field reducing the $\vec{E} \times \vec{B}$ drift velocity ($v_E = E/B$).

Although no steady state was established, these dynamics were repeated throughout the current pulse; specifically, vortices were formed on the curved electrode at $r \sim 5.2\text{cm}$, merged at smaller radii, moved towards the anode at the right-angled bend and drifted to the load boundary next to the coaxial anode. A plot of the electric field strength at 44ns is shown in Figure 4.45. The electric fields associated with space charge of the electron vortices centred at radii of 3.5 and 4.85cm are clearly visible. We have included a vector plot to show the direction of the electric field in Figure 4.46. Here we see that the electric field at the centre of the vortex was essentially zero, as the line electric field was shielded by the space charge. The space charge electric field was directed towards the centre of the vortex; this lead to field reversal on the cathode electrode below the vortices, suppressing further electron emission and re-trapping current in the bound part of the sheath here [31]. The electric field strength was highest on the anode side of the vortex at $r = 3.5\text{cm}$. This was consistent with the MITL theory discussed in section 2.3 of chapter 2, where the centroid of the electron sheath charge acted as a virtual cathode for the line electric field. Considering the current carried by the vortices, this was directed clockwise around the vortex, consistent with the counter-clockwise electron drifts. The current density was highest near the centre of the vortex, consistent with the higher charge density and electric field strength ($v_E = E/B$) here. The magnetic field associated with this current opposed the field associated with the bound current in the electrodes. The magnitude of the vortex current was $\sim 40\text{kA}$, compared to the multi-mega ampere bound current, such that the magnetic field was not modified significantly compared to the case with no particles.

In Figure 4.43, the load currents for simulations with and without particle creation are compared, showing minimal current loss in the particle case. At early times, $< 60\text{ns}$,
as shown in Figure 4.44, we found that the vortices did connect with the anode electrode at the right angled bend and in the coaxial part of the line. As such, electrons were lost to the anode, however this loss was minimal compared to the bound current. At later times, the vortices formed in the radial part of the line, were found to miss the anode electrode as they were transported around the corner, as shown in the plot of the electron density at 112ns in Figure 4.47. As such, the anode surface temperature, which was a diagnostic of the magnitude of the electron deposition, was not seen to exceed 400K by the end of the current pulse; note that the usual threshold used for anode plasma formation is 700K.

The inner MITL simulations were repeated with the inclusion of a Hydrogen plasma injected from the cathode. As was done in the 3D DPHC convolute simulations, described in section 4.4, pairs of electron and proton macroparticles were injected throughout the vacuum cell next to the electrode surface. We used the same desorption rate
of 0.0075mlns$^{-1}$, that was found to match the loss current in the 3D convolute simulations. Similarly, the initial velocities were sampled from a Maxwellian distribution of proton velocities at 3eV. As the simulation cell size of 200µm was still at least several hundred times the plasma Debye length ($<1µm$), energy conserving quadratic spline interpolation was again used to mitigate the numerical electron heating instability [68].

Plots of the electron and ion density taken at 80ns, are shown in Figure 4.48 and 4.49, respectively. Here we found a dense, $>10^{15}cm^{-3}$ plasma was formed on the electrode surface. This was established by 40ns and remained tightly bound to the electrode for the entire current pulse. On the curved part of the cathode electrode at $r=5.3cm$, plasma was observed to penetrate the a-k gap and then be transported in the negative radial direction. Apart from here, the cathode plasma remained constrained within two computational cells, $\sim 400µm$, of the electrode. This was a result of the large magnetic field strength, which ranged between 20 and 200T, preventing significant collisional cross field transport. Note that as the strength of the magnetic field was inversely proportional to the radius and all of the bound current flowed through the single inner MITL, the magnetic field strength was larger in the inner MITL compared to the convolute.

From Figure 4.48, we found an unstable electron sheath was formed in the a-k gap by electrons emitted from the cathode plasma. As in the SCL emission only simulations, electron vortices were formed in the sheath. In the plasma case, the number of vortices and their size were increased and reduced, respectively. The vortices were again seeded from the plasma on the curved part of the cathode electrode at $r\sim5.3cm$, which represented a region of more rapid vacuum impedance increase due to the reduction in the
In addition to the electron sheath, we also found that an ion sheath was formed within the a-k gap by protons emitted from the cathode plasma, as shown in Figure 4.49. The proton Lamor radii in the gap were less than the gap spacing and as such the protons were observed to $\vec{E} \times \vec{B}$ drift in the same direction as the electrons, such that the ions essentially followed the electron distribution. For example, comparing Figure 4.48 and 4.49, at the positions of the electron vortices, the ion density was also increased.

Earlier time plots of the electron and ion density at 26ns are shown in Figure 4.50 and 4.51, respectively. At this time, cathode plasma creation had just begun in a single cell at a radius of $\sim5.2$cm. From the electron density plot we see a vortex had also formed in the electron sheath above this plasma cell. As shown in Figure 4.46, the electric field associated with the vortex space charge was directed towards the centre of the vortex. This opposed the line electric field on the cathode plasma surface and
drew ions from the plasma, as shown in Figure 4.51. This process continued throughout
the current pulse, resulting in the a-k gap being filled with the low density ion sheath
as shown in Figure 4.49. At the curved part of the cathode electrode at a radius of
\( \sim 5.2 \text{cm} \), vortices were found to periodically form and be transported towards the load;
the magnitude of the proton density drawn into the a-k gap in this way was increased
when the electron vortices were forming and decreased when they drifted away along
the line.

Note that a low density ion sheath was also seen to fill the majority of the a-k gaps
in the 3D convolute simulations, consistent with these higher resolution inner MITL
simulations. It is proposed that the mechanism for this in the 3D simulations was field
reversal at the cathode surface due to the vortices in the electron sheath formed above
the cathode plasma.

As shown in Figure 4.50, the electron sheath formed from the cathode plasma, con-
nected with the anode electrode. However, as was found in the SCL electron emission only simulation, the electron flow current loss was minimal and the anode electrode temperature did not exceed 400K. As such, the 120kA difference between the convolute and load currents, found in the 3D couple convolute and inner MITL simulations, was not reproduced. In the coupled simulations, the current loss came from an electron sheath formed next to the anode, from particles transported into the inner MITL from the convolute. Additionally, at later times in the current pulse, we found a relative dense plasma filled the inner MITL, again from particles transported from the convolute. Neither of these structures was reproduced in the 2D inner MITL simulations; the fact that the 2D simulations did not match the level of current loss found in the coupled convolute and inner MITL simulations, was therefore not surprising. As such, we attempted to model the electron current entering the inner MITL, from the convolute, in the 2D inner MITL simulations, using a number of methods. Firstly, we extending the radius of the simulation domain; although the electron flow current was increased, the sheath remained closely bound to the cathode electrode. We therefore attempted to directly inject electrons closer to the anode electrode, at the simulation domain boundary; however, this was also not very successful and resulted in spurious EM wave reflections at the PIC domain-circuit boundary that significantly perturbed the simulated current drive. Finally, we attempted to form an electron sheath on the anode by turning off the magnetic field in the particle push for particles above a certain radius; again, this was not successful and only resulted in the upstream electron current being shunted to the anode electrode.

Following these unsuccessful attempts to reproduce the 3D simulation results, we concluded that to consistently simulate the current loss mechanism within the inner MITL, would require higher resolution coupled simulations of the inner MITL and convolute. One way to achieve this would be to use variable grid spacing, where higher resolution would be used within the inner MITL and coarser resolution within the convolute, to allow tractable simulations. Alternatively, separate convolute and higher resolution inner MITL simulations could be run in tandem, with the EM field and particle information passed between the simulations. Both cases would require significant modifications to the code and as such were left as future work.

In terms of the cathode plasma evolution within the inner MITL, as discussed above,
for the 2D simulations we used the same fully ionised, Hydrogen plasma desorption rate and initial temperature that was found to match the current loss in the 3D DPHC simulations. As the bound current was higher in the inner MITL compared to the convolute, the sensitivity of the simulated current loss to these free parameters in the plasma creation model should also be investigated. Additionally, no measurements of the plasma within the inner MITL have been made; as such unlike the convolute, there is no experimental evidence that the plasma is predominantly Hydrogen. Again, the sensitivity of the simulated current loss to the plasma ion species could also be investigated. In order to constrain the model with the measured convolute and inferred load current, we should initially simulate the compact wire-array loads and electrode geometries considered in [2,3]. Here, the initial load radius was 1cm, compared to the 2cm loads used in the simulations described above. As such, the compact array simulations will give higher peak magnetic field strengths and therefore be more stressing on the simulation time step. Although these were 2D simulations, due to the nature of the cathode plasma, where the highest density plasma remained bound to the cathode, efficient domain decomposition was difficult. As such, the compact wire array simulations were also left as further work.

### 4.15 Chapter Summary

In this chapter, fully kinetic 3D PIC simulations of a π/12 extent of the Z DPHC and inner MITL, including a small part of the radial lines, using the code described in chapter 3, were presented. We modelled a large diameter Aluminium wire array Z-pinch load with an initial radius of 2cm, height of 2cm and total mass of 4.09mg. Simulations that included only SCL electron and ion emission directly from the cathode and anode electrodes respectively, predicted the formation of an unstable, but magnetically insulated (electron Larmor radii < a-k gap spacing) electron sheath in the radial lines. The insulation was lost in the convolute, where electrons crossed the a-k gap at the magnetic nulls and impacted the anode, as well as wrapping around and impacting the downstream side of the anode posts. However, the magnitude of this electron flow current loss was found to be well below the 10% current loss measured at peak current. This result was consistent with equivalent LSP and Quicksilver simulations and circuit models including
only an electron flow current loss, as reviewed in section 2.6 in chapter 2.

Consistent with the recent spectroscopic plasma measurements made on ZR [17, 59], a fully ionised Hydrogen plasma was injected at $0.0075 \text{mln s}^{-1}$ with an initial temperature of $3 \text{eV}$, throughout the first cell next to the cathode electrode. With SCL ion emission from the anode electrode where the surface temperature exceeded 700K due to electron bombardment, the simulated current loss at peak current was increased to $\sim 2 \text{MA}$, consistent with the 10% experimental loss. As in the SCL emission only simulations, a magnetically insulated but unstable electron sheath was formed in the radial lines. Within the convolute, magnetic insulation was again lost and electrons impacted the anode at the positions of the magnetic nulls and on the downstream sides of the anode posts. The enhancement of the current loss compared to the SCL emission only simulations, came mainly from the cathode plasma penetrating the a-k gap on the downstream side of the anode posts, reducing the effective a-k gap spacing from 1cm to $\sim 2 \text{mm}$ and enhancing the electron loss rate to the anode across this gap. The plasma penetration came partly from plasma being transported from the upstream inner edge of the cathode holes, along magnetic field lines which collected on the downstream side of the anode posts. In addition, plasma which had expanded into the central magnetic null from the downstream cathode, was transported into the downstream sides of the anode posts, consistent with the direction of the $\vec{J} \times \vec{B}$ force, enhancing the plasma penetration into the a-k gap. Electron deposition on the upstream side of the anode posts was also enhanced by plasma penetrating into the magnetic nulls here.

The magnetic field topology was found to be identical for simulations with and without particles. The electron flow current was on the order of $100 \text{kA}$, such that the bound current dominated the magnetic field in the sheath regions. Within the plasma, the magnetisation was estimated to range between 40 and 1000, consistent with Hall like transport of the magnetic field into the plasma [16].

Our simulated current loss at peak current, was consistent with experimental measurements [2, 17] and the equivalent LSP simulation results [16]. The LSP simulations also found that the current loss was enhanced on the downstream side of anode posts, where the plasma penetration was partly due to plasma being transported from the inner edge of the upstream cathode, along field lines around the posts and collecting on the downstream side of the posts; the role of the plasma formed in the central null was
not highlighted in the LSP study [16]. We also observed additional late time plasma
dynamics; between 100 and 104ns, a plasma short was formed across the downstream
a-k gap of the bottom post. The short was subsequently transported in the positive
z-direction by the $\mathbf{J} \times \mathbf{B}$ force, opening the gap on the downstream side of the bottom
post and increasing the plasma density in the top post-hole gap and eventually, in the
inner MITL.

When plasma injection started at the same time as SCL electron emission, our sim-
ulations predicted a current loss of up to 1MA, at early times ($<10$MA). This was found
to be significantly larger than the experimental measurements [2, 17] and equivalent
LSP results [16]. This early time over prediction of the current loss was found to be
insensitive to refinements made in the spatial, temporal steps and particle statistics and
although it was reduced by $\sim50\%$ at later times, was still higher than experiment, using
linear interpolation.

The measured current loss at early times was found to be in better agreement with
our SCL emission only simulations. Here, the magnitude of the current loss decreased
up to $\sim10$MA, due to improving magnetic insulation in the electron sheath in the radial
lines with increasing current. As such, better agreement with the measured current loss
was achieved by delaying the time at which plasma creation began after SCL electron
emission; this delay was consistent with the time taken for the plasma to fill the cell next
to the cathode electrode and was a lower limit, as the assumed expansion velocity of
3cm$\mu$s$^{-1}$, was at the higher end of the measured scale [17]. Without the delay, the high
early time current loss in our simulations was consistent with Quicksilver results [58],
which did not introduce a delay to the start of the plasma creation [18]. It was not
ascertained whether the LSP model introduced a delay.

With no particle creation within a radius of 5cm, our 3D simulations predicted
a current loss of $\sim120$kA at peak current within the inner MITL, due to electrons
transported from the radial lines and convolute, being lost to the anode electrode in
the radial section. Due to the poor spatial resolution in the inner MITL in the 3D
simulations, we carried out a separate series of higher resolution 2D cylindrical r-z
simulations of the inner MITL. Both SCL emission only and cathode plasma simulations
were carried out; in both cases the level of current loss seen in the 3D simulations could
not be reproduced. In the 3D simulations, an electron sheath was formed next to the
anode electrode in the inner MITL from electrons transported from the convolute; this was not reproduced in the 2D inner MITL only simulations which had a radial extent of 6.4 cm and attempts to reproduce this sheath structure were unsuccessful. In addition, in the 3D simulations, plasma was transported into the inner MITL from the convolute; at peak current, plasma at a density comparable to the convolute filled the inner MITL. As such, it was concluded that to consistently investigate the current loss within the inner MITL, higher resolution coupled convolute and inner MITL simulations were required.

Although they did not reproduce the current loss, the 2D simulations were useful for studying the dynamics of the unstable electron sheath and the formation of a low density ion sheath, which were also observed in the 3D DPHC simulations. In the 2D simulations the cathode plasma remained tightly bound to the electrode due to the higher magnetic field strength associated with the higher currents and smaller radii. As in the 3D convolute plasma simulations, a low density, $\sim 10^{12-13}$ cm$^{-3}$, ion sheath was formed throughout the a-k gap from ions emitted by the cathode plasma. This was driven by field reversal on the cathode plasma surface due to the space-charge electric field associated with vortices formed in the electron sheath above the plasma.

The computational overhead of the fully kinetic simulations was substantial. At relatively coarse spatial resolutions, approximately one month of wall-clock time on 384 processors was required to reach peak current. Although the measured current loss of 10% at peak current was matched, the long run times precluded a thorough parameter scan of desorption rates, initial temperatures and plasma ion species. Additionally, it was not possible to establish convergence in the spatial cell size; this seemed particularly important due to the large discrepancy between the ion thermal energy and the electric potential energy in the a-k gap. In 1D studies the cathode plasma transport was found to be strongly dependent on the grid cell size [18]. With the goal of minimising the current losses within the current convolute and assessing new convolute designs, the fully kinetic model was not a practical design tool. The time step was governed by the requirement to resolve the electron cyclotron frequency; this was found to be necessary to accurately model the electron sheath dynamics and magnetic field transport in the plasma. In section 4.12, of this chapter, an attempt was made to reduce the run time by sub-cycling the particle push under the EM field solution; this was unsuccessful as the sub-cycling reintroduced the numerical electron heating instability, significantly
modifying the plasma dynamics and current loss prediction. Over the next two chapters we will investigate alternative methods to reduce the computational overhead of the convolute plasma simulations by assuming collisionality and treating either the electron or both the electron and ion plasma components using a less computationally intensive fluid model. The lower density plasma and charged particle sheath require a kinetic description; as such to accurately model the current loss mechanism, which is driven by a loss of electrons from the sheath to the anode, a hybrid fluid-kinetic model was required. In the next chapter we will investigate the applicability of a single fluid MHD model to the convolute plasma, as well as develop a hybrid MHD-PIC model, the basis of which will be formed by implementing our PIC code in the Gorgon MHD code [79].
Chapter 5

Magneto-hydrodynamics Model and Simulations

Gorgon [79], is an explicit, parallel, 3D resistive MHD code, used to simulate HEDP experiments ranging from Z-pinches [99,100], to laboratory astrophysics [79,101,102] and laser plasma interactions. The code solves the equations of magneto-hydrodynamics (MHD), describing the conservation of mass, Eqn.(5.1), momentum, Eqn.(5.2) and internal energy, Eqn.(5.3-5.4), in finite differenced form, on a discrete simulation grid. Here, \( \rho \), is the mass density, \( \vec{v} \), the fluid velocity, \( p_{i,e} \), the ion and electron fluid pressures, \( \vec{j} \), the plasma current density and \( \epsilon_{i,e} \), the ion and electron fluid internal energy densities. The system of equations, Eqn.(5.1-5.4), are evolved using the split scheme of Gentry et al. [103].

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \tag{5.1}
\]

\[
\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla (p_i + p_e) + \vec{j} \times \vec{B} \tag{5.2}
\]

\[
\frac{\partial \epsilon_i}{\partial t} + \nabla \cdot (\epsilon_i \vec{v}) = -p_i \nabla \cdot \vec{v} - \nabla \cdot \vec{q}_i + \Delta_i \epsilon \tag{5.3}
\]

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\[
\frac{\partial \epsilon_e}{\partial t} + \nabla \cdot (\epsilon_e \vec{v}) = -p_e \nabla \cdot \vec{v} - \nabla \cdot \vec{q}_e + \eta \left| \vec{j} \right|^2 - \Lambda + \Delta_{ei} \tag{5.4}
\]

The momentum equation, Eqn.(5.2), is solved in the single fluid approximation, whilst the energy equations, Eqn.(5.3) and Eqn.(5.4), are solved separately, allowing the ion and electron fluid temperatures to be out of thermodynamic equilibrium. For a quasi-neutral plasma with singly charged ions, the mass density, velocity and current density are related to the two-fluid parameters in Eqn.(5.5-5.7). Here, \(M\) and \(m\) are the masses of the ion and electron species respectively [69].

\[
\rho \equiv n_i M + n_e m \approx n (M + m) \tag{5.5}
\]

\[
\vec{v} \equiv \frac{1}{\rho} \left( n_i M \vec{v}_i + n_e m \vec{v}_e \right) \approx \frac{M \vec{v}_i + m \vec{v}_e}{M + m} \tag{5.6}
\]

\[
\vec{j} \equiv e \left( n_i \vec{v}_i - n_e \vec{v}_e \right) \approx ne (\vec{v}_i - \vec{v}_e) \tag{5.7}
\]

The energy equations are coupled through the energy exchange terms, \(\Delta_{ei} = -\Delta_{ie}\). Ohmic heating is described by \(\eta \left| \vec{j} \right|^2\), where \(\eta\) is the plasma resistivity and radiation losses included through \(\Lambda\). The system of equations, Eqn.(5.1-5.4) are closed by assuming the internal energy is related to the pressure by the ideal gas equation of state (EoS); for the ions this relation is given in, Eqn.(5.8) and for the electrons in Eqn.(5.9), where \(Q\) is the ionization potential energy and is a function of the average plasma ionisation \(Z\) [79]. The plasma ionisation is calculated from an average-ion Thomas-Fermi model [104]. The adiabatic index is taken to be \(\gamma = 5/3\) [79]. More modern versions of Gorgon have replaced the ideal gas EoS with tabulated data; this was necessary to accurately model the aluminium liners in the MagLif experimental concept [105]. However, in this study we have exclusively assumed an ideal gas EoS.

\[
\epsilon_i = \frac{p_i}{\gamma - 1} \tag{5.8}
\]

\[
\epsilon_e = \frac{p_e}{\gamma - 1} + Q(Z) \tag{5.9}
\]
The ion and electron thermal fluxes are evolved using Eqn. (5.10-5.11), where $\kappa_{i,e}$ are the thermal conductivities and $T_{i,e}$, the ion and electron fluid temperatures [79]. Both $\eta$ and $\kappa$ are calculated using Braginskii like transport coefficients [72] and include the effects of neutral collisions [106]. With a non-zero magnetic field, the transport coefficients parallel and perpendicular to the field lines can differ by many orders of magnitude. As such, the transport equations should strictly be split into components parallel and perpendicular to the magnetic field lines. For simplicity in Gorgon, all directions are assumed to be perpendicular to the magnetic field and a cell centred average of the magnetic field is used to calculate the transport coefficients.

$$q_i = -\kappa_i \nabla T_i$$ (5.10)

$$q_e = -\kappa_e \nabla T_e$$ (5.11)

Gorgon is novel, in that it uses explicit differencing exclusively. Here, the extra restrictions placed on the time and spatial steps for stability, over an equivalent implicit solution, have been offset by efficient parallelisation; Gorgon has demonstrated nearly linear scaling up to 12,000 processors. A key feature of the model, allowing this efficient parallelisation, is the EM field solver, which is described in the next section [107].

### 5.1 Vector Potential Field Solution

Gorgon uses a novel EM field solver to evolve the magnetic field, where the vector potential $\vec{A}$, is the fundamental quantity. In this scheme, the displacement current is maintained in Maxwell’s equations, allowing wave solutions in the large vacuum regions present in typical Gorgon simulations. This is in contrast to standard MHD codes and older versions of Gorgon, where the magnetic field over the whole simulation domain was updated via the induction equation and the vacuum was treated as a highly resistive medium, through which the magnetic field could quickly diffuse into the plasma regions of interest. For stability at the vacuum-plasma boundary, an implicit field solution was required; this represented a significant fraction of the total simulation time. Now, the vacuum region is still specified with a large resistivity, however this is only used to
enforce wave solutions in the vacuum [107]. The vector potential scheme was chosen to simply enforce \( \nabla \cdot \vec{B} = 0 \) in the plasma regions [108].

The vector potential is related to the magnetic field through Eqn.(5.12).

\[
\vec{B} = \nabla \times \vec{A}
\]  

(5.12)

Substituting Eqn.(5.12) into Faraday’s law, Eqn.(3.13), yields an expression for the electric field, Eqn.(5.13), where \( \varphi \) is the scalar potential.

\[
\vec{E} = -\frac{\partial \vec{A}}{\partial t} - \nabla \varphi
\]  

(5.13)

In the MHD approximation, the plasma is assumed to be quasi-neutral, \( n_e = \bar{Z} n_i = n \), and the charge density is taken to be zero [69]. In this limit, the scalar potential term in Eqn.(5.13) can be neglected [107].

The electrical properties of the plasma are described by a generalised Ohm’s law, Eqn.(5.14) [60,69].

\[
\vec{E} + \vec{v} \times \vec{B} = \eta \vec{j} + \frac{1}{en_e} \left( \frac{M m n}{e} \frac{\partial}{\partial t} \left( \frac{j}{n} \right) + (M - m) \vec{j} \times \vec{B} + m \nabla p_e - M \nabla p_i \right)
\]  

(5.14)

For slow motions, where inertial i.e. cyclotron frequency effects are unimportant, the \( \partial / \partial t \) term can be neglected; in the limit \( m/M \to 0 \) this gives Eqn.(5.15), where the \( \vec{j} \times \vec{B} \) term is known as the Hall current term [69].

\[
\vec{E} + \vec{v} \times \vec{B} = \eta \vec{j} + \frac{1}{en_e} \left( \vec{j} \times \vec{B} - \nabla p_e \right)
\]  

(5.15)

The Hall term can be neglected when \( B/\eta \) is much less than \( en_e \) i.e. \( \omega_{ce} \ll \nu_{ei} \) [69], where \( \omega_{ce} \) is the electron cyclotron frequency and \( \nu_{ei} \) is the electron-ion collision frequency. In typical systems to which Gorgon is applied, such as wire array Z-pinches, this is generally true. If we also assume that the pressure term is negligible, then the second term on the right hand side of Eqn.(5.15), can be neglected. As such, in Gorgon, the electrical properties of the plasma, are obtained from the simplified generalised Ohm’s law given in Eqn.(5.16) [107].

\[
\left( \vec{E} + \vec{v} \times \vec{B} \right) = \eta \vec{j}
\]  

(5.16)
Rearranging Eqn.(5.16) for the plasma current density, $\vec{j}$, and substituting it into Ampere’s law, including the displacement current, gives an equation for the evolution of $\vec{A}$, Eqn.(5.17), in the plasma [79].

$$\frac{\partial^2 \vec{A}}{\partial t^2} = -c^2 \nabla \times \nabla \times \vec{A} - \frac{\mu_0 c^2}{\eta} \left( \frac{\partial \vec{A}}{\partial t} - \vec{v} \times \nabla \times \vec{A} \right)$$  \hspace{1cm} (5.17)

Remembering that $\vec{E} = -\partial \vec{A}/\partial t$, Eqn.(5.17) is integrated to give the electric field at a time $t + \Delta t$, in terms of the field at time $t$, Eqn.(5.18), where $\Delta t$ is a small time step. Here, the terms involving the curl of $\vec{A}$ are assumed to be constant over $\Delta t$ [107].

$$\vec{E}(t + \Delta t) = \vec{E}(t)e^{-\frac{c^2 \mu_0}{\eta} \Delta t} - \frac{\eta}{\mu_0} \left( \nabla \times \nabla \times \vec{A} - \frac{\mu_0}{\eta} \vec{v} \times \nabla \times \vec{A} \right) \left( e^{-\frac{c^2 \mu_0}{\eta} \Delta t} - 1 \right)$$  \hspace{1cm} (5.18)

As will be shown in section 5.4, this expression is equivalent to taking an exponential difference of Ampere’s law, Eqn.(3.15), including the generalised Ohm’s law, Eqn.(5.16) [108]. In the vacuum limit, $\eta \to \infty$ and $\vec{v} = 0$ and Eqn.(5.18) reduces to a wave solution. In the plasma limit, $\eta \to 0$ and the solution describes the standard magnetic field diffusion and advection in the plasma. The vector potential at the new time is updated using $\vec{E} = -\partial \vec{A}/\partial t$. For stability, the field solver time step is taken to be $dt \leq x_{\text{min}}/2.5c$. This is typically smaller than the hydrodynamic time step, such that the field solver is sub-cycled under the fluid update [107].

The model allows flexibility in the choice of the numerical speed of light. For typical Gorgon simulations this is set to $c/10$, reducing the number of field solver sub-cycles and giving an overall speed up in the simulation run time. This is valid as $c/10$ is still larger than the highest plasma wave velocities of interest [107].

### 5.2 Hybrid Plasma Model

As discussed in chapter 4, the 3D kinetic PIC simulations of the cathode plasma evolution in the DPHC were computationally intensive, even with relatively poor spatial resolutions. To reduce the run-time and subsequently access improved spatial resolutions, we investigated the applicability of using the MHD model to simulate the plasma in the convolute. This is not without precedence; Jennings has used Gorgon to simulate
a Carbon plasma at a relatively higher density, in both the Z DPHC and inner MITL.

In our study, we focussed on modelling the lower density Hydrogen plasma, $\sim 10^{13-16}$ cm$^{-3}$, considered in the PIC simulations; as discussed previously, this is consistent with measured plasmas in the ZR convolute [17,59] and published PIC simulation results [16].

In the PIC simulations, the long run times were a result of resolving the large density gradients between the plasma and sheath, $\sim 10^{12-16}$ cm$^{-3}$ i.e. using many relatively small weight macroparticles, whilst resolving the electron cyclotron frequency in the large magnetic field generated by the high current. The hydro time step in Gorgon is set by the requirement to resolve the fastest wave speed; this is typically the Alfven velocity, which is given in Eqn.(5.19) and is typically less restrictive than the cyclotron frequency. As such, where the PIC convolute simulation took over one month, an equivalent MHD simulation of the plasma, would take less than one day to run.

$$v_A \equiv \frac{B}{(\mu_0 \rho)^{1/2}} \quad (5.19)$$

However, the MHD model makes a number of assumptions and approximations about the plasma. As the convolute plasma density was up to six orders of magnitude lower than the typical minimum density considered in Z-pinch simulations, for which Gorgon had been developed, the range of the applicability of the model must be considered.

Where the MHD approximation is definitely not applicable, is in the low density $\sim 10^{12-13}$ cm$^{-3}$ electron and ion sheath that is formed from the plasma. Here, finite space-charge and kinetic effects (to capture the instability) are important. As the current loss was driven by electron losses from the sheath to the anode electrode, in order to simulate the full convolute system, a hybrid model was therefore proposed; the denser plasma would be treated using the fluid description, whilst the lower density plasma and sheath would be described with the kinetic PIC model. The fluid and kinetic components would then be coupled through a common EM field solver and algorithms to consistently transfer plasma between the descriptions.

To this end, we implemented our PIC model, which was described in chapter 3, in Gorgon. Over the remainder of this chapter, we will describe the implementation and code modifications, as well as discuss test simulations of the Z DPHC.
5.3 Validity of the Fluid Approximation

The fluid plasma model is derived by taking velocity moments of the kinetic Vlasov-Fokker-Plank (VFP) equation. Here, each component of the plasma is assumed to be in local thermodynamic equilibrium (LTE), where the velocities are distributed according to a Maxwellian, characterised by a temperature \([60,109]\).

For the resulting transport equations and coefficients to be an accurate description of the plasma, all average quantities in the plasma must change slowly compared to the thermalisation time, \(\tau\) i.e. \(d/dt \ll 1/\tau\) and not vary significantly over distances comparable to those traversed by particles between collisions i.e. \(L \gg l\), where \(L\) is the characteristic scale length over which all quantities vary significantly, \(\nabla \sim 1/L\).

For zero magnetic field, the particles are assumed to follow straight line trajectories between collisions of length \(l \sim v_{th}\tau\), where \(v_{th}\) is the thermal velocity of the Maxwellian distribution. In a strong magnetic field, the spatial requirement is modified; in the simplest case, the particle orbits across the magnetic field are bounded by the Larmor radius, \(r_L\), such that the conditions for validity are now \(L_\perp \gg r_L\) and \(L_\parallel \gg l\). However, this is complicated by drift motions, which occur with a velocity of \(v_d\) and represent a displacement between collisions; the specific value for \(v_d\) is dependent on the geometry of the system \([72\).

There is an additional condition for accuracy in magnetised systems, as the effect of the magnetic field is not included in the calculation of the collisions. This simplification is valid when the Larmor radius is larger than the Debye length i.e. \(r_L \gg \lambda_D\) \([72\).

Considering a Hydrogen plasma at 3eV, as was loaded into the PIC convolute simulations, the density ranged between \(\sim 10^{13-16}\text{cm}^{-3}\). The electron-electron, ion-ion and electron-ion thermalisation times were calculated using Eqn.(3.7) and Eqn.(3.8) and the discussion in section 3.1.3; the results are shown in Table 5.i \([72\).

Comparing the electron-ion thermalisation time, \(\tau_{ei}\), with the current discharge time of 100ns, we see that up to \(10^{15}\text{cm}^{-3}\), \(\tau_{ei}\) is at least four times longer. As such, the electron and ion temperatures could separate, requiring separate energy equations for accuracy.

The Courant time step, represents the shortest time over which information about
Table 5.1: Thermalisation times for a fully ionised Hydrogen plasma at $T_e = T_i = 3$ eV for a range of densities.

<table>
<thead>
<tr>
<th>$n$ (cm$^{-3}$)</th>
<th>$\tau_{ee}$ (s)</th>
<th>$\tau_{ii}$ (s)</th>
<th>$\tau_{ei}$ (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{13}$</td>
<td>$1.8 \times 10^{-8}$</td>
<td>$1.1 \times 10^{-6}$</td>
<td>$3.3 \times 10^{-5}$</td>
</tr>
<tr>
<td>$10^{14}$</td>
<td>$2.0 \times 10^{-9}$</td>
<td>$1.2 \times 10^{-7}$</td>
<td>$3.7 \times 10^{-6}$</td>
</tr>
<tr>
<td>$10^{15}$</td>
<td>$2.3 \times 10^{-10}$</td>
<td>$1.4 \times 10^{-8}$</td>
<td>$4.3 \times 10^{-7}$</td>
</tr>
<tr>
<td>$10^{16}$</td>
<td>$2.7 \times 10^{-11}$</td>
<td>$1.7 \times 10^{-9}$</td>
<td>$5.0 \times 10^{-8}$</td>
</tr>
<tr>
<td>$10^{17}$</td>
<td>$3.3 \times 10^{-12}$</td>
<td>$2.0 \times 10^{-10}$</td>
<td>$6.1 \times 10^{-9}$</td>
</tr>
<tr>
<td>$10^{18}$</td>
<td>$4.2 \times 10^{-13}$</td>
<td>$2.5 \times 10^{-11}$</td>
<td>$7.7 \times 10^{-10}$</td>
</tr>
</tbody>
</table>

Changes in the plasma could be transmitted across a computational cell. For a typical cell size of 500 $\mu$m used in the MHD simulations, $\Delta t_{C_{ourant}} \sim 2.5 \times 10^{-13}$ s. Comparing this to the electron thermalisation time, $\tau_{ee}$, in Table 5.1, we see that $\Delta t_{C_{ourant}}$ is shorter over the entire density range coincided. However, the hydro time step is set by the Alfven wave speed; as such, changes in the plasma will in fact be transmitted on this time scale. Considering the convolute plasma parameters, the time associated with the Alfven speed, $\Delta t_A$, ranged between $\sim 2.5 \times 10^{-10}$ and $2.1 \times 10^{-11}$ s, which was comparable to $\tau_{ee}$ between densities of $10^{15}$ and $10^{16}$ cm$^{-3}$. However, below $10^{15}$ cm$^{-3}$, $\tau_{ee}$ $> \Delta t_A$, such that the assumption of LTE for the electrons is less valid below this density. In fact, at $10^{14}$ cm$^{-3}$, $\tau_{ee} \sim 100 \Delta t_A$ for the majority of the current pulse. As $\tau_{ii} \sim \left( \frac{m_p}{m_e} \right)^{1/2} \tau_{ee} \sim 42 \tau_{ee}$ [71, 72], the validity of the assumption that the ions are in LTE is even worse; between densities of $10^{14}$ and $10^{16}$ cm$^{-3}$, $\tau_{ii}$ ranges between 120 and 1.7 ns.

As $\tau_{ei}$ and $\tau_i$ scale as $T^{3/2}$, reducing the temperature to 1 eV improves the validity of the fluid approximation. Now, $\tau_{ee} = 0.48$ ns at a density of $10^{14}$ cm$^{-3}$. However, $\tau_{ii}$ is still 3.5 ns at $10^{15}$ cm$^{-3}$, which is $\sim 175 \Delta t_A$. In terms of applying the MHD model to the convolute plasmas, the validity of the approximation for the ions is therefore questionable. However, the MHD model has been successfully used to simulate the early time evolution of a plasma-opening-switch (POS), which had similar densities and temperatures to the convolute plasma [86]. As the electron-ion thermalisation time was
Table 5.ii: Electron and ion mean-free-paths, $l$, with $B=0$T for 1, 3 and 10eV at a range of densities.

<table>
<thead>
<tr>
<th>$n$ (cm$^{-3}$)</th>
<th>1 (1eV) (m)</th>
<th>1 (3eV) (m)</th>
<th>1 (10eV) (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{13}$</td>
<td>2.5x10$^{-3}$</td>
<td>1.9x10$^{-2}$</td>
<td>1.7x10$^{-1}$</td>
</tr>
<tr>
<td>$10^{14}$</td>
<td>2.8x10$^{-4}$</td>
<td>2.1x10$^{-3}$</td>
<td>1.9x10$^{-2}$</td>
</tr>
<tr>
<td>$10^{15}$</td>
<td>3.4x10$^{-5}$</td>
<td>3.4x10$^{-4}$</td>
<td>2.2x10$^{-3}$</td>
</tr>
<tr>
<td>$10^{16}$</td>
<td>4.2x10$^{-6}$</td>
<td>4.0x10$^{-5}$</td>
<td>2.5x10$^{-4}$</td>
</tr>
<tr>
<td>$10^{17}$</td>
<td>5.4x10$^{-7}$</td>
<td>4.8x10$^{-6}$</td>
<td>2.8x10$^{-5}$</td>
</tr>
<tr>
<td>$10^{18}$</td>
<td>7.7x10$^{-8}$</td>
<td>6.1x10$^{-7}$</td>
<td>3.4x10$^{-6}$</td>
</tr>
</tbody>
</table>

estimated to be either longer than, or a significant fraction of, the current discharge time, this necessitates the use of separate electron and ion energy equations; as described at the start of this chapter, Gorgon includes separate energy equations for the electrons and ions.

In the directions parallel to the magnetic field and within the magnetic nulls, assuming $T_e = T_i$, then the mean-free-paths (mfps) for the electrons and ions, are comparable [71, 72]. These are given at 1, 3 and 10eV for a range of densities in Table 5.ii. Again considering the typical simulation cell size of $\Delta x = 500\mu m$, used in the MHD simulations, at 1eV we see that at densities of $10^{14}$cm$^{-3}$ and above $l < \Delta x$. However, this threshold is shifted up to $10^{15}$ and $10^{16}$cm$^{-3}$ at 3 and 10eV, respectively. Considering the PIC convolute simulations results, in the radial lines we found that the plasma was relatively uniform parallel to magnetic field lines along the $\theta$-direction, such that we could take the characteristic scale length $L_{||}$ to be longer than the cell length anyway. However, in the magnetic nulls and along field lines within the convolute, $\Delta x$ should still set the plasma scale length. Here the path lengths will be given by Table 5.ii and as such the assumption that the mfp’s are shorter than the cell size is not valid for the full density range.

In the convolute simulations, the magnetic field in the plasma was both a function of the time in the current pulse and the radial coordinate. Considering the radial lines, between 30 and 120ns, the magnetic field strength ranged between $\sim 4$ and 8T,
corresponding to electron, $r_{Le}$, and ion, $r_{Li}$, Larmor radii of between 2.2 and 1.3µm and 93 and 55µm, respectively; therefore, at worse $r_{Li} \sim 0.19\Delta x$.

On the downstream side of the bottom post, the magnetic field strength ranged between 8 and 17T, with corresponding electron and ion Larmor radii of 1.4 to 0.67µm and 60 to 28µm, respectively. On the downstream side of the top post, the magnetic field was approximately twice as large, with Larmor radii of therefore approximately half the bottom post values. In the magnetised regions, both the electron and ion Larmor radii were therefore at least ten times smaller than the cell size.

The MHD model makes a number of further approximations, mainly in the simplification of the generalised Ohm’s law, which is used to calculate the electrical properties of the plasma, as discussed in section 5.1. Here, the Hall term was neglected assuming that the electron cyclotron frequency was much smaller than the electron-ion collision frequency, i.e. $\omega_{ce} << \nu_{ei}$ or $\omega_{ce} \tau_{ei} << 1$, where $\omega_{ce} \tau_{ei}$ is the magnetisation of the plasma [60, 69, 109]. Taking the electron-ion momentum transfer time, $\tau_{ei} \sim \tau_{ee}$, this decreases with increasing plasma density and from Table 5.1, is equal to 0.027ns at density of $10^{16}$cm$^{-3}$ and temperature of 3eV. The magnetic field strength in the convolute ranges between 5 and 8T in the radial lines, 5 and 15T on the downstream side of the bottom anode post and 10 and 30T on the downstream side of the top post. Taking the lowest value of 5T gives a magnetisation of $\omega_{ce} \tau_{ei} \sim 200$, which is not consistent with the limit $\omega_{ce} \tau_{ei} << 1$. For lower density and higher magnetic field strengths, the magnetisation is larger, such that it was concluded that neglecting the Hall term was not a valid assumption over the entire range of the convolute plasma parameters. A method to consistently and stably include the Hall term in the Gorgon EM field solution, will be described in section 5.4.2.

In this study, we have not considered the effects of neglecting the pressure term in the generalised Ohm’s law. We do however note that this term was not included in the MACH2 model of the POS [86], due to issues regarding the fact that in the single fluid approximation, energy was advected with the fluid and not the electron drift velocity. Further investigation into this term was therefore left as further work.
5.4 Electromagnetic Field Solution

The novel, explicit field solver, described in section 5.1, which allows wave solutions in the vacuum [79, 107], is one of the main features of Gorgon that made it applicable to simulating transmission line systems. However, the assumption of quasi-neutrality, which was used to justify neglecting the scalar potential part of the electric field, will only be valid for the MHD description of the plasma [107].

Initially, it was thought that the neglect of the scalar potential in the standard A-field solver precluded its use for modelling the electron sheath formed in the convolute, which has a non-zero space-charge. As such we investigated retaining the scalar potential in Eqn.(5.13). On substitution of Eqn.(5.13) in Ampere’s law, in addition to Eqn.(5.16), to evolve the vector potential, $\vec{A}$, an additional Poisson equation for the scalar potential, $\phi$, would also have to be solved. This is an elliptical partial differential equation [110] and therefore typically requires an iterative solution, which are difficult to efficiently parallelise. We tested a number of solution methods, ranging from direct matrix inversion, through to various implementations of the Jacobi iteration method [93]. For solutions in 3D, we found that the alternating-direction-implicit (ADI) method converged the fastest [110]. However, this still required tens of iterations per time step; as at each iteration the grid information had to be passed on the domain boundaries, the solution was very slow on multiple processes. In addition, electrode and vacuum boundary conditions were more complicated to implement than the EM scheme used in the PIC model. With the aim of implementing the PIC model in Gorgon, we therefore developed a new EM solver, based on the Yee scheme [83] described in section 3.4, which updated the electric and magnetic fields directly.

Following section 3.4, the change in the magnetic field was obtained from Faraday’s law, Eqn.(5.20), whilst the change in the electric field followed from Ampere’s law, including the displacement current, Eqn.(5.21) [62,107].

$$\frac{\partial \vec{B}}{\partial t} = -\vec{\nabla} \times \vec{E} \quad (5.20)$$

$$\vec{\nabla} \times \vec{B} = \mu_0 \vec{j} + \frac{1}{c^2} \frac{\partial \vec{E}}{\partial t} \quad (5.21)$$
Now \( \vec{j} = \vec{j}_p + \vec{j}_{\text{plasma}} \), where \( \vec{j}_p \) is the macroparticle current and \( \vec{j}_{\text{plasma}} \) the plasma currents. The plasma current was given by the generalised Ohm’s law, Eqn.(5.22). Note that we initially neglected the Hall term, as was done in the standard Gorgon field solver [107].

\[
\vec{j}_{\text{plasma}} = \frac{1}{\eta} (\vec{E} + \vec{v} \times \vec{B})
\]

(5.22)

For second order accuracy, the electric and magnetic fields were again leap-frogged in time [62, 63, 83]. Substituting Eqn.(5.22) in Eqn.(5.21), the resulting equation was differenced as in Eqn.(5.23). Here, the electric field in the plasma current was treated implicitly and set to the new time step \( t^{n+1} \); this was found to improve the stability properties of the model [12].

\[
\vec{E}^{n+1} \left( 1 + \frac{\mu_0 c^2 \Delta t}{\eta} \right) = \vec{E}^n + \frac{\mu_0 c^2 \Delta t}{\eta} \left[ \frac{\eta}{\mu_0} \left( \vec{\nabla} \times \vec{B}^{n+1/2} - \vec{j}_p^{n+1/2} \right) - \vec{v}^n \times \vec{B}^{n+1/2} \right]
\]

(5.23)

Recasting Eqn.(5.23) as an exponential difference, Eqn.(5.24) [108]; with \( \vec{B} = \vec{\nabla} \times \vec{A} \), we see that this is equivalent to Eqn.(5.18) in the standard A-field solution.

\[
\vec{E}^{n+1} = e^{-\frac{\mu_0 c^2 \Delta t}{\eta}} \vec{E}^n + \left( 1 - e^{-\frac{\mu_0 c^2 \Delta t}{\eta}} \right) \left[ \frac{\eta}{\mu_0} \left( \vec{\nabla} \times \vec{B}^{n+1/2} - \vec{j}_p^{n+1/2} \right) - \vec{v}^n \times \vec{B}^{n+1/2} \right]
\]

(5.24)

The magnetic field was then updated via the difference of Eqn.(5.20) given in Eqn.(5.25). Note that the magnetic field leads the electric field by half a time step; to obtain the magnetic field at the full time \( t^{n+1} \), it was averaged as \( \vec{B}^{n+1} = \left( \vec{B}^{n+1/2} + \vec{B}^{n+3/2} \right) / 2 \) [62].

\[
\vec{B}^{n+3/2} = \vec{B}^{n+1/2} - \Delta t \vec{\nabla} \times \vec{E}^{n+1}
\]

(5.25)

Taking the curl of the equation used to update the vector potential from the electric field, \( \vec{E} = -\partial \vec{A} / \partial t \) in the Gorgon solver, with \( \vec{B} = \vec{\nabla} \times \vec{A} \), we see that this is just Faraday’s law, Eqn.(5.20). As such, our scheme was completely equivalent to the standard Gorgon A-field solver! In the PIC model, the electric field solution was made consistent with Gauss’s law i.e. the scalar potential, by ensuring that the macroparticle current,
\( \vec{j}_p \), satisfied the continuity equation, Eqn.(3.16) in section 3.3 of chapter 3. As such, if we employed the same macroparticle current interpolation scheme in the hybrid model, then either EM field solution scheme could be used. We decided to continue with the direct electric and magnetic field solution, as it had already been coupled to the relevant circuit and electrode boundary conditions in the PIC model.

As in section 3.4, the curl terms, \( \vec{\nabla} \times \vec{E} \) and \( \vec{\nabla} \times \vec{B} \), were calculated using the staggered Yee-mesh to ensure second order accuracy in the spatial step [83].

Taking the vacuum limit, \( \eta \to \infty \) i.e. \( e^{-\mu_0 c^2 \Delta t/\eta} \to 1 \) and \( \left(1 - e^{-\mu_0 c^2 \Delta t/\eta}\right) \to -\mu_0 c^2 \Delta t/\eta \), and \( \vec{v} = 0 \), Eqn.(5.23) reduces to the standard PIC expression for the electric field update. Taking the plasma limit, \( \eta \to 0 \) i.e. \( e^{-\mu_0 c^2 \Delta t/\eta} \to 0 \), Eqn.(5.23) reduces to Eqn.(5.26)

\[
\vec{E}^{n+1} = \frac{\eta}{\mu_0} \vec{\nabla} \times \vec{B}^{n+1/2} - \vec{v}^n \times \vec{B}^{n+1/2} \tag{5.26}
\]

Substituting Eqn.(5.26) into Eqn.(5.25), gives Eqn.(5.27), where we have set \( \vec{j} = \left(\vec{\nabla} \times \vec{B}\right)/\mu_0 \) (Ampere’s law without the displacement current) and \( \vec{j}_p = 0 \); Eqn.(5.27) is an explicit difference of the standard magnetic field induction equation.

\[
\vec{B}^{n+3/2} = \vec{B}^{n+1/2} - \Delta t \left(\eta \vec{j} - \vec{v}^n \times \vec{B}^{n+1/2}\right) \tag{5.27}
\]

In practice, the resistivity was used to switch between the plasma and vacuum limits. In the vacuum an artificially large resistivity was set, which forced the standard EM wave solution. In the plasma, the full expression, given in Eqn.(5.24), was used [107].

For stability, a time step of \( \Delta t = \Delta x_{\text{min}}/2.5c \), where \( \Delta x_{\text{min}} \) was the smallest grid length, was required [107]. As can be seen from the denominator, this was \( \sim \Delta t_{\text{Courant}}/2.5 \). The extra stability constraint came from the solution in the plasma regions. Note that if the electric field in the generalised Ohm’s law was included explicitly, i.e. \( \vec{E}^n \) instead of \( \vec{E}^{n+1} \), in Ampere’s law, then the stability constraint on the time step was even more severe [12].

As the electron inertia was neglected in the generalised Ohm’s law, we assumed that the electrons were sufficiently mobile such that the electric field instantaneously drove a current in the plasma given by Eqn.(5.28) [107]. This quantity was calculated after each time the electric field was updated. The electric field was defined on the cell edges,
as such the plasma current was also defined here. The plasma resistivity was calculated from the plasma density, temperature and magnetic field strength and as such was cell centred. To calculate Eqn. (5.28), the resistivity was first spatially averaged to the cell edges. In 3D, this was a four cell average; a cell was only included in the average if its density was above a vacuum threshold.

\[ \tilde{J}_{\text{plasma}}^{n+1} = \frac{\tilde{E}^{n+1}}{\eta} \]  

(5.28)

5.4.1 Evaluation of the \( \vec{v} \times \vec{B} \) Term

Following the standard Gorgon solver, the \( \vec{v} \times \vec{B} \) term in Eqn. (5.24), was evaluated using an upwind difference scheme [107]. The fluid velocity was cell centred; the relevant component of the velocity in the cross product was therefore first spatially averaged to be coincident with the edge centred electric field components. In 3D, this was a four point average. The product with the magnetic field was then formed with the cell face centred component in the upwind direction of the averaged edge centred fluid velocity. For second order accuracy, the fluxes were corrected using the vanLeer scheme [79,111].

In practice, direct application of Eqn. (5.24), in the plasma cells was unstable; the electric field in the plasma was found to grow to unphysical, large values, driving a current that heated the plasma until the simulation crashed. This issue followed from including the \( \vec{v} \times \vec{B} \) term directly into the electric field update, Eqn. (5.24). The standard Gorgon A-field solver actually includes this term in the magnetic field update directly; adopting this methodology in our direct solver gave stable results.

Taking the \( \vec{v} \times \vec{B} \) term out of Eqn. (5.24), the magnetic field update, Eqn. (5.25), was modified to give Eqn. (5.29). Note that for the macroparticle push step and diagnostic purposes, we stored a separate electric field array which included the \( \vec{v} \times \vec{B} \) term.

\[ \vec{B}^{n+3/2} = \vec{B}^{n+1/2} - \Delta t \left( \vec{\nabla} \times \vec{E}^{n+1} - \vec{\nabla} \times \vec{v}^m \times \vec{B}^{n+1/2} \right) \]  

(5.29)

To ensure that the magnetic field satisfied \( \vec{\nabla} \cdot \vec{B} = 0 \), a constrained transport scheme was used to evaluate \( \vec{\nabla} \times \vec{v} \times \vec{B} \) [112,113]; this simply involved calculating and storing all of the \( \vec{v} \times \vec{B} \) terms first, using the upwind difference described above and then calculating the spatial gradients using these common values. Note that this was significantly simpler.
than the Flux-Constrained transport schemes [110], used for the same purpose in other codes [108]. As the $\vec{v} \times \vec{B}$ terms were calculated on the cell edges, the same Yee difference [83] that was used for the $\nabla \times \vec{E}$ term, was also used for $\nabla \times \vec{v} \times \vec{B}$ term, ensuring second order accuracy in the calculation of the spatial gradient [62,63].

Note that the fluid velocity in Eqn.(5.29), was taken from the old time step, $t^n$. As discussed above, the field solver time step was typically shorter than the hydro step and was therefore sub-cycled. In the standard A-field solver, $\vec{v}^n \times \vec{B}^n$ was calculated once, before the start of the sub-cycling [107]. In contrast, we recalculated the quantity at each sub-cycle, using the latest value for the magnetic field, assuming the fluid velocity was constant over the hydro step.

5.4.2 Evaluation of the Hall Term

As describe in section 5.3, the neglect of the Hall term in the generalised Ohm’s law, Eqn.(5.15), was no longer valid for the relatively low density convolute plasmas. For accuracy in the convolute simulations, the Hall term was therefore included in the field solution; this introduced an additional, non-linear magnetic field advection term into the induction equation [56,86].

Retaining the Hall term, whilst still neglecting the inertial and pressure terms, the generalised Ohm’s law can be rearranged to give the plasma current as in Eqn.(5.30) [60,69]. In the last expression, we have identified $-\vec{j}_{\text{plasma}}/en_e$, with the electron drift velocity, $\vec{v}_e$.

$$\vec{j}_{\text{plasma}} = \frac{1}{\eta} \left( \vec{E} + \vec{v} \times \vec{B} - \frac{1}{en_e} \vec{j}_{\text{plasma}} \times \vec{B} \right) = \frac{1}{\eta} \left( \vec{E} + \vec{v} \times \vec{B} + \vec{v}_e \times \vec{B} \right)$$ (5.30)

Substitution of Eqn.(5.30) into Ampere’s law gives Eqn.(5.24), including the extra $\vec{v}_e \times \vec{B}$ term. As was found for the $\vec{v} \times \vec{B}$ term, direct inclusion of the Hall term in the electric field update was unstable. Following the $\vec{v} \times \vec{B}$ scheme, the Hall current was instead included directly in the magnetic field update as in Eqn.(5.31). Again, for the macroparticle push step and diagnostic purposes, the Hall term was also added to the separate electric field array which included the $\vec{v} \times \vec{B}$ term.
\[\vec{B}^{n+3/2} = \vec{B}^{n+1/2} = \Delta t \left( \vec{\nabla} \times \vec{E}^{n+1} - \vec{\nabla} \times \vec{v}^{n} \times \vec{B}^{n+1/2} - \vec{\nabla} \times \vec{v}_{e}^{n+1/2} \times \vec{B}^{n+1/2} \right) \]  

(5.31)

Note that we used the current at the latest time, \(\vec{j}_{\text{plasma}}^{n+1}\) (consistent with \(\vec{E}^{n+1}\)), in the Hall term; we found that the results were insensitive to using a temporal average of the values at the old and new time step.

The cross product, \(\vec{v}_{e} \times \vec{B}\), was again evaluated using an upwind difference scheme [107]. As the plasma current was defined on the cell edges, some spatial averaging was required. Initially, the separate components of \(\vec{j}_{\text{plasma}}^{n+1}\) were averaged from their staggered positions; this was found to give rise to a checker-board instability in the magnetic field. This could be removed by first averaging each component of the current density to the cell centre, consistent with the \(\vec{j} \times \vec{B}\) force calculation in the momentum equation and then using the same averaging as was used for \(\vec{v}\) to form \(\vec{v} \times \vec{B}\), as described in the previous section.

To form \(\vec{v}_{e}\) from \(\vec{j}_{\text{plasma}}\), the plasma electron number density was required, which was a cell centred quantity. To obtain the cell centred electron drift velocity two schemes were tried; in the first, the density was averaged to the cell edges and \(\vec{v}_{e}\) calculated before being averaged to the cell centre. In the second, the current density was first averaged to the cell centre and the cell centred density used to form \(\vec{v}_{e}\). Again, the results were found to be insensitive to this choice; for simplicity the second scheme was adopted.

Finally, the cross product with the differential operator, \(\vec{\nabla} \times \vec{v}_{e} \times \vec{B}\), was again evaluated using the constrained transport method [112,113] i.e. \(\vec{v}_{e} \times \vec{B}\) was first calculated and stored on the grid and the spatial gradients calculated using common values.

The above implementation of the Hall term was found to be stable with the standard EM field solver time step of \(\Delta t = \Delta x_{\text{min}}/2.5c\) [107]. An issue that threatened this stability, was the occurrence of lower density cells with \(v_{e} > c\). A fix for this issue, using the plasma resistivity, will be discussed in the next section, but for safety we also included a numerical limiter in the field solver itself. Here, a hard limit of \(v_{e} \leq c\) was enforced. In fact, by lowering this limit, the rate of the magnetic field advection could be varied.
5.5 MHD Z DPHC Simulations

To test the stability of the field solver, including the Hall term and the fluid transport algorithms at the relatively low convolute plasma densities, we initially carried out a series of MHD plasma only simulations of the Z DPHC convolute. Here, we additionally wanted to investigate if the plasma evolution and dynamics observed in the PIC simulations could be reproduced at least qualitatively by the fluid model.

These simulations used the same electrode geometry, Figure 4.1 and load and transmission line circuit models, as the PIC simulations presented in chapter 4. However, the cell size was reduced to $\Delta r = \Delta z = 500\mu m$ and $\Delta \theta = \pi/12/40$ radians (half the PIC cell size along each axis). We again applied reflective conditions at the $\theta$-boundaries and modelled a $\pi/12$ extent along the $\theta$-direction i.e. half of a single layer of the 12 post convolute.

The electrodes were again assumed to be perfect conductors; the parallel components of $\vec{E}$ and the perpendicular components of $\vec{B}$, to the electrode surface, were set to zero after each field update. Additionally, the parallel component of the plasma current was also set to zero on the electrode surface. The coupling of the simulation grid to the circuit models was identical to the PIC simulations, as described in section 4.2 in the previous chapter, due to the equivalence of the EM field solution in the vacuum cells.

5.5.1 Vacuum Cut-off Density Threshold

As discussed at the beginning of this chapter, Gorgon is an Eulerian code; the numerical grid is fixed and the plasma is transported through it. As such, at the plasma-vacuum interface low density plasma cells are formed, which introduce short time scales i.e. high Alfven speeds, Eqn.(5.19), into the simulation. To maintain practical simulation time steps, it is therefore necessary to define a lower plasma mass density cut-off $\rho_{vac}$, below which a cell is forced to be vacuum. This is necessary anyway, as the fluid approximation becomes less accurate at lower densities, as discussed in section 5.3. To further control the time step, Gorgon includes a modification which reduces the Alfven speed to a user defined value, $s_{max}$, by self-consistently increasing the inertia during the Lagrangian acceleration step [114]. Care must be taken that $s_{max}$ is larger than the fastest process
of interest in the system.

The implementation of a lower density cut-off introduces a mass conservation error into the advection step. To avoid quickly filling the entire volume with low density plasma, only a single layer of cells on the surface of the plasma are allowed to be below \( \rho_{\text{vac}} \). In these cells, the density was initially set to \( \rho_{\text{vac}}/10 \) and only became part of the plasma proper when the density was greater than or equal to \( \rho_{\text{vac}} \). Any mass which was transported out of the transition cells, into the vacuum, was lost from the simulation. It was therefore important to set the threshold low enough to capture all of the densities of interest.

In typical Gorgon simulations of Z-pinches, \( \rho_{\text{vac}} = 10^{-4} - 10^{-2} \text{kgm}^{-3} \). From the PIC simulations, we found that the Hydrogen plasma density ranged between \( \sim 10^{13-16} \text{cm}^{-3} \), corresponding to mass densities of \( 10^{-8} \) to \( 10^{-5} \text{kgm}^{-3} \). As such, the lower density threshold had to be lowered significantly from the Z-pinch case. Considering the accuracy of the fluid approximation, section 5.3, we chose \( \rho_{\text{vac}} = 10^{-7} \text{kgm}^{-3} \), corresponding to a number density of \( 10^{14} \text{cm}^{-3} \). Below this density, the ion thermalisation time was estimated to be longer than the current discharge and the mfp in the directions parallel to the magnetic field and in the zero magnetic field null regions, was a significant fraction of the a-k gap spacing. However, even at this threshold, the applicability of the fluid model to the ion component of the plasma was questionable.

### 5.5.2 Time Step and EM Solver Sub-cycling

The EM solver was sub-cycled under the hydro solution using a time step of \( \Delta t = \Delta x_{\text{min}}/2.5c \). Here, the minimum grid length was \( \Delta x_{\text{min}} = 1.9\Delta \theta \text{cm} \), where a minimum radius of 1.9cm was used, as in the PIC simulations. Below this radius the solution transitioned to 2D cylindrical r-z coordinates, where uniformity along the \( \theta \)-direction was assumed. Additional, as we were ultimately interested in the EM wave propagation in the transmission lines, the physical value for the speed of light, c, was used. The hydro time step was set by the time for an Alfven or sound wave to propagate across the minimum cell length, \( \Delta x_{\text{min}} \). Here, we set \( s_{\text{max}} = 0.1c \) to limit the maximum Alfven velocity. This was higher than typical values of \( \sim 2 \times 10^6 \text{ms}^{-1} \) used in Z-pinch simulations, to reflect the lower density of the convolute plasma. We found that the
simulations were insensitive to further reducing the hydro time step. For example, we ran the hydro solution with the EM solver time step, i.e. without sub-cycling and obtained very similar results.

5.5.3 Plasma Creation Model and Electrode Boundary Conditions

Following the phenomenological cathode plasma creation model used in the PIC simulations, we modelled the plasma creation process by loading a fully ionised Hydrogen plasma directly into the first vacuum cell next to the electrode, at a user defined desorption rate, \( \nu_{\text{desorp}} \), in units of monolayers (1ml=10^{15} \text{cm}^{-2}) per nanosecond. The mass of plasma injected in each cell at each time step was then calculated from \( \Delta m = \nu_{\text{desorp}} A_{\text{cell}} \Delta t \), where \( \Delta t \) was the time step in nanoseconds and \( A_{\text{cell}} \) was the area of the electrode cell surface in cm\(^2\). The particles were loaded uniformly throughout the cell; if the density of the cell was less than \( \rho_{\text{vac}}/10 \) then the injected mass was stored until \( \sum_t \Delta m/V \geq \rho_{\text{vac}}/10 \). Here, \( V \) is the volume of the cell, consistent with the assumption that plasma was created uniformly throughout the volume and \( \sum_t \), denotes the sum over the time steps until the condition was met. As discussed in section 4.9 of the previous chapter, in the PIC simulations we found that we could control the early time current loss by adding a delay to the start of the plasma creation, to account for the finite expansion velocity. In the MHD simulations, we did not include such a delay; however, the minimum density requirement did introduce a delay of several nanoseconds.

Plasma creation began when the normal component of the electric field exceeded 240kVcm\(^{-1}\), the threshold for neutral desorption and ionisation \([16, 21]\). In Gorgon, the density is cell centred; as such the creation algorithm was applied to the centre of the electrode surface faces. The normal components of the electric field used in the threshold test, were therefore spatially averaged from the cell edges to the cell centre.

In the PIC simulations, the initial velocities of the electron and ion macroparticles were sampled from a Maxwellian distribution at a temperature of 3eV. Following section 5.3, we decided to load the MHD plasma at a lower temperature of 1eV, as the fluid approximation was more accurate. This temperature was also used to calculate the energy to add to the plasma components, assuming an ideal gas EoS and full ionisation.
This energy was stored in the creation algorithm and then self-consistently added to the plasma, along with the other source terms, when the energy equations were solved to update the plasma temperature.

The baseline PIC plasma simulations used a desorption rate of $0.0075 \text{mln s}^{-1}$; due to the electrode boundary conditions, which will be discussed below, we found that this rate lead to plasma densities of $>10^{23} \text{cm}^{-3}$ in the source cell, which was approximately one hundred times higher than the plasma formed in the PIC simulations. As such, the plasma desorption rate was tuned in the MHD case to control the peak density in the source cells.

The plasma boundary conditions at the electrode surface were a difficult part of the model. In the PIC simulations, a sheath was formed at the cathode electrode to drive the return current; physically this return current is carried by the ions [27]. In the PIC simulations, this was supplemented by a SCL electron current [94]. This boundary layer could not be easily modelled in the quasi-neutral MHD plasma model.

We tried a range of electrode boundary conditions to approximate the PIC results. The results which will be presented in section 5.5.5, allowed a finite pressure, but set the force to zero in the boundary cell; this was found to prevent significant mass loss to the electrode due to the pressure gradient (the pressure was set to zero within the electrode). However, a finite fluid velocity at the electrode boundary was allowed; as such, there was a finite mass flux (using the velocity averaged to the cell faces) across the electrode surface. In practice this was small, such that the plasma desorption rate had to be reduced below the PIC simulation value to reproduce a similar density in the source cell, as discussed above. We were not completely satisfied with this treatment and further development is therefore required.

For the convolute simulations, we found that the code kept crashing in the ionisation routines, which calculated an average ionisation, $\bar{Z}$, based on a Thomas-Fermi average atom model [79]. To avoid this issue and following the PIC simulations, we assumed the plasma remained fully ionised throughout the current pulse. As such, the ionisation routine was skipped over and $\bar{Z}$ set to one in all the plasma cells.
5.5.4 Controlling the Electron Drift Velocity

Assuming the electrons carry the plasma current, the electron drift velocity is given by Eqn.(5.32), where $\vec{v}$ is the bulk fluid velocity [86]. A problem that was quickly encountered when modelling the low density convolute plasma, was superluminal electron drift velocities, $v_e > c$, in the lowest density cells. This typically occurred at the vacuum-plasma interface where, due to the skin effect [19], the electric field and therefore plasma current were largest.

$$\vec{v}_e = \vec{v} - \frac{\vec{j}}{en_e} \quad (5.32)$$

These high currents heated the plasma to temperatures of $> 10^5 \text{eV}$, through a combination of Ohmic and PdV heating. Additionally, the inclusion of the Hall term in the magnetic field update became unstable as the magnetic field could be advected across a cell in less than the time step. Note that this issue was also found to occur with both the standard A-field solver and the direct E and B solver without the Hall term, such that the new field solution and Hall current could be ruled out as the cause of the problem; inclusion of the Hall term did however make the simulation crash earlier, due to its dependence on the electron drift velocity.

The unphysical electron drift velocities followed from neglecting the inertial term in the generalised Ohm’s law, Eqn.(5.14), where this approximation was least valid in the lower density plasma [60, 69]. An attempt was made to include the inertial term in the Gorgon EM field solution; however, the validity of the resulting scheme was not clear. As an alternative, we therefore investigated controlling the electron drift velocity by modifying the plasma resistivity.

The electrons were assumed to instantaneously carry the current consistent with the electric field according to Eqn.(5.28). Here, we see that the current is inversely proportional to the plasma resistivity. Physically, when the drift velocity is larger than the sound speed, the lower-hybrid instability is excited. This generates additional scattering of the electrons from the lower-hybrid plasma wave, raising the effective electron collision frequency and giving an anomalous resistivity. Anomalous resistivity has already been included in the standard Gorgon resistivity calculation; the term is proportional to the ratio of the squares of the electron drift and sound speeds [115]. On its own, this
was insufficient to maintain \( v_e < c \). As such, we tried increasing the anomalous collision frequency by making it proportional to the fourth power of the ratio of the wave speeds; again we found that this was not sufficient.

Taking this idea further, we found that the electron drift velocity could be controlled by artificially increasing the plasma resistivity. Here, we were essentially forcing the lowest density plasma cells to be closer to vacuum, which is not completely unphysical. This scheme is not dissimilar to the more standard MHD codes, where there is no wave solution and the vacuum is treated as a highly resistivity medium through which magnetic field can quickly diffuse [86, 107].

Combining \( \vec{j} = \vec{E}/\eta \) with \( \vec{v}_e = -\vec{j}_e/e n_e \), an expression for the resistivity in terms of the drift velocity can be obtained, as in Eqn.(5.33).

\[
\eta = \frac{E}{e n_e v_e} 
\]  

(5.33)

From Eqn.(5.33), we calculated a limiting resistivity, \( \eta_{\text{limit}} \), by forcing \( v_e \) to take a user defined value of \( v_{e,\text{limit}} \). In Gorgon, the resistivity is calculated at the cell centres. To form the currents from the electric fields on the cell edges, the cell centred resistivity was spatially averaged to these positions. Initially, we applied Eqn.(5.33) at the cell edges and replaced the spatially averaged resistivity with the maximum of the standard and limited value. We found that this method gave non-satisfactory results. Instead, the cell centred values of the resistivity were modified directly as follows; first, the electric fields on the edges of the cell were tested and the largest used in Eqn.(5.33), to obtain the limiting resistivity. The resistivity in the cell was then set to the larger of the standard and limiting resistivity; we additionally only allowed a \( \pm 5\% \) change to the value from the old time step, in order to avoid rapid transitions between the plasma and vacuum limits in the field solution. If this was not included, the electric field in the vacuum contained high frequency noise. In the convolute simulations, we limited the electron drift velocity to \( v_{e,\text{limit}} = 0.1c \) in Eqn.(5.33). It should be noted that superluminal electron drift velocities were also encountered in MACH2 simulations of the POS. In this code, the Hall term was implemented in the induction equation using an implicit method and the electron drift velocity was numerically limited to \( v_e \leq c \) in the solution [86].

An undesirable by product of increasing the resistivity to control the electron drift
velocity, was that the Ohmic heating ($\eta \vec{j}^2$), was artificially high in the lower density surface cells. Here, we found that the electron temperature exceeded $\sim 1$keV. As such, Ohmic heating was turned off in the plasma surface cells; this was justified by the fact that we were modelling the lower density plasma as being closer to a vacuum, as opposed to a highly collisional plasma.

5.5.5 Results

The Z DPHC model was run with the code modifications and simulation parameters described above. Slices of the simulated plasma density taken at 0 (through the anode posts) and 15 (between the anode posts) degrees at 70, 110 and 120ns, are shown in Figure 5.1-5.3. The number density is plotted in units of m$^{-3}$ on a logarithmic scale; these
Considering the plots at 70ns, Figure 5.1, we see that a plasma with a peak density of $\sim 10^{16}\text{cm}^{-3}$, was formed across the surface of the cathode electrode emission region. Comparing this plot with the equivalent PIC result, Figure 4.21 in chapter 4, we found that the MHD plasma had remained more tightly bound to the cathode electrode, such that the plasma penetration into the a-k gap, especially on the downstream side of the anode posts, was significantly smaller.

At the later times of 110 and 120ns, Figure 5.2 and 5.3, respectively, in the 0 degree slices we found that the MHD plasma penetrated further into the a-k gap on the downstream side of the top anode post. Additionally, we observed a small amount of penetration on the upstream side of the top post, consistent with the position of the (1)
Figure 5.5: Slices of the magnitude of the magnetic field strength in Tesla, taken at 0 (though the anode posts) and 15 (between the anode posts) degrees, at 120ns. Note the results have been plotted on a log scale.

magnetic null. Similarly, in the 15 degree slices, the plasma had started to penetrate into the a-k gap at the position of the (3) magnetic null in the level B line. However, comparing these plots to the equivalent PIC simulation results at these times in chapter 4, we again found a much smaller level of plasma penetration into the post-hole a-k gaps; this was especially true on the downstream side of the bottom anode post.

A plot of the magnitude of the electric field at 120ns, is shown in Figure 5.4. Here, we found that the MHD plasma had shielded the cathode electrode from the line electric field, such that the vacuum-plasma interface was the effective cathode surface. This result was consistent with the PIC simulations, where the cathode plasma screened the electric field. At this time, on the downstream side of the top anode post, where the plasma had penetrated the gap, the a-k gap had been reduced to \( \sim 3\text{mm} \) and the electric field strength increased accordingly. Similarly, in the 0 and 15 degree slices respectively, this can also be seen where the plasma had begun to penetrate the gaps at the positions of the (1) and (3) magnetic nulls. Note that we have plotted the total electric field, including the \( \vec{v} \times \vec{B} \) and Hall terms.

Slices of the magnetic field strength at 120ns are shown in Figure 5.5. Comparing this plot with the case with no plasma, Figure 4.6 in chapter 4, we found that the magnetic field was able to penetrate the MHD plasma and was dominated by the bound current in the electrodes. Again, this result was consistent with the PIC plasma simulations; in the MHD case the magnetic field transport in the plasma was due to a combination of resistive diffusion and the Hall advection term.
Figure 5.6: Slices of the electron temperature, in units of eV on a logarithmic scale, taken at 0 (though the anode posts) and 15 (between the anode posts) degrees, at 120ns.

Figure 5.7: Slices of the ion temperature, in units of eV on a logarithmic scale, taken at 0 (though the anode posts) and 15 (between the anode posts) degrees, at 120ns.

The electron and ion temperatures at 120ns are shown in Figure 5.6 and 5.7, respectively. These results are plotted in eV on a logarithmic scale. For the plasma in the radial lines and start of the convolute, $r > 10\text{cm}$, both the ion and plasma temperatures were $\sim 10\text{-}60\text{eV}$; the lower end of this range was typical of experimentally measured cathode plasmas [16,17,21,27]. However, we found that within the convolute, most notably on the downstream side of the top anode post in the 0 degree slice and between radii of 6 and 8cm in the level A line in the 15 degree slice, that the plasma temperature was unphysical with a temperature of $>1\text{keV}$

We systematically turned off the source terms in the electron and ion energy equations, Eqn.(5.3) and Eqn.(5.4). In the lower temperature regions, we found that the main heating mechanism was due to an energy correction scheme; here, the kinetic
energy was advected with the plasma and compared to the kinetic energy calculated from the fluid momentum. Any discrepancy was added as an additional heat source in the ion component [113]. However, this did not account for the significantly higher temperatures in the other regions of the plasma.

Turning off Ohmic heating in the electron component, similarly had little effect on the results. The Gorgon advection scheme includes an artificial viscosity, in order to broaden shocks so they can be accurately captured by the spatial mesh. This introduces an additional work term in the energy equation [103]; however, setting the viscosity to zero was also found to have little effect on the plasma temperature. As such, the large plasma heating was attributed to the PdV work term.

Comparing the temperature maps, Figure 5.6 and 5.7, to the magnetic field strength plots, Figure 5.5, we found that the highest temperature regions correspond to the regions of largest magnetic field strength. For example, in the 15 degree slice in the level A line, there is a clear correlation between the start of the higher magnetic field region at a radius of 6cm and the highest temperatures in the electron component of the plasma. Similarly, the magnetic field strength on the downstream side of the top anode post was approximately twice as large as the bottom post (due to the current addition), again consistent with the higher temperatures at the top compared to the bottom post. It was therefore concluded that the excessive PdV heating was due to the magnetic field pinning the plasma close to the electrode, with the \( \vec{j} \times \vec{B} \) force doing the work to heat the plasma. As such, the plasma dynamics, specifically the plasma penetration into the downstream side of the top anode post, which was in qualitative agreement with the PIC simulation results, were due to non-physical behaviour of the MHD model.

In the MHD simulations of a POS system mentioned previously [86], it was stated that the PdV term in the electron energy equation was set to zero. This was justified on the grounds that the electron internal energy in the single fluid model was being convected at the fluid and not the electron drift velocity, which could lead to artificially large temperature gradients [86]. We tried this in our simulations, but still observed large ion temperatures. Turning off all source terms in both energy equations, the resulting plasma density at 120ns is plotted in Figure 5.8.

Here, the plasma temperature remained below 10eV and as such, the plasma remained closely bound to the cathode electrode throughout the current pulse; none of
the dynamics found in the PIC simulations, which reduced the effective a-k gap in the convolute, were reproduced. It was therefore concluded that the single fluid MHD model was not applicable to modelling the Z DPHC cathode plasma.

As discussed in section 5.3, generally the fluid approximation becomes more valid with increasing density and/or decreasing temperature [71, 72]. As such, we expect the MHD model developed in this chapter, to be more applicable to the ZR convolute, where the peak plasma density is expected to be \( \sim 100 \) times higher than on Z [15,17], as well as future higher power machines, where again we expect the plasma formed from the electrodes to be higher density.

## 5.6 Hybrid Simulations

As discussed in section 5.2, we proposed a hybrid MHD-PIC model to simulate the full convolute plasma and sheath system. To this end, we implemented our PIC code in Gorgon. In parallel to the work described above to assess the applicability of modelling the Z convolute plasma as an MHD fluid, the EM field coupling and schemes to transfer plasma particles between the MHD and PIC components of the hybrid model, were investigated. Although we ultimately concluded that the MHD model was not applicable to Z, we will describe this work with a view to modelling the higher density plasmas in ZR and future higher power pulsed power machines.

The PIC routines were called from within the Gorgon EM field solver. As discussed
in section 3.10 of chapter 3 and in section 4.5 of the previous chapter, to efficiently resolve the electron cyclotron frequency, the PIC time step was dynamically reduced. As the EM field solver was sub-cycled under the hydro solution, based on the Courant condition, we included an additional level of sub-cycling within the EM solver time step. In order to avoid re-centring the EM fields and particle velocities and positions at the start of every step, the PIC time step was again set to an integer division of the EM field solution step. We used a common spatial mesh for the MHD and PIC components of the model.

5.6.1 MHD Load-PIC Convolute Plasma Simulations

To test the common EM field solver, we initially repeated the 3D fully kinetic PIC convolute plasma simulations, but extended the grid along the z-axis, such that the load could be simulated using the MHD model. Due to the coarse cell size, the individual wires of the array could not be resolved; instead the load was initialised as a shell of aluminium plasma with a total mass of 4.09mg, an initial radius of 2cm and a length of 2cm, consistent with the 0D load parameters [16]. The simulation was driven with the same transmission line circuit and effective source voltage as used in the fully kinetic simulations and particles were loaded within the radial lines and convolute using the SCL emission and cathode plasma creation models, described in the previous chapter; again, no particle creation was allowed below a radius of 5cm due to the poor spatial resolution. As the load was approximated as a shell, the MHD implosion followed the 0D trajectory shown in Fig 4.4, in section 4.3 of the previous chapter. As such, the convolute plasma evolved consistently with the PIC simulations using the 0D load model. The simulation was stable and conserved energy to the few percent level and charge to machine-round off, such that we were confident in the method used to couple the MHD and PIC components through the EM field solver.

As discussed in section 3.4.1 in chapter 3, the presence of relativistic electrons in the convolute PIC simulations gave rise to noise in the electric field which disrupted the sheath. This was removed using a low pass spatial filter [86]; it was found that the same filtering could be applied to the electric field in the vacuum cells of the coupled MHD-PIC simulations. However, its application in the MHD plasma cells gave rise to unstable
simulations. As such, the plasma resistivity was used as a switch for the filtering in the hybrid simulations.

As was found in the convolute simulations presented in the previous chapter, electron and ion macroparticles created within the radial lines and convolute were transported into the load region through the inner MITL. To prevent the time step getting too small, the kinetic particles were terminated if they were transported below a radius of 1cm in the load region. In practice, the particles were slowed down in the MHD plasma using a kinetic-fluid Coulomb collision algorithm, which will be described in section 6.6 of the next chapter; this modelled interactions between the kinetic electron and ion particles and the MHD fluid. Higher resolution simulations using this coupled MHD load-PIC convolute plasma model would be of interest for studying the current loss within the inner MITL. Here, a spatial resolution of 100μm would be sufficient to approximate the discrete nature of the wires in the array and give a more realistic implosion. This could be achieved using variable grid spacing [62] to better resolve the load in the inner MITL, whilst allowing tractable simulations of the convolute with a coarser mesh. Alternatively, the load and power feed could be modelled on separate grids, with additional MPI routines to self-consistently set the boundary conditions between the two regions.

5.6.2 MHD-PIC Convolute Plasma Simulations

Returning to the hybrid model of the electrode plasma; here, the goal was to treat the densest part of the plasma as an MHD fluid and transition to a PIC description in the lower density plasma and charged particle sheaths, where the fluid approximation was no longer valid. We investigated a number of schemes to achieve this goal. As we were not attempting to accurately simulate the plasma in the Z convolute, the MHD plasma creation rate and vacuum cut-off density were increased to mitigate the unphysical plasma heating encountered for the relatively low density convolute plasma, as discussed above. In this way we could investigate the hybrid modelling techniques in the convolute electrode geometry, with a more realistic fluid plasma temperature.

In the simplest case, we considered describing all of the plasma as an MHD fluid, from the surface of which a SCL electron current could be drawn to source the electron
sheath. In this way, the plasma would essentially act as a moving cathode electrode. This model was inspired by both the kinetic PIC simulation results, where the cathode plasma was found to penetrate the a-k gap with a surface density of approximately $5 \times 10^{13} \text{cm}^{-3}$, acting as the effective cathode and the 1D diffusion model described in [27] and reviewed in section 2.2 of chapter 2, where the electron sheath was modelled using the Child-Langmuir SCL current, with a dynamic gap spacing set by the expanding fluid plasma front.

In practice, at each time step, the SCL emission particle creation algorithm described in section 3.9.1 of chapter 3, was applied at the surface of the MHD plasma defined by the vacuum density cut-off, $\rho_{\text{vac}}$. In addition to electrons, protons were also emitted at the SCL emission limit, if the charge calculated in Eqn. (3.81), was positive. This modelled the formation of the proton sheath, formed by particles emitted from the cathode plasma, observed in the fully kinetic PIC plasma simulations.

This model was found to be inadequate for two main reasons; firstly, sourcing electrons and ions in this way introduced a charge conservation error, which was found to generate unphysical electric fields that significantly disrupted the sheath. Secondly, due to the Eulerian nature of the MHD plasma transport, when the surface cell exceeded the vacuum density, the emission surface moved an entire cell further into the a-k gap. This left a large fraction of the electron sheath inside the new plasma cell. As such, we could not consistently model the SCL emission surface gradually moving across the cell, as in the fully kinetic PIC plasma simulations.

The charge conservation issues encountered with the previous scheme, could be mitigated in a similar way to the cathode plasma creation model in the fully kinetic plasma simulations; here, pairs of electron and ion macroparticles were sourced on the surface of the plasma cell with equal velocities. The electron flux from the plasma surface was set by the random flux [27] calculated from the density and temperature of the MHD plasma. Again, the kinetic ions modelled the plasma return current, consistent with the 1D cathode plasma model described in [27]. Additionally, they provided a source of protons which could be drawn into the gap by any field reversal on the plasma surface, again consistent with the fully kinetic plasma simulations. In this method, we were relying on the spatial resolution being adequate to self-consistently enforce the SCL emission condition. Mass and energy were conserved by subtracting the values for the
new PIC particles from the source fluid cell. Although the charge conservation error was mitigated, we still encountered the same issue relating to the Eulerian plasma transport; specifically, a large part of the sheath was trapped inside the plasma as it expanded into the gap.

The above issues, together with the fact that the MHD fluid approximation is likely to be invalid in the lowest density part of the plasma from which the sheath is formed, lead us to consider an alternative hybrid scheme. Here, a PIC plasma was sourced throughout the cell next to the surface of the MHD plasma and allowed to evolve self-consistently into the a-k gap; specifically, the electron and ion sheath could be formed as in the fully kinetic PIC model. The idea was to again source the plasma in the MHD description in the first cell next to the electrode. In order to conserve mass, energy and momentum, the PIC particle source was coupled to the MHD advection step. Here, the normal split Lagrangian acceleration and Eulerian advection scheme was used to transport plasma into the vacuum gap; now, instead of resetting the parameters of the fluid cell if its density was below $\rho_{\text{vac}}/10$, the fluid density, temperature and momentum were used to source PIC particles using the plasma creation algorithm described in section 3.9.3 of chapter 3. Specifically, the mass was used to calculate the new particle weights, whilst the velocities were initialised as a sum of the average fluid velocity and a random component sampled from a Maxwellian distribution at the fluid temperature. This sampling was again carried out using the Box-Muller scheme [93].

As described above, the model would result in a single layer of MHD plasma cells next to the cathode electrode sourcing PIC plasma. As such, the run time saving would not be significant. To achieve the desired hybrid plasma evolution, the PIC plasma in a cell would need to be transitioned to the MHD description, once the fluid approximation became valid. In the test simulations, we considered a simple density threshold to trigger this transition, but more thorough tests would be warranted. Here, the issue was transitioning the PIC plasma in a conservative way, with the added complication of ensuring that the quasi-neutrality of the single-fluid MHD plasma was taken into account. As the density of the MHD fluid was cell centred, we initially tried interpolating the PIC plasma parameters to the cell centres using NGP weighting. The resulting electron and ion charges were then tested and if the lower of the two was greater than the transition threshold, it and an equal fraction of charge from the PIC particles in...
the other species were deleted from the active particle list and replaced with an MHD fluid with the averaged parameters. Here, the fluid electron and ion temperatures were set from the kinetic energy of the PIC particles, assuming an ideal gas EoS. Although simple, this transition scheme was found to give large charge conservation errors, as the PIC density was defined on the cell corners for the EM field solution. These errors were again found to lead to the formation of unphysical electric fields that significantly disrupted the remaining PIC component of the plasma.

A number of other schemes were tested to try and achieve a conservative PIC to MHD transition; however, we were unable to reconcile this with the staggered positions of the MHD mass density and interpolated PIC charge density on the spatial mesh. Either the MHD or PIC parameter definitions could be shifted by half a cell to coincide with the other, however the positions of the electric and magnetic fields could then not be made consistent.

5.7 Chapter Summary

The run time of an MHD convolute plasma simulation at 500µm was found to be less than one day, compared to over one month for the fully kinetic PIC simulations. The MHD model would therefore provide the desired reduction in computational overhead; however the model makes a number of simplifying assumptions compared to the fully kinetic PIC model. In the first part of this chapter, the applicability of the single fluid, two temperature MHD (Gorgon) code to simulating the Hydrogen cathode plasma in the Z DPHC was therefore assessed. Typical Gorgon simulations of wire array Z-pinches use a vacuum cut-off density of between $10^{-4}$ and $10^{-2}$kgm$^{-3}$; this was reduced significantly to $10^{-7}$kgm$^{-3}$, corresponding to a proton density of $10^{14}$cm$^{-3}$, in order to capture the lower density convolute plasma (up to $10^{16}$cm$^{-3}$). The cathode plasma was sourced by injecting MHD plasma at a fixed rate, into the vacuum cell next to the electrode. A generalised Ohm’s law was used to determine the electrical properties of the MHD plasma. A number of assumptions made in this expression for Z-pinch applications were determined to be invalid at the lower convolute plasma densities. Specifically, the neglect of the inertial term lead to unphysical, super-luminal electron drift velocities in the lower density plasma cells, due to an over prediction of the plasma current. An
ad-hoc correction, where the plasma resistivity was artificially increased, was found to be sufficient to control the electron drift velocities in the convolute simulations.

The Hall term can typically be neglected in Z-pinch applications as $\omega_{ce} \tau_{ei} \ll 1$, where $\omega_{ce}$ is the electron cyclotron frequency and $\tau_{ei}$ is the electron-ion collision time. For the convolute plasma $\omega_{ce} \tau_{ei} > 232$; for accuracy the Hall term, which represents a non-linear advection of the magnetic field in the plasma, was therefore reintroduced into the generalised Ohm’s law. Gorgon includes a novel A-field solver, which gives EM wave solutions in the vacuum and transitions to an explicit solution of the standard MHD induction equation in the plasma. We developed an equivalent field solution scheme which updated the electric and magnetic fields directly, based on the Yee scheme [83] used in our PIC model and described in chapter 3; it was found that the Hall term could be successfully included in the explicit field solution, if it was added directly to the magnetic field. The solution was unstable if the term was first used to update the electric field. Consistent with the fully kinetic PIC simulations presented in the previous chapter, the magnetic field with and without the MHD cathode plasma, was identical.

In the MHD case, the magnetic field transport in the plasma was from a combination of resistive diffusion and advection from the Hall term. However, the plasma penetration into the a-k gap was significantly under predicted by the MHD model compared to the PIC results, even where the PdV work term had heated the plasma to unphysical temperatures ($>10^5$eV). It was therefore concluded that the single fluid MHD model was not applicable to modelling the Z DPHC cathode plasma.

Generally, the fluid approximation becomes more valid with increasing density and/or decreasing temperature [71, 72]. As such, we expect the MHD model to be more applicable to the ZR convolute, where the peak plasma density is expected to be ~100 times higher than on Z [15, 17], as well as future higher power machines, where we again expect the plasma formed from the electrodes to be higher density. To model the current loss, which was driven by electron losses from the sheath formed from the cathode plasma, to the anode electrode, a kinetic model of the sheath is required. To this end, we investigated methods to couple our PIC code to Gorgon, to form a hybrid model. Here, we found that the MHD and PIC models could be coupled through a common field solver where, as in the standard PIC model, the macroparticle current was added as a source term in Ampere’s law. To self-consistently model the sheath formation from the
cathode plasma, a number of schemes to transfer plasma between the particle based PIC and fluid MHD descriptions were investigated. Schemes where the sheath particles were sourced directly from the MHD plasma surface could not accurately model the sheath penetration into the a-k gap. Sourcing a PIC plasma throughout the cells next to the MHD plasma surface was more successful, as the sheath could naturally form from the lower density PIC plasma. However, to reduce the computational overhead compared to a fully kinetic model, the PIC plasma would need to transition to the MHD description when the fluid approximation was valid; a scheme to achieve this conservatively, going directly from a fully kinetic PIC description of the plasma to the MHD fluid, could not be established.

This issue initially motivated us to investigate the inertial two-fluid plasma model, which will be described in the next chapter. This was implemented as an extension of our PIC code described in chapter 3. Here, an Eulerian transport model was developed, which could be coupled directly to the Gorgon advection routines and used to conservatively transition the fully kinetic PIC plasma to the MHD description, through an intermediate two-fluid description. This three component model will be motivated further at the end of the next chapter. Initially, the applicability of modelling the Z DPHC convolute with a two-component hybrid model, comprising an inertial fluid description of the higher density plasma and a fully kinetic description of the lower density plasma and charged particle sheaths, will be considered.
In chapter 5, the Gorgon MHD code was used to simulate the Z DPHC cathode plasma. We found that neglecting the electron inertia in the generalised Ohm’s law gave rise to electron drift velocities, \( \vec{v}_e \sim -\vec{j}/en_e \), that exceeded the speed of light; as \( \vec{j} = \vec{E}/\eta \), this was mitigated with an ad-hoc correction to the plasma resistivity, \( \eta \). Additionally, we found that the penetration of the cathode plasma into the a-k gap was under predicted, compared to the equivalent PIC simulations, even where the MHD plasma had been heated to unphysical temperatures. However, the fluid model offered large reductions in the run time compared to the fully kinetic model. These failings of the MHD model, but reduction in computational overhead of a fluid model, prompted us to investigate the applicability of an inertial two-fluid plasma model to simulating the convolute plasmas. Here, by retaining the electron mass, the magnitude of the plasma current was naturally controlled.

As discussed in section 5.3 of chapter 5, the fluid approximation, which assumes the components of the plasma are in LTE, is accurate if the thermalisation time of the plasma components is short compared to the timescales of interest [72]. As \( \tau_{ee} \sim \left( \frac{m_e}{m_i} \right)^{1/2} \tau_{ii} \), this is typically a better approximation for the electron, than the ion component [71]. In fact, for the higher end of the expected convolute plasma temperate scale (10eV), \( \tau_{ii} \)
exceeds tens of nanoseconds, such that the accuracy of the approximation is questionable. Where this is the case, but the approximation is still valid for the electron component, the two-fluid model has the flexibility to treat the ions kinetically, whilst retaining fluid electrons. In terms of improving the accuracy of the predicted ion mfps compared to the fully kinetic PIC model, we also investigated the applicability of this more standard hybrid model to simulating the plasma in the convolute [62]. Here, part of the electron population was treated as a fluid, whilst the whole ion population was treated kinetically, with an additional model to describe the Coulomb interactions between the fluid and PIC components of the plasma.

The fluid approximation is definitely not accurate in the low density sheath, $10^{12−13}\text{cm}^{-3}$, formed by particles emitted from the plasma, where kinetic effects are important. To model the full convolute system, we therefore still propose a hybrid model. To simplify the link between the fluid and kinetic descriptions, common transport and field solution algorithms would be desirable. Such a model has been implemented in the LSP PIC code [94,116]; following the decision to develop our own PIC code discussed in section 3.2, we implemented our own version of the two-fluid model in our PIC code, which was described in chapter 3. Again, this allowed complete control over the physics algorithms and was particular important for the hybrid code, as many components of the model, when applied to the convolute simulations, could be classed as ‘experimental’. The LSP hybrid model has been used to simulate high-power diodes [94], a dense plasma focus (DFP) and other magnetic plasma systems, such as laboratory plasma jets [116]; to the authors knowledge, no results for hybrid simulations of the Z DPHC have been published.

A major difference in our implementation of the hybrid fluid PIC model was the exclusive use of explicit differencing; this was again done to allow easier parallelisation. The published LSP hybrid simulations used both an implicit particle push and EM field solution [94,116]; this allowed the time step to under resolve the plasma frequency, $\omega_{pe}\Delta t >> 1$ for the relatively high density plasma, $n_i \sim 10^{17}\text{cm}^{-3}$, considered [116]. As in our implementation, an energy conserving force interpolation was used to allow stable simulations with $\Delta x/\lambda_e >> 1$ [94,116].
6.1 Numerical Model

The inertial two-fluid model was implemented as an extension of the PIC model described in chapter 3. As such, it was essentially a particle based, MC solution of the two-fluid momentum and energy equations. As for the kinetic component, the fluid was represented by a relatively small number of simulation macroparticles; each macroparticle was a Lagrangian mass point in the fluid and carried, in addition to its velocity, charge and mass, a temperature. This temperature defined the distribution of particle velocities according to a Maxwellian, assuming LTE, such that the thermal and directed components of the velocity were separated [94]. The electrical properties of the fluid plasma were self-consistently calculated using the standard PIC method of coupling the plasma current to a numerical grid for a solution of Maxwell’s equations and then applying the resulting fields on the grid to the particles [116]. In the fully kinetic PIC model, Coulomb interactions between the plasma components were modelled with a binary collision algorithm described in section 3.8 of chapter 3; fluid-fluid and kinetic-fluid Coulomb interactions were treated with different models.

At each time step, the fluid macroparticle charge, momentum and thermal energy were interpolated to the numerical grid (the same grid used for the EM field solution), from which the fluid number density, \( n_{e,i} \), averaged fluid velocity, \( \vec{V}_{e,i} \) and temperature, \( T_{e,i} \), were calculated [94]. We assumed an ideal gas EoS, such that the energy density was related to the temperature by \( E_{e,i} = \frac{3}{2} n_{e,i} k_b T_{e,i} \). For consistency with the field solution, the natural choice was to interpolate these quantities to the cell corners. To differentiate the individual macroparticle velocities from the averaged grid velocities, the former is labelled with the lower case, \( \vec{v}_{e,i} \), whilst the latter is labelled with the upper case, \( \vec{V}_{e,i} \).

The system of two-fluid equations used to evolve the plasma parameters are given in Eqn.(6.1-6.4). Here, Eqn.(6.1-6.2), correspond to momentum conservation in the electron and ion plasma components, whilst Eqn.(6.3-6.4), correspond to energy conservation, respectively [72].

\[
m_e \frac{d\vec{v}_e}{dt} = -\frac{\vec{V} P_e}{n_e} - e \left( \vec{E} + \vec{v}_e \times \vec{B} \right) + \frac{\vec{R}_e}{n_e}
\]  

(6.1)
To close the energy equation, we assumed an ideal gas EoS, such that the electron and ion pressures were given by \( P_e = n_e k_b T_e \) and \( P_i = n_i k_b T_i \), respectively. The electron-ion momentum, \( \vec{R}_{e,i} \), and energy exchange, \( Q_{e,i} \), terms and thermal fluxes, \( \vec{q}_{e,i} \), will be discussed in sections 6.2 and 6.3, respectively.

For simplicity, we neglected the plasma viscosity and thermo-electric forces in Eqn.(6.1-6.4); this approximation should be investigated in further work.

### 6.2 Momentum Equation Solution

Comparing the fluid Eqn.(6.1-6.2) with the standard PIC, Eqn.(3.2), equations of motion in the non-relativistic limit, we see they differ by the addition of a pressure gradient, \(-\vec{\nabla} P/n\), and drag, \( \vec{R}/n \), force term in the fluid case [116]. The former models intra-, whilst the latter models the effect of inter-species collisions. Forms for the drag terms, in the limit of high magnetic field normal to the direction of the relative fluid velocity, are given in Eqn.(6.5) [72, 116]. Here, \( \tau_e = \tau_{ei} \), where \( \tau_{ei} \) was defined in Eqn.(3.7) and gives a measure of the electron-ion momentum exchange time due to Coulomb collisions in the weakly coupled plasma limit [72].

\[
m_i \frac{d\vec{v}_i}{dt} = -\frac{\vec{\nabla} P}{n_i} + Z_i e \left( \vec{E} + \vec{v}_i \times \vec{B} \right) + \frac{\vec{R}_i}{n_i} \tag{6.2}
\]

\[
\frac{3}{2} n_e \frac{dT_e}{dt} = -P_e \vec{\nabla} V_e - \vec{\nabla} \vec{q}_e + Q_e \tag{6.3}
\]

\[
\frac{3}{2} n_i \frac{dT_i}{dt} = -P_i \vec{\nabla} V_i - \vec{\nabla} \vec{q}_i + Q_i \tag{6.4}
\]

Note that the momentum equations, Eqn.(6.1-6.2), were used to evolve the velocities of the individual fluid macroparticles, \( \vec{v}_{e,i} \). In Eqn.(6.5), we are calculating the drag of the individual fluid macroparticles from one component of the plasma, with the grid-averaged velocity of the other [116]. This was found to be more accurate than our
initial implementation of the model, where the drag force between the averaged fluid velocities was first calculated on the grid according to

$$\vec{R}_{e/i} = -\frac{m_e e}{\tau_e} \left( \vec{V}_{e/i} - \vec{V}_{i/e} \right),$$

before being interpolated to the macroparticles. In this case, particles with different velocities experienced the same force, resulting in particles streaming through the plasma. In the new scheme, the force felt by an individual particle was proportional to its velocity, which was more accurate [117]. Note that in order to form Eqn.(6.5), the relevant grid velocity, $\vec{V}_{e/i}$, was first interpolated to the macroparticle position.

The pressure of each component of the plasma was calculated from the grid averaged densities and temperatures and as such, was a grid quantity, defined at the cell corners. The pressure force $-\vec{\nabla} P/n$, was also calculated on the grid at the cell corners, following the differencing scheme used in Gorgon [79]. Here, the gradient was approximated by the finite difference given in Eqn.(6.6).

$$\vec{\nabla} P_{i,j,k} = \frac{\partial P}{\partial r} \hat{i} + \frac{1}{r} \frac{\partial P}{\partial \theta} \hat{j} + \frac{\partial P}{\partial z} \hat{k} = \left( \frac{P_{i+1,j,k} - P_{i-1,j,k}}{2 \Delta r} \right) \hat{i} + \left( \frac{P_{i,j+1,k} - P_{i,j-1,k}}{2 r_i \Delta \theta} \right) \hat{j} + \left( \frac{P_{i,j,k+1} - P_{i,j,k-1}}{2 \Delta z} \right) \hat{k} \quad (6.6)$$

In this way, the gradient included information about the pressures in the surrounding cells. As noted in [94], at the electrode surfaces, the pressure force was set to zero in order to avoid excessive PdV heating of the plasma. At the edge of the fluid plasma region within the a-k gap, we also found that it was necessary to replace Eqn.(6.6), with a single sided difference that included only nodes with a non-zero fluid density. This prevented unphysical, large forces being applied to the fluid macroparticles in this region, which acted to force the plasma into the a-k gap. After calculating the gradient, $\vec{V} P$, in this way, it was divided by the fluid density and the resulting force interpolated to the fluid macroparticles.

In practice, the fluid update was called at the end of the normal PIC cycle, shown in Figure 3.1, before the standard Boris push to update the particle velocities and positions. As such, the drag and pressure forces were used to update the fluid macroparticle velocities using the central difference in time shown in Eqn.(6.7), before the Lorentz force was applied.
\[ \tilde{v}_{e,i}^{n+1/2} = \tilde{v}_{e,i}^{n-1/2} + \frac{\Delta t}{m_{e,i}} \left( -\frac{\tilde{V}_{e,i}}{n_{e,i}} + \frac{\tilde{R}_{e,i}}{n_{e,i}} \right) \]  

(6.7)

Note that we used the 3-velocity in Eqn.(6.5) and Eqn.(6.7); consistent with the standard PIC macroparticles, we actually stored the relativistic quantity, \( \tilde{u} = \gamma \tilde{v} \), for each fluid particle. At the start of the fluid update step, we therefore calculated \( \gamma = (1 + u^2/c^2)^{1/2} \) and formed the 3-velocity from \( \tilde{v} = \tilde{u} / \gamma \) [62]. After the fluid particle velocities had been updated according to Eqn.(6.7), we calculated \( \gamma = 1 / (1 - v^2/c^2)^{1/2} \) and formed the \( u \)'s as \( \tilde{u} = \gamma \tilde{v} \). This method assumed that the fluid macroparticle velocities were always non-relativistic i.e. \( \gamma \sim 1 \); this condition was enforced in the fluid to kinetic particle transition algorithm, as will be discussed in section 6.5.

With a non-zero magnetic field, strictly we should have split the drag force, Eqn.(6.5), into components parallel and perpendicular to the magnetic field [72]. For simplicity, we followed Gorgon and assumed that all directions were perpendicular to the magnetic field; the Braginskii fits in [72], for the drag term were then used. For the drag force, this was not such a bad approximation; in the limit of a strong magnetic field, \( R_{\parallel} \sim 0.51 R_{\perp} \), so that we over predicted the magnitude of the force by at most a factor of two in the parallel directions [72].

### 6.3 Energy Equation Solution

To calculate the change in the fluid temperatures over a time step, \( \Delta T_{e,i} \), the Lagrangian energy equations, Eqn.(6.3-6.4), were solved explicitly on the grid. To update the temperatures of the individual fluid macroparticles, \( \Delta T_{e,i} \) was then interpolated from the grid to the macroparticles [94,116].

The right hand sides of Eqn.(6.3-6.4) are comprised of terms describing PdV heating, thermal conduction and collisional energy exchange between the electron and ion plasma components, respectively. Considering these terms first, \( Q_{e,i} \), are given in Eqn.(6.8) [72].

\[
Q_e = \frac{m_e}{n_e \tau_e} \left( \tilde{V}_e - \tilde{V}_i \right)^2 - \frac{3m_e}{m_i} \frac{n_e}{\tau_e} (T_e - T_i)
\]

\[
Q_i = \frac{3m_e}{m_i} \frac{n_e}{\tau_e} (T_e - T_i)
\]

(6.8)
For the electrons, the first term on the rhs of $Q_e$ describes Ohmic heating, whilst the second is the energy exchanged with the ion component through Coulomb collisions; this term is proportional to the temperature difference and acts to bring the plasma components into thermodynamic equilibrium. The ion term, $Q_i$, includes only the collisional energy exchange [72]; note that this term is inversely proportional to $(m_i/m_e)\tau_e$, consistent with the fact that energy exchange in electron-ion Coulomb collisions is less efficient than momentum exchange, by a factor of the mass ratio [71].

The PdV work term, $P\nabla \tilde{V}$, was evaluated following the differencing scheme used in Gorgon. Here, the cell corner grid velocities were first averaged to the cell edges, using a two-point average. The gradient was then formed according to Eqn.(6.9) and was therefore centred at the cell corners; this was multiplied by the pressure, $P_{i,j,k}$, which was also defined at the cell corners, to give the work done.

\[
\nabla \tilde{V}_{av} = \frac{1}{r} \frac{\partial}{\partial r} (rV_{av,r}) + \frac{1}{r} \frac{\partial V_{av,\theta}}{\partial \theta} + \frac{\partial V_{av,z}}{\partial z} \\
= \frac{\left(r_{i+1/2}V_{av,r,i+1/2,j,k} - r_{i-1/2}V_{av,r,i-1/2,j,k}\right)}{r_i \Delta r} \\
+ \frac{(V_{av,\theta,i,j+1/2,k} - V_{av,\theta,i,j-1/2,k})}{r_i \Delta \theta} + \frac{(V_{av,z,i,j,k+1/2} - V_{av,z,i,j,k-1/2})}{\Delta z} \tag{6.9}
\]

The thermal fluxes, $\tilde{q}_{e,i}$, are defined in Eqn.(6.10) [72].

\[
\tilde{q}_e = -\kappa_e \nabla T_e \\
\tilde{q}_i = -\kappa_i \nabla T_i \tag{6.10}
\]

The thermal conductivities, $\kappa_{e,i}$, were taken from Braginskii [72]. Again, with a non-zero magnetic field, the thermal fluxes should strictly be split into components parallel and perpendicular to the magnetic field. We initially implemented such a split, however we found that splitting the temperature gradient in Eqn.(6.10), in this way, gave large variations in the fluxes over single cells due to the square grid. For simplicity, we therefore followed Gorgon and assumed that all directions were perpendicular to the magnetic field. In this case the thermal conductivities took the form, $\kappa_{e,i} \sim n_{e,i} T_{e,i}/m_{e,i} \omega_{ce,i}^2 \tau_{e,i}$ [72]. Unlike the drag terms, Eqn.(6.5), the parallel and perpendicular components of the thermal conductivity could differ by many orders of mag-
nitude and as such, this assumption was less accurate in this case. However, in the purely kinetic PIC simulations described in chapter 4, we found that the convolute plasma was relatively uniform along the $\theta$-direction in the radial lines. As such, we do not expect large temperature gradients parallel to the magnetic field in these regions. However, this was not generally true along field lines and at the magnetic nulls within the convolute.

The thermal conductivities were calculated on the cell corners, such that the thermal fluxes, Eqn.(6.10), were calculated by first averaging the conductivities to the cell edges and then multiplying by the gradient of the cell corner temperatures, which were also centred on the cell edges. The gradient of the cell edge centred thermal flux, $\vec{q}_{av} = \left( \kappa \vec{V} T \right)_{av}$, was then calculated at the cell corners for use in Eqn.(6.3-6.4). As we differenced the energy equations explicitly in time, this placed hard limits on the maximum values of $\kappa_{e,i}$ allowed for stability [110]. In the regions with non-zero magnetic field, we found $\kappa$ was typically below this limit; however, within the magnetic nulls, the limit was exceeded. As the thermal diffusion model was not accurate in these regions anyway, we simply limited $\kappa_{e,i}$ to be less than the stability threshold.

The above described terms were combined to give the change in the fluid temperature on the grid, according to the explicit difference given in Eqn.(6.11).

$$\Delta T_{e,i} = \frac{2}{3} \rho_{e,i} \left( -P_{e,i} \vec{V} V_{e,i} - \vec{V} \vec{q}_{e,i} + Q_{e,i} \right)$$ (6.11)

The change, $\Delta T_{e,i}$, was then interpolated to the fluid macroparticles to calculate the new particle temperatures. As was found in [94], a small amount of the fluid kinetic energy was lost in the momentum interpolation step. A similar issue was also found in the Gorgon advection step; energy conservation was enforced by advecting the fluid kinetic energy with the fluid and comparing this to the kinetic energy calculated from the fluid momentum [113]. Similarly, in the two-fluid model, the fluid particle kinetic energy was also interpolated to the grid at the start of the fluid update and compared to the kinetic energy calculated from the averaged grid velocities. Any difference was added as thermal energy to $\Delta T_{e,i}$, before the change was interpolated to the fluid macroparticles. Note that in the single fluid Gorgon model, the thermal energy was added to the ions.
6.4 EM Field Solution

In Gorgon, a generalised Ohm’s law was used to determine the electrical properties of the fluid plasma [69]. In contrast, the fluid PIC model used the same EM field solution method for the fluid and kinetic particles. Specifically, the changes in the individual fluid macroparticle positions, due to the velocities updated from the EM and fluid forces, were used to interpolate the fluid current to the grid. Along with the kinetic macroparticle current, this was used as a source term in Ampere’s law to self-consistently evolve the electric and magnetic fields on the grid [62]. In this way, finite Larmor radius effects, such as the Hall current, were included self-consistently [116].

In terms of the practicality of the hybrid model, a common EM field solution scheme also ensured charge conservation when transitioning fluid particles to the kinetic description.

6.5 Fluid to Kinetic PIC Transition

In the hybrid plasma simulations, the macroparticles were created using the cathode plasma creation model described in section 4.4; however, the macroparticles were now initialised in the fluid description. Here, instead of sampling a Maxwellian distribution at a user defined temperature to set the initial electron and ion macroparticle pair velocities, they were simply given this initial temperature (as well as a small directed velocity to initially move them away from the electrode). A key component of the hybrid model was therefore the transition of the macroparticles from the fluid to the kinetic PIC descriptions. The threshold for this transition was a trade-off between the reduced run-time of the fluid and the accuracy of the PIC treatments. In [86], a range of criteria for transitioning between an MHD and PIC description of a plasma opening switch (POS), based on the relative accuracy of the fluid and PIC models, were derived. In our model, we followed the simpler method of [94, 116] and transitioned the fluid particles based on a comparison of their thermal and kinetic energy, associated with their temperature and directed momentum, respectively; nominally, when the kinetic energy exceeded ten times the thermal energy, the fluid macroparticle was transitioned.
to the kinetic description. In the transition, the particle charge remained constant, but a random component was added to the velocity, sampled from a Maxwellian distribution at the fluid particle temperature. This sampling was again carried out along each velocity axis separately using the Box-Muller method [93], described in section 3.9.3 of chapter 3. Note that due to this sampling of the random component of the particle velocity, neither the momentum nor the kinetic energy were conserved in individual transitions; however, on average, over many such transitions, these properties were statistically conserved [94]. The simulation particle statistics could be improved by splitting the fluid particles into multiple smaller weight kinetic particles in the transition step; here the Maxwellian at the fluid particle temperature was sampled separately for each of the new kinetic particles.

The fluid model assumed non-relativistic particles; this was enforced by adding an additional test of the kinetic energy, as was discussed in section 6.2. If the velocity of a fluid particle exceeded 0.1c, which corresponds to \( \sim 2.5\text{keV} \) for electrons, then the particle was transitioned to the kinetic description. In practise, the fluid particles were typically transitioned well before this, due to the relatively low temperature of the convolute plasma.

With these transition criteria, a typical hybrid convolute plasma simulation would proceed as follows. The plasma particles were loaded in the fluid description in the higher density source cells next to the electrode and allowed to evolve. As the plasma penetrated the a-k gap, fluid particles in the lower density cells on the plasma surface were accelerated by the electric field and transitioned to the kinetic description, such that the low density sheath was modelled with the standard kinetic PIC model, as required for accuracy. To supplement the ion return current to the cathode electrode, SCL electron emission was continued from the cathode electrode throughout the simulation, as discussed in section 4.4 [94]. As such, these electrons were also loaded initially as fluid particles; for SCL emission in non-plasma emission cells, an additional if statement was included in the transition algorithm to instantly transfer them to the kinetic description.

For simulations using a modified fluid electron transport scheme, aimed at reducing the total number of simulation particles, an additional test of the local plasma density was added to the transition algorithm. This modification will be described in section 6.10.
6.6 Coulomb Interactions between the Kinetic and Fluid Particles

As discussed at the start of this chapter, the two-fluid model allowed the flexibility to model the convolute plasma using a more standard hybrid model; specifically, part of the electron population was treated as a fluid, whilst retaining a kinetic ion description. In this case, an additional model to include the effects of Coulomb collisions between the kinetic ions and fluid electrons was included in the code [118]; in the two-fluid description the energy and momentum exchanged in these inter-species interactions were modelled with the drag, Eqn.(6.5), and energy exchange, Eqn.(6.8), terms in the momentum and energy equations, respectively [94, 116]. Additionally, in both the two-fluid and electron fluid simulations, we could have the case where a kinetic electron was transported into either a fluid electron or ion cell or a kinetic ion was transported into a fluid ion cell. As such, we implemented a general collision algorithm due to Sherlock [118], treating the interaction of a test particle with charge $Z$, velocity $\vec{v}$ and mass $m$, with a background of field particles of charge $Z_f$, with velocities distributed according to a Maxwellian at a temperature of $T_f$, drifting with the average fluid velocity, $\vec{u}$. The mean thermal velocity of the field particles is related to the temperature according to $v_{th} = \sqrt{2T_f/m_f}$, where $m_f$ is the mass of the field particles [118]. This is a MC solution of the VFP equation, Eqn.(3.1) and Eqn.(3.9), discussed in section 3.1.3 of chapter 3. Here, the Coulomb collisions are included as an additional force in the macroparticle equations of motion [61]; the corresponding response of the fluid particles is included by enforcing energy and momentum conservation; here, the change in the kinetic particle energy and momentum due to the collisions, is added to the fluid [118].

Treating the kinetic PIC particle as the test particle, its velocity was first transformed to the local rest frame of the fluid according to $\vec{c} = \vec{v} - \vec{u}$. The fluid velocity used in this expression was for the simulation cell, centred on the grid corner, in which the particle lay; in fact, all of the fluid parameters appearing in the expressions below were defined in this way. For simplicity, the particle velocity was then rotated such that it was directed along the z-axis, $\vec{w}$, according to Eqn.(6.12). Here, $c_{\perp} = \sqrt{c_x^2 + c_y^2}$, $c = \arccos(c_z/c)$ and $\phi = \arccos(c_z/c_{\perp})$. Note that in practice, this rotation was not done implicitly,
but the rotation angles were calculated and used to perform the reverse rotation after
the particle velocity had been updated due to the collisions [118].

\[
\begin{pmatrix}
0 \\
0 \\
w_z
\end{pmatrix} = 
\begin{pmatrix}
\cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \\
-\sin \phi & \cos \phi & 0 \\
\sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta
\end{pmatrix}
\begin{pmatrix}
c_x \\
c_y \\
c_z
\end{pmatrix}
\]

(6.12)

The change in the test particle velocity due to the Coulomb interactions was calcu-
lated from the Chandresekhar diffusion coefficients, Eqn.(6.13-6.15). Here, Eqn.(6.13)
describes the slowing down and is deterministic, whilst Eqn.(6.14-6.15) describe diffu-
sion in velocity space parallel and perpendicular to the initial particle velocity and are
treated stochastically [71, 118]. These expressions were derived in the weakly coupled
plasma limit by taking statistical averages over many small angle binary interactions,
which dominate over a few large angle interactions. For a Maxwellian distribution of
field particle velocities, only these three diffusion coefficients are independent and non-
zero [71].

\[
\frac{\partial w_\parallel}{\partial t} = -A \left( 1 + \frac{m}{m_f} \right) \frac{G(w/v_{th})}{v_{th}^2}
\]

(6.13)

\[
\frac{\partial w_\parallel^2}{\partial t} = A \frac{G(w/v_{th})}{w}
\]

(6.14)

\[
\frac{\partial w_\perp^2}{\partial t} = A \frac{Erf(w/v_{th}) - G(w/v_{th})}{w}
\]

(6.15)

The parameter A and function G(x), are given in Eqn.(6.16) and Eqn.(6.17), respec-
tively [118]. Here, n_f is the density of field particles and ln\Lambda is the Coulomb logarithm;
this results from applying upper and low cut-offs in the integration over the impact pa-
rameter in the calculation of Eqn.(6.13-6.15) [60, 71], for which we used the form given
in [73]. In Eqn.(6.17), Erf(x) is the error function, which was evaluated numerically
using an efficient scheme taken from [93].

\[
A = \frac{Z^2 Z_f^2 e^4 n_f \ln \Lambda}{2\pi m^2 e_0^2}
\]

(6.16)

\[
G(x) = \frac{Erf(x) - x \frac{\partial Erf(x)}{\partial x}}{2x^2}
\]

(6.17)
The contribution to the change in the parallel component of the particle velocity, \( \Delta w_z \), from the slowing down was calculated using a simple explicit difference, as in Eqn.(6.18). Here, \( \Delta t \) is the simulation time step [118].

\[
\Delta w_z = \Delta t \frac{\partial w_\parallel}{\partial t} \quad (6.18)
\]

The contribution to the change in the parallel component of the particle velocity, from parallel diffusion, was calculated from the standard deviation, \( \sigma_\parallel = \sqrt{\Delta t \partial w_\parallel^2 / \partial t} \), according to Eqn.(6.19). Here, \( \hat{N}(\sigma) \) represents the operation of choosing a random number from a Gaussian distribution with a standard deviation of \( \sigma \) [118]; an algorithm taken from [93] was used for this purpose.

\[
\Delta w_z = \hat{N}(\sigma_\parallel) \quad (6.19)
\]

Similarly, the change in the perpendicular components of the particle velocity, \( \Delta w_\perp \), due to perpendicular diffusion was given by Eqn.(6.20), where \( \sigma_\perp = \sqrt{\Delta t \partial w_\perp^2 / \partial t} \). This was split between the \( x \) and \( y \) components by choosing a second random angle, \( \theta_\perp \), between 0 and \( 2\pi \) radians, according to \( \Delta w_x = \Delta w_\perp \cos \theta_\perp \) and \( \Delta w_y = \Delta w_\perp \sin \theta_\perp \) [118].

\[
\Delta w_\perp = \hat{N}(\sigma_\perp) \quad (6.20)
\]

The test particle velocity was then updated to the new time as \( \vec{w}^{n+1} = \vec{w}^n + \Delta \vec{w} \) and transformed back to the fluid rest frame, \( \vec{c}^{n+1} \), by applying the inverse of the rotation in Eqn.(6.12). The particle velocity was then finally transformed to the lab frame according to \( \vec{v}^{n+1} = \vec{c}^{n+1} + \vec{u} \) [118].

To conserve energy and momentum, the change in the particle kinetic energies and momenta were summed over the particles and added to the fluid in the cell in which the particle lay. The momentum added to each fluid cell, \( \Delta \vec{P} \), is given in Eqn.(6.21). Here, \( \Delta \vec{p}_i \), is the change in the momentum of the \( N \) PIC particles in the cell due to the collisions and \( w_i \) is the particle weight i.e. the number of physical particles that each macroparticle represents. The above changes in velocity due to the collisions were calculated for a single physical particle; it was assumed that the change was the same for all the particles which the macroparticle represented [118].
\[
\Delta \vec{P} = - \sum_{i=1}^{N} w_i \Delta \vec{p}_i \quad \text{(6.21)}
\]

The total energy added to the fluid cell, \( \Delta E \), is given in Eqn.(6.22), where \( \Delta k_i \), is the change in kinetic energy of the individual PIC particles in the collisions [118].

\[
\Delta E = - \sum_{i=1}^{N} w_i \Delta k_i \quad \text{(6.22)}
\]

The total energy was split between the kinetic and thermal energy of the fluid. The change in the fluid kinetic energy in each cell, \( \Delta K \), was calculated from the change in the momentum, as in Eqn.(6.23). Here, \( \vec{P}_f \) is the fluid momentum, \( M_f \) the mass of fluid in the cell and \( \Delta \vec{P} \), was defined in Eqn.(6.21) [118].

\[
\Delta K = \frac{(\vec{P}_f + \Delta \vec{P})^2}{2M_f} - \frac{(\vec{P}_f)^2}{2M_f} \quad \text{(6.23)}
\]

Finally, the change in the thermal energy of the fluid in each cell, \( \Delta U \), was given by a difference of the change in the total and kinetic energies, as in Eqn.(6.24) [118].

\[
\Delta U = \Delta E - \Delta K \quad \text{(6.24)}
\]

In practice, the PIC-fluid collision algorithm was called before the temperature update, calculated from the energy equation, was interpolated to the particles; the change in thermal energy due to collision was converted to a change in temperature of the fluid as \( \Delta T_{\text{coll}} = \frac{2}{3} \frac{\Delta U}{N} \), where \( N \) is the number of particles, and added to \( \Delta T \) in Eqn.(6.11), before being interpolated to the fluid macroparticles. The change in momentum due to PIC-fluid collisions, \( \Delta \vec{P} \), was also interpolated to the fluid macroparticles at this time.

For accuracy, the time step had to well resolve the shortest collisional interaction time. To enforce this condition, three time scales for slowing down and parallel and perpendicular diffusion were defined, as in Eqn.(6.25) [118].
\[ \tau_s = \frac{w}{\partial w_\parallel/\partial t} \]
\[ \tau_\parallel = \frac{w^2}{\partial w_\parallel^2/\partial t} \]
\[ \tau_\perp = \frac{w^2}{\partial w_\perp^2/\partial t} \]  \hspace{1cm} (6.25)

The PIC particle collisions with the fluid were then sub-cycled using a time step calculated from the minimum, \( \Delta t_p = t_{min} \min \left( \tau_s/2, \tau_\parallel/2, \tau_\perp/2 \right) \), where \( t_{min} = 1/40 \), such that the time step for each particle enforced at least 40 steps for the shortest collision time. Note that each PIC particle was sub-cycled with its own time step up to the new time.

The PIC-fluid collision model was also implemented in the Gorgon hybrid MHD-PIC model to treat collisional interactions when a PIC particle was transported into an MHD fluid cell. This same model has also been used to track other fast ion species in Gorgon simulations of burning plasmas in ICF and gas puff experiments [119].

6.7 Two-fluid Simulation Results

The hybrid plasma simulations used the same phenomenological creation algorithm as the fully kinetic simulations. Initially, we carried out simulations where both the electron and ion species were created as fluid macroparticles; we will refer to these as two-fluid simulations. In this case, the inter-species collisions were described by the drag force and energy exchange terms described in section 6.2 and 6.3, respectively.

We initially repeated the 2D kinetic simulations of the cathode plasma in the inner MITL described in section 4.14.2 of chapter 4, using the two-fluid hybrid model. These simulations were run with the same spatial resolution of \( \Delta r = \Delta z = 200 \mu m \) and initial time step of \( \Delta t = 0.5 \Delta t_{Courant} \).

We found that the electrical diagnostics from the hybrid simulation were almost identical to the fully kinetic case; specifically, no significant current loss was predicted to be occurring within the inner MITL. However, some discrepancies in the plasma and charged particle sheath formation and evolution were identified.
Figure 6.1: Plots of the densities of the fluid (top) and kinetic (bottom) components of the electron species, taken at 80ns from the two-fluid hybrid simulation, plotted on a logarithmic scale in units of $m^{-3}$.

Figure 6.2: Plots of the densities of the fluid (top) and kinetic (bottom) components of the ion species, taken at 80ns from the two-fluid hybrid simulation, plotted on a logarithmic scale in units of $m^{-3}$.

Plots of the simulated electron and ion density taken at 80ns are shown in Figure 6.1 and 6.2, respectively. Here, we have plotted the fluid and kinetic components of each species separately.

We found that transitioning the fluid particles when their kinetic energy exceeded ten times their thermal energy, the hybrid model behaved as expected; specifically, the dense plasma next to the cathode electrode was represented with fluid particles, whilst both the lower density electron and ion sheaths were represented with kinetic particles. From Figure 6.2, we also see that by this time the most mobile plasma, on the curved part of the cathode electrode at a radius of $\sim5.2$cm, had transitioned to the kinetic description. Comparing this with the ion density from the fully kinetic simulation at the same time, Figure 4.49 in chapter 4, we see that the hybrid simulation was more diffusive at this
location. This was also true of the plasma in the radial part of the electrode; in the hybrid simulation the plasma expanded to cover an additional computational cell here.

Differences in the electron sheath structure were also identified; comparing the hybrid electron density, Figure 6.1, with the fully kinetic simulation, Figure 4.48 in chapter 4, although similar electron vortex structures were formed, the peak densities at the centres of the vortices were reduced in the hybrid case. However, a direct comparison was difficult, due to the unstable nature of the sheath which was seeded differently by run to run variations in the random sampling used in the particle creation algorithms.

The hybrid simulations ran approximately four times faster than the equivalent fully kinetic case. This reduction in the computational overhead was due to two factors. Firstly, the hybrid simulations were run with approximately ten times larger particle weights (i.e. less particles), in the fluid plasma cells. This was possible as we were no longer relying on having a large number of particles per cell in order to accurately sample the velocity distribution, as a Maxwellian had been assumed [116]. As discussed in section 6.5, good particle statistics in the low density sheath were maintained by splitting the fluid particles in the kinetic transition step. Here, the same maximum particle weight of $10^{-12} \text{C}$ used in the particle creation algorithms in the fully kinetic simulations was enforced. Secondly, as the inter-species collisions were modelled with energy exchange and drag force terms on the grid, the binary collision algorithm, described in section 3.1.3 of chapter 3, did not need to be called for the fluid particles. In the kinetic simulations, sorting and ordering the particles arrays and then calculating the collision for each pair was a large part of the total computational overhead.

The hybrid two-fluid model was next applied to the 3D convolute plasma simulations. Again, for testing purposes, these simulations were run with the same spatial and temporal resolutions as the baseline fully kinetic simulations; specifically, $\Delta r = \Delta z = 1\text{mm}$ and $\Delta \theta = \pi/12/20$ radians and $\Delta t_{\text{initial}} = 0.5\Delta t_{\text{Courant}}$.

In these initial simulations, we found that all of the fluid particles were quickly transitioned to the kinetic description. The onset of the transitions coincided with a rapid increase in the energy conservation error to over 100% of the total simulation energy. Systematically turning off terms in the fluid energy and momentum update equations, this error was attributed to the drag force, Eqn.(6.5) in the momentum equations. For particles at the edge of the fluid plasma region, the drag force was
unphysical, due to a large relative velocity between the electron and ion fluids driven by electrons being accelerated into the sheath by the line electric field. Here, the fluid particles were being accelerated above 0.1c and transitioned to the kinetic description. A weaker form of this issue could have also been responsible for the more diffusive plasma transport observed in the two-fluid hybrid versus fully kinetic 2D inner MITL simulations discussed above. Here, the weaker effect was due to the higher magnetic field strength limiting the magnitude of the relative velocity, compared to the DPHC simulations.

We initially thought that this issue could be mitigated with finer spatial resolutions; here, a smaller fraction of the fluid particles in the bulk plasma would sample the velocity at the edge of the fluid plasma. We reran the hybrid simulations with spatial resolutions of 500\(\mu\)m and 250\(\mu\)m; note that due to the increased computational overhead, neither of these simulations were run for the full current pulse. However, in both cases we found the same issue with the drag force accelerating particles to unphysical velocities. The current associated with the motion of these particles generated large electric fields that significantly perturbed the plasma and sheath behaviour.

The fluid-kinetic transition algorithm was called after the EM field update and before the fluid update, such that fluid particles which had been accelerated above the energy threshold in the current time step had already been transitioned and were not included in the grid average. As such, the problem could only be mitigated by either transitioning the fluid particles to the kinetic description sooner, or defining a fluid plasma density threshold below which the drag force was set to zero. The former solution was not satisfactory, as it was found that a significant fraction of the plasma would need to be transitioned. The latter solution was also found to be not very robust, where setting a single global threshold was not sufficient to prevent the problem for the whole current pulse; as such, the simulations had to be regularly restarted with an adjusted threshold.
6.8 Fluid Electrons, Kinetic Ions Simulation Results

Following the issues found when applying the two-fluid model to the 3D convolute plasma simulations, we investigated the applicability of the more standard hybrid model; now, part of the electron population was treated as a fluid, but the whole ion population was treated kinetically. In this case, the electron-ion Coulomb collision interactions were modelled with the Sherlock [118] scheme described in section 6.6. Returning to the discussion of the applicability of the fluid approximation, we have already stated that this was questionable for ions in the convolute plasma; this was therefore a further justification for the fully kinetic treatment of the ion population considered below.
We again initially applied the hybrid model to the 2D inner MITL simulations. As for the two-fluid case, the electrical diagnostics were consistent with the fully kinetic simulations and predicted no significant current loss. Plots of the simulated electron and ion densities at 80ns, are shown in Figure 6.3 and 6.4, respectively. Here, the fluid and kinetic components of the electron species have been plotted separately (note that there was no fluid ion component in these simulations).

As for the two-fluid case, the hybrid simulation evolved as expected; specifically, the dense plasma on the cathode electrode was represented by fluid particles, whilst the lower density electron and ion sheaths were represented by kinetic particles. Now, comparing the ion density, Figure 6.4, to the fully kinetic result, Figure 4.49 in chapter 4, we found that the fluid electron only hybrid simulation was in better qualitative agreement than the two-fluid case; specifically, the plasma on the curved part of the cathode electrode at a radius of 5.2cm was less diffuse. Similarly, comparing the hybrid electron density, Figure 6.3, with the fully kinetic simulation, Figure 4.48 in chapter 4, we found that the fluid electron only simulation was also in better qualitative agreement than the two-fluid case; specifically, the peak electron densities in the vortices was higher. However, we again note that in general, the hybrid simulation plasma was still more diffusive than the fully kinetic simulation.

The run time of the fluid electron only 2D simulations, was longer than the equivalent two-fluid simulations. This was due to both the requirement for more kinetic ion macroparticles per cell in the plasma cells to give good statistics in the sheath and the application of the binary collision algorithm to model ion-ion collisions. However, the run time was still approximately half that of the fully kinetic simulations, due to the use of fewer electron fluid macroparticles in the plasma cells and the treatment of electron-ion collisions using the computational more efficient kinetic-fluid collision model, which did not require the particle arrays to be sorted and involved fewer floating-point operations for each kinetic particle.

The fluid electrons, kinetic ions, hybrid model was applied to the 3D convolute plasma simulations. Again, the same spatial and temporal resolutions as the baseline fully kinetic PIC simulations were used. Compared to the two-fluid hybrid simulations, we found this model to be much more robust; specifically, the energy conservation was close to that of the fully kinetic simulations and the issue with the electron-ion collisional
interactions at the fluid-kinetic plasma interface, found in the two-fluid simulations, was not encountered. However, the savings in the computational overhead made in these 3D simulations, were significantly less than the approximately 50% reduction achieved in the 2D inner MITL simulations described above. The reason for this was twofold; firstly, a significant fraction of the plasma was found to be in the kinetic description relatively early in the current pulse. Slices of the simulated fluid and kinetic electron densities taken at 40ns at 0 (through the anode posts) and 15 (between the anode posts) degrees, are plotted in Figure 6.5 and 6.6, respectively. Slices of the ion density are also plotted in Figure 6.7; note that all of the ions were in the kinetic description.
Figure 6.7: Slices of the simulated density of the kinetic ion species, taken at 40ns at 0 (through the anode posts) and 15 (between the anode posts) degrees, plotted on a logarithmic scale in units of m$^{-3}$.

Comparing the ion density, Figure 6.7, with the fully kinetic simulation at the same time, Figure 4.11 in chapter 4, in the 0 degree slices the plasmas were qualitatively similar on the radial lines and upstream side of the anode posts. However, comparing the 15 degree slices, especially in the level C and D lines, the plasma was more diffuse in the hybrid case and had expanding further into the a-k gap by this time. This more diffusive plasma transport, which was also observed in the 2D inner MITL simulations as described above, will be considered further in section 6.10. Additionally, comparing the 0 degree slices on the downstream sides of the anode posts, at the bottom post the penetration was larger in the fully kinetic simulation; the higher density plasma, $\sim 10^{15}$cm$^{-3}$, covered $\sim 2$, compared to $\sim 1$ grid cell in the hybrid simulation.

Considering the electron density, although the cathode plasma was initialised as fluid particles, by this time a significant fraction of the plasma had transitioned to the kinetic description. This was especially true on the level C and D lines, due to a combination of the electrode stair stepping and the higher voltages, resulting in the fluid particles sampling higher electric field strengths. As such, we investigated varying the fluid-kinetic transition criteria to control the fraction of the cathode plasma in the fluid description. A discussion of this work is left to the end of section 6.10, while we first address the second part of the reason for a smaller reduction in the computational overhead in the hybrid convolute versus the inner MITL simulations.

The major part of the saving in the computational overhead in the 2D hybrid inner MITL simulations, came from reducing the number of fluid macroparticles per cell in
the dense plasma regions. We found that we could not make such a large saving in the 3D convolute simulations, as the fluid plasma density gradient was larger. In the 2D simulations, the fluid plasma macroparticles remained constrained within two computational cells above the electrode surface, such that the plasma was well approximated by a small number of larger weight particles. However, in the convolute simulations, the plasma extended over several computational cells. As with the standard kinetic simulations, the fluid particles therefore had to be created with weights that were small enough to give good statistics in the lower density plasma cells. As such, we still required a relatively large number of particles per cell in the hybrid simulations, such that the run time saving was not significant. This problem would persist to finer spatial resolutions; to obtain larger run time savings in the hybrid simulations of the DPHC, we therefore investigated implementing a modified transport scheme, which will be described in the next section.

6.9 Eulerian Particle Push

To efficiently treat gradients in the plasma density, an Eulerian transport model was included; this was inspired by a similar option available in the LSP code [94,116]. Here, after the fluid force and temperature update had been applied to the fluid macroparticles, their parameters were remapped to the grid nodes and they were removed from the active particle list. These old particles were replaced by a single new macroparticle on each grid node, created with the grid averaged charge, velocity and temperature. In this way, each component of the fluid plasma was treated with approximately one particle per cell, significantly reducing the number of simulation particles required to resolve the gradient in the plasma density [116]. This transport scheme is similar to the donor cell method implemented in Gorgon. Here, the transport is split into a Lagrangian acceleration, followed by an Eulerian advection step [103]. Compared to the PIC model, the initial Lagrangian step to update the fluid momentum is identical, but the advection step differs in that fluxes through the cell faces are used to transport the mass and internal energy in Gorgon, whereas the fluid PIC scheme transports these parameters by explicitly moving the fluid elements consistent with the fluid velocity and then interpolating these quantities from the updated positions to the grid. Another example of the Lagrangian-
Eulerian remap technique, applied to the solution of the MHD equations in 3D is given in [113].

As with any Eulerian transport scheme, a lower density cut-off must be set in order to prevent the entire grid being filled with low density plasma. In the fluid PIC model, this meant that after remapping to the grid and removing the old fluid particles, new particles with charges below a certain threshold were never created. This represented a charge conservation error, such that if the threshold was set too high, then unphysical electric fields were established which significantly perturbed the plasma and sheaths. We found that a threshold of $10^{-15}$ gave a good trade off between charge conservation and population control. Here, the peak charge conservation error, calculated using Eqn.(4.8) as described in section 4.13 of the previous chapter, increased from $\sim 10^{-11}$ without to between $\sim 10^{-5}$ and $10^{-4}$, with remapping. We implemented a partial correction to the divergence of the electric field to try and control this error [120,121]. This was applied after the normal electric field update and was effectively a single iteration of the Jacobi iterative solution of the Poisson equation [121]. As such, it was not a full correction and it was therefore found that the error could not be significantly reduced below $10^{-5}$. A full correction was possible, however this would require a converged solution of the Poisson equation [62]. As discussed in section 5.4 of the previous chapter, in relation to incorporating the scalar potential in the Gorgon A-field solver, a solution of the Poisson equation in 3D over split domains was inefficient. As such, a full correction was not attempted; in any case, an error of $\sim 10^{-5}$ did not appear to significantly disrupt the plasma and charged particle sheath evolution in the simulations.

Note that a charge of $10^{-15}$, typically corresponded to a plasma density for which the fluid approximation was not accurate. As such, a second density threshold was defined; the energy and fluid part of the momentum equations, in cells with a density below this threshold, were not evolved. In the hybrid simulations of the inner MITL and convolute described below, a threshold of $10^{12} \text{cm}^{-3}$ was used.

The interpolation scheme used to remap the fluid parameters to the grid must be linear for the method to be conservative. As such, we could not employ the second order quadratic spline interpolation used in the baseline kinetic simulations and the hybrid simulations presented above. Initially, we implemented the model using the linear interpolation scheme described in section 3.7 of chapter 3. Note that in order
to conserve charge in the EM field solver, the current and force interpolation were also reduced to first order; for the energy conserving electric field interpolation, this forced NGP interpolation in the longitudinal directions [68].

The linear interpolation scheme was found to give unsatisfactory results for a number of reasons. Firstly, remapping to the cell corners meant particles were created on the electrode surfaces in each step; these particles could be easily lost to the electrode, representing a large loss of charge as the plasma density was typically highest here. If this was not corrected, an excess of positive space charge was formed on the electrode surface, resulting in the formation of an unphysical sheath. We implemented two schemes to mitigate this problem. At first, we simply added the charge of any fluid particles that impacted an electrode to the closest node on the electrode surface. However, this led to an excess of negative space charge on the surface, as it precluded charge being re-trapped in the electrode and again an unphysical sheath was formed. Better results were obtained if the charge of the fluid particle that entered an electrode cell was linearly interpolated from below the electrode surface. However this required additional code modifications in the particle tracker, which was described in section 3.6.1 of chapter 3. Note that in the LSP model, the charge of particles that impacted an electrode was added to the surface nodes [116]. Secondly, due to the perfect conducting electrode boundary conditions used in the EM field solution, a particle created on the electrode surface felt no electric field parallel to the surface. As such, the more mobile electron species was found to rapidly propagate along the electrode surface, again leading to unphysical charge imbalances. We attempted to mitigate this issue, by forcing the parallel components of the momentum to be zero on the electrode surface, but this was found to be not very consistent. An ultimate fix for all of the above issues, was to not include particles lying within a cell of the electrode surface in the remapping step; however, this defeated the point of the Eulerian transport scheme, as the highest plasma densities and therefore particle numbers, were present in these cells.

A further issue encountered with first order interpolation, was related to the application of both the EM and fluid forces. Energy conserving force interpolation forces the electric field in the longitudinal direction to be interpolated with a NGP scheme [68]. This resulted in the simulation particles experiencing a piece-wise electric field as they crossed a simulation cell boundary, which as discussed in section 4.10 of chapter 4, was
found to be insufficient for modelling the ion transport at the plasma-vacuum interface. When an ion was emitted from a plasma cell it experienced the full line electric field instantly, such that the plasma remained confined to the electrode [18].

In terms of the application of the fluid forces by first order interpolation, initial simulations found that all of the fluid particles were quickly transitioned to the kinetic description. This was found to be due to the pressure force at the vacuum plasma interface; this could be mitigated using higher order interpolation as each fluid particle sampled a larger proportion of the plasma.

As discussed in chapter 3, in the standard linear interpolation scheme, each macroparticle has an effective size of a single grid cell, whilst in the quadratic spline interpolation scheme, each macroparticle has an effective size of two grid cells along each axis [62]. The deficiencies of applying the standard linear interpolation scheme to the Eulerian fluid model, led us to seek an alternative interpolation scheme, which was linear (for conservative remapping), but increased the effective particle size to cover two computational cells (for improved accuracy). This could be achieved by modifying the quadratic spline weights, Eqn.(3.48) and Eqn.(3.49), as in Eqn.(6.26) [68], by simply removing the square from the half-grid wights, \( \vec{w}_\pm \), in the definition of \( \vec{w}_\pm \), to give trapezium shaped particles. Here, \( \vec{x} \) is the particle position, \( \vec{X}_{i-1/2,k-1/2} \) is the position of the bottom left hand corner of the half-grid cell in which the particle lies and \( \Delta \vec{x} \) is the grid cell size.

\[
\begin{align*}
\vec{w}_\pm &= \frac{1}{2} (\vec{u}_\pm) \\
\vec{w}_0 &= 1 - \vec{w}_+ - \vec{w}_- \\
\vec{u}_\pm &= \frac{\vec{x} - \vec{X}_{i-1/2,k-1/2}}{\Delta \vec{x}}
\end{align*}
\]  
(6.26)

We could not find any references for this interpolation scheme in the literature; as such we initially tested its energy conservation properties i.e. did it mitigate the numerical electron heating instability when \( \Delta x >> \lambda_D \)? To this end we reran the baseline fully kinetic 3D convolute and 2D inner MITL plasma simulations with the new interpolation. Here, we found that the energy conservation was excellent and on a par with the results using the quadratic spline interpolation scheme.
As in the quadratic spline scheme discussed in section 3.7 of chapter 3, the new interpolation scheme was transitioned to the standard first order interpolation to the full grid cells, for particles within half a cell of the electrode surface, in order to avoid interpolating charge inside the electrodes [68]. Compared to the quadratic scheme, our linear interpolation scheme coupled a larger fraction of the particle charge inside the electrode during the transition. However, as discussed in section 3.7.1.3 of chapter 3, this was not a charge conservation error, but an inaccuracy when coupled to the SCL emission algorithm [68]. Test 3D and 2D plasma simulations found that this did not adversely affect the results, which were consistent with simulations using quadratic spline interpolation.

Referring to Eqn.(6.26), for particles within the vacuum cells, the natural choice now was to remap their parameters to the cell centres. As such the half-grid weights, $\vec{u}_\pm$, were used to interpolate the fluid parameters here after the fluid update. The old fluid particles were killed and a single new particle created at the centre of each cell, with the averaged parameters. This mitigated the issues found with the standard linear interpolation scheme, relating to creating particles on the electrode surfaces. However, due to the transition to first order interpolation, particles within half a cell of the electrode could not be included in the remap to the cell centres conservatively. This effectively created a second vacuum-plasma interface, half a cell above the electrode surface, at which the minimum particle threshold was applied. In initial simulations we found that the surface cells were filled with many small weight particles at this threshold of $\sim 10^{-15}$C, such that the hybrid simulation actually used many more particles than the equivalent fully kinetic simulation.

To control the number of macroparticles within the surface cell we initially implemented a particle coalescence algorithm, as described in section 3.13 of chapter 3. Here, $N$ particles were replaced with $M$ particles, where $M < N$, which conserved charge, momentum and temperature on the grid; energy conservation was ensured by adding a scaled random component to the momentum of each new particle [97]. However, we found that this algorithm failed over 90% of the time to reduce the particle number, due to the mixed interpolation used at the electrode surface.

As the positions of the small weight particles were clustered about the cell centre at which they were sourced in the remapping step, we found a simpler method to control
the fluid particle population here; we simply replaced these smaller weight particles with a single particle, with a weight given by the sum of the smaller particle weights, created at the weight averaged position given in Eqn.(6.27). Similarly, the new particle carried the weight averaged velocity and temperature as in Eqn.(6.28). Here, $F$, refers to a component of the velocity and temperature respectively.

\[
\vec{x}_{\text{new}} = \frac{\sum_{i=1}^{N_{\text{old}}} w_i \vec{x}_{\text{old},i}}{\sum_{i=1}^{N_{\text{old}}} w_i} \tag{6.27}
\]

\[
F_{\text{new}} = \frac{\sum_{i=1}^{N_{\text{old}}} w_i F_{\text{old},i}}{\sum_{i=1}^{N_{\text{old}}} w_i} \tag{6.28}
\]

This scheme was found to introduce a charge conservation error smaller than that associated with the remapping itself, such that it did not adversely affect the simulation results. However, we found that kinetic energy could be lost in the averaging process in Eqn.(6.28). To converse energy, we therefore also summed the kinetic energies of the old particles; this was compared to the kinetic energy calculated from the new particle velocity and any difference was added as thermal energy and the new particle temperature was updated accordingly [113].

In terms of applying the EM forces, this interpolation scheme maintained first order weighting of the electric field in the longitudinal directions, such that ion transport at the vacuum-plasma was more accurately treated [18, 68]. Additionally, this scheme, which sampled 27 grid points in 3D, was found to be more robust in applying the pressure force, such that the issues encountered using the standard linear interpolation scheme, were mitigated.

### 6.10 Eulerian Transport Simulation Results

We initially repeated the 2D hybrid inner MITL simulations using the Eulerian transport scheme. The model was run with both the fluid electron only and two-fluid plasma descriptions. In the two-fluid case, the remapping was only applied to the electron species [116]; as the ions are less mobile than the electrons, remapping them was found to significantly modify the plasma transport. Note, that although the two-fluid model
Figure 6.8: Plots of the simulated density of fluid (top) and kinetic (bottom) components of the electron species, taken at 80ns, plotted on a logarithmic scale in units of m$^{-3}$, from the fluid electron only simulations with electron remapping.

Figure 6.9: Plots of the simulated density of kinetic (bottom) ion species, taken at 80ns, plotted on a logarithmic scale in units of m$^{-3}$, from the fluid electron only simulations with electron remapping.

was not applied to the 3D convolute simulations, due to the issues described in section 6.7, it was included in the 2D tests.

The electron and ion densities at 80ns taken from the fluid electron only simulation are shown in Figure 6.8 and 6.9, respectively. Here, the fluid and kinetic components of the electron species have been plotted separately.

Comparing the hybrid ion density, Figure 6.9, with the fully kinetic simulation, Figure 4.49 in chapter 4, qualitative agreement between the plasma and ion sheath distributions were found. This was consistent with the hybrid simulations with no electron remapping discussed in section 6.8. However, considering the electron density, Figure 6.8, with electron remapping we found that the fluid electrons filled the a-k gap
with a density $>10^{12}\text{cm}^{-3}$, comparable to the kinetic electron sheath density. This resulted in the kinetic sheath being 'smeared out', where the electron vortices were not as clearly defined as in the fully kinetic simulation shown in Figure 4.48 in chapter 4.

Equivalent results were found when the Eulerian transport scheme was applied to the two-fluid simulations. In this case, the 'smearing out' of the kinetic electron sheath by the fluid electrons in the a-k gap was more severe.

These more diffusive results with electron remapping resulted from an attempt to avoid creating many small weight PIC particles in the fluid-kinetic transition step. As discussed above, the charge cut-off used in the remap step was $10^{-15}\text{C}$. This was one thousand times smaller than the minimum charge assigned to particles in the SCL and plasma creation algorithms. To avoid creating many small weight particles at the fluid-kinetic plasma interface, only fluid particles with a charge greater than $10^{-12}\text{C}$ (the lower limit in the creation algorithms) could be transitioned. Without this condition, the kinetic electron population was found to increase rapidly and any savings in the computational overhead made in the fluid region were offset. The fluid electron sheath formed in the a-k gap in the simulations described above was due to electron fluid macroparticles below this threshold expanding from the interface into the a-k gap. With only the kinetic energy as the transition criteria, when the charge of these fluid cells exceeded $10^{-12}\text{C}$, their kinetic energy was not sufficient for them to be transitioned to the kinetic description.

To mitigate this issue, we initially tried to implement an effective plasma-vacuum interface tracker, similar to the scheme employed in Gorgon. Here, only a single layer of cells on the plasma surface were allowed to be below the vacuum cut-off density; everywhere else in the volume, the density was reset to $\rho_{\text{vac}}/10$. As such, the plasma filled the volume a layer of cells at a time; only when the cell density exceeded the vacuum cut-off did it became part of the plasma proper. However, we found that applying this scheme to the PIC fluid model resulted in large charge conservation errors, which gave rise to unphysical electric fields that disrupted the plasma and sheath.

Instead, the low density fluid electron sheath was removed by including an additional transition criteria, based on the local electron density, in the fluid-kinetic transition algorithm. For each fluid macroparticle above the $10^{-12}\text{C}$ charge threshold, as well as a comparison of its thermal and kinetic energy, the local electron density (including both
Figure 6.10: Plots of the simulated density of the fluid and kinetic components of the electron species, taken at 80ns, plotted on a logarithmic scale in units of m$^{-3}$, from the fluid electron only simulations with electron remapping, including the electron density transition criteria.

Figure 6.11: Plots of the simulated ion density, taken at 80ns, plotted on a logarithmic scale in units of m$^{-3}$, from the fluid electron only simulations with electron remapping, including the electron density transition criteria.

The fluid and kinetic components) was sampled; if the density was below a threshold of $10^{15}$ cm$^{-3}$, then the fluid particle was transitioned to the kinetic description, as described in section 6.5. This density sampling could be carried out in a number of ways; we chose to test the density at the eight corners of the full grid cell in which the particle lay. If the density at none of these positions was above the threshold, then the particle was transitioned. This scheme was chosen in preference to simply testing the density at the grid node at the centre of the particle half-grid cell, in order to avoid transitioning remapped particles, which could have a large weight, directly on the edge of the fluid plasma.

The electron and ion densities at 80ns taken from the 2D inner MITL fluid electron,
kinetic ion simulations with electron remapping and the modified transition scheme, are shown in Figure 6.10 and 6.11, respectively. Again, the fluid and kinetic components of the electron density have been plotted separately. Considering the electron density, Figure 6.10, we found that the inclusion of the electron density transition threshold minimised the penetration of the fluid electrons into the a-k gap. Note that there was still a low density fluid sheath present, but its density was several orders of magnitude lower than the kinetic sheath and as such, it did not perturb the simulation. The distribution of electrons in the sheath was in better agreement with the fully kinetic result shown in Figure 4.48 in chapter 4; specifically, the smaller scale of the electron vortices formed in the sheath was consistent. Again, the ion density, Figure 6.11, was in qualitative agreement with the fully kinetic result, Figure 4.49. To reemphasise, we did not expect an exact match due to the run to run variations in the particle creation algorithms seeding the sheath instability differently.

The Eulerian transport scheme was applied to the 3D convolute fluid electrons, kinetic ions hybrid plasma simulations. As was found in the 2D inner MITL simulations discussed above, without the additional density transition criteria, the fluid electrons were found to penetrate the a-k gap and form a sheath with an equivalent density to the kinetic component; this was again found to significantly alter the distribution of the sheath electrons compared to the fully kinetic simulation. This could be removed by applying the same electron density transition threshold of $10^{13}\text{cm}^{-3}$.

The kinetic ion density at 40ns is plotted in Figure 6.12. Comparing this to the fully kinetic simulation at the same time, Figure 4.11 in chapter 4, as was found in the case with no electron remapping, the plasma was more diffuse, especially in the level C and D lines in the hybrid case. Considering the 0 degree slice, in the level D line, we also now found a higher penetration here, as well as the reduced plasma penetration on the downstream side of the bottom post identified in the results with no electron remapping.

The fluid and kinetic electron densities at 40ns are plotted in Figure 6.13 and 6.14, respectively. As was found in the simulations with no electron remapping, a significant fraction of the plasma had transitioned to the kinetic description relatively early in the current pulse. Considering the electron density, this was again especially true in the conical level C and D line. As such, the saving in computational overhead of the hybrid model, even with remapping giving approximately one electron particle in the fluid cells,
was minimal.

Returning to this issue, which was raised at the end of section 6.8, we investigated varying the energy threshold for the fluid-kinetic transition in order to control the fraction of the plasma in the fluid description. In [94], for high power diode simulations using a similar hybrid plasma model, the kinetic energy threshold for the transition, was set to a fraction of the electric potential in the gap. In this case a threshold of 25keV was used; this was significantly larger than the thermal energy threshold used in our inner

Figure 6.12: Slices of the simulated ion density at 0 (through the anode posts) and 15 (between the anode posts) degrees, taken at 40ns, plotted on a logarithmic scale in units of m$^{-3}$, from the fluid electron only simulations of the DPHC with electron remapping, including the electron density transition criteria.

Figure 6.13: Slices of the simulated density of the fluid component of the electron species, at 0 (through the anode posts) and 15 (between the anode posts) degrees, taken at 40ns, plotted on a logarithmic scale in units of m$^{-3}$, from the fluid electron only simulations of the DPHC with electron remapping, including the electron density transition criteria.
Figure 6.14: Slices of the simulated density of the kinetic component of the electron species, at 0 (through the anode posts) and 15 (between the anode posts) degrees, taken at 40ns, plotted on a logarithmic scale in units of $m^{-3}$, from the fluid electron only simulations of the DPHC with electron remapping, including the electron density transition criteria.

MITL and convolute simulations so far, due to the relatively low plasma temperature of $<10\text{eV}$. As such, we repeated the 2D inner MITL fluid electron only simulations with the kinetic energy transition threshold set ten times higher, i.e. the fluid particles were transitioned when their kinetic energy exceeded one hundred times their thermal energy. Note that this energy was around 1keV, which was lower than the relativistic criteria of $\sim2.5\text{keV}$. The electron density transition criterion was also included to avoid filing the a-k gap with a relatively high density electron fluid.

The simulated electron and ion densities at 80ns are plotted in Figure 6.15 and 6.16, respectively, where the electron species has been split into its fluid and kinetic components. Comparing the electron density, Figure 6.15, to the lower energy transition case shown in Figure 6.10, we found that increasing the transition threshold, forced the plasma on the curved part of the cathode electrode, at a radius of $\sim5.2\text{cm}$, to remain in the fluid description. As such the run time was reduced. However, we found that the plasma and electron sheath dynamics were modified compared to the fully kinetic simulation; specifically, by this time a plasma of density $\sim5\times10^{13}\text{cm}^{-3}$ had penetrated approximately half way into the a-k gap. In the fully kinetic simulation, the plasma remained bound closely to the electrode. In the hybrid case, the enhanced plasma penetration also modified the vortex structure in the sheath. Here, we found the vortices sourced at a radius of 5.2cm, were significantly larger and had lower peak densities, than
Figure 6.15: Plots of the simulated density of the fluid and kinetic components of the electron species, taken at 80ns, plotted on a logarithmic scale in units of m$^{-3}$, from the fluid electron only simulations with electron remapping and a higher kinetic energy transition threshold.

Figure 6.16: Plots of the simulated ion density, taken at 80ns, plotted on a logarithmic scale in units of m$^{-3}$, from the fluid electron only simulations with electron remapping and a higher kinetic energy transition threshold.

in the equivalent fully kinetic simulation, as shown in Figure 6.15.

Applying the same increase in the fluid particle kinetic energy transition threshold to the 3D hybrid convolute plasma simulations, slices of the resulting fluid and kinetic components of the electron density at 50ns are plotted in Figure 6.17 and 6.18, respectively. Comparing the fluid and electron components to the results with a lower energy transition threshold at the earlier time of 40ns, Figure 6.13 and 6.14, we found that a larger fraction of the higher density plasma had remained in the fluid description as desired. As such, the run time was reduced.

However, in a similar way to the 2D simulations, the plasma was found to be more diffusive in the hybrid case. Slices of the ion density taken at 50ns from the hybrid
Figure 6.17: Slices of the simulated density of the fluid component of the electron species, at 0 (through the anode posts) and 15 (between the anode posts) degrees, taken at 50ns, plotted on a logarithmic scale in units of $m^{-3}$, from the fluid electron only simulations of the DPHC with electron remapping and a higher kinetic energy transition threshold.

Figure 6.18: Slices of the simulated density of the kinetic component of the electron species, at 0 (through the anode posts) and 15 (between the anode posts) degrees, taken at 50ns, plotted on a logarithmic scale in units of $m^{-3}$, from the fluid electron only simulations of the DPHC with electron remapping and a higher kinetic energy transition threshold.

Figure 6.19: The equivalent plots from the fully kinetic simulation are shown in Figure 6.20. Considering the 15 degree slices, we found that the plasma was significantly more diffusive in the hybrid simulation. A similar comparison was applicable in the level C and D radial lines in the 0 degree slices. In contrast, on the downstream sides of both the top and bottom anode posts, the plasma penetration was reduced in the hybrid compared to the fully kinetic simulations. As discussed in section 6.7, similar differences in the plasma evolution between the hybrid and fully kinetic
Figure 6.19: Slices of the simulated ion density at 0 (through the anode posts) and 15 (between the anode posts) degrees, taken at 50ns, plotted on a logarithmic scale in units of m$^{-3}$, from the fluid electron only simulations of the DPHC with electron remapping and a higher kinetic energy transition threshold.

Figure 6.20: Slices of the simulated ion density at 0 (through the anode posts) and 15 (between the anode posts) degrees, taken at 50ns, plotted on a logarithmic scale in units of m$^{-3}$, from the fully kinetic PIC simulations described in chapter 4.

Simulations were observed, but to a lesser extent, in the simulations with no electron remapping. As such, part of the difference in the plasma evolution could have come from a deficiency in the fluid-kinetic collision algorithm, compared to the fully kinetic binary collision model.

A comparison of the convolute currents from the hybrid and fully kinetic simulations is shown in Figure 6.21. Here we found that the currents agreed relatively well up to $\sim$44ns, at which point the hybrid simulation under predicts the fully kinetic result. As such, the current loss predicted by the hybrid model was $\sim$0.5MA larger at this time,
6.11 Chapter Summary

With the goal of mitigating issues found when applying the single fluid MHD model to simulating the convolute plasma, whilst reducing the computational overhead compared to the fully kinetic PIC model, in this chapter we developed an inertial two-fluid hybrid model of the Z DPHC and inner MITL. This was based on a similar model in LSP [94,116] and was implemented as an extension of the PIC model described in chapter 3, by including a pressure and drag force in the equation of motion, to model intra- and inter-species Coulomb collisions and solutions of separate energy equations to update the temperatures of the fluid particles.

Two types of hybrid model were investigated; a two-fluid description, where both the densest parts of the electron and ion components of the plasma were treated as a fluid and an electron fluid only description, where the whole ion population was treated kinetically. The two-fluid model was found to not be applicable to simulating the 3D DPHC, as the drag force used to model the inter-species momentum exchange via Coulomb collisions gave rise to unphysical forces. The fluid electrons, kinetic ions model was more robust, however the reduction in the computational overhead compared to the fully kinetic PIC model was small; this was due to the requirement for relatively large numbers of fluid...
particles per cell, in order to accurately resolve the plasma density gradient.

The computational overhead was reduced by using an Eulerian transport scheme for the fluid electrons [94,116]. This was implemented successfully using a linearized version of the quadratic spline interpolation scheme, described in chapter 3 [68]. With the addition of a local electron density test in the fluid-kinetic particle transition step, the electron fluid could be modelled with approximately one particle per cell. However, simulations of the Z DPHC found that a large fraction of the fluid transitioned to the kinetic description early in the current pulse, minimising the run-time saving. The fraction of the plasma in the fluid description could be controlled by increasing the fluid to kinetic transition energy threshold; however this resulted in more diffusive plasma transport in the radial lines. The current loss prediction compared to the fully kinetic PIC simulation result, therefore increased. Additionally, in all cases, the penetration of the plasma into the a-k gap on the downstream side of the anode posts was reduced in the hybrid simulations compared to the fully kinetic PIC results; this was a key deficiency of the model as the evolution of the plasma in this part of the convolute was found to give the largest enhancement to the current loss in the fully kinetic simulations, as discussed in chapter 4.

Increasing the spatial resolution in the hybrid Eulerian transport simulations would partly mitigate the more diffusive plasma evolution. However, unlike the MHD convolute model, which ran in less than 24 hours, compared to one month for the fully kinetic PIC simulation, even with electron remapping giving approximately one electron macroparticle per fluid cell, the reduction in the computational overhead of the inertial fluid hybrid model would not significantly off-set the increase in the overhead from improving the spatial resolution. As such, although the fluid model developed in this chapter was found to be more physically applicable than the MHD model presented in chapter 5, it would not achieve the desired reduction in the run time of the Z DPHC plasma simulations compared to the fully kinetic PIC model.

However, as discussed at the end of the last chapter, the inertial fluid description could be used as an intermediate step in hybrid MHD-PIC simulations of higher density plasma systems, such as the ZR DPHC and future higher-power facilities. In fact, this was the initial motivation for investigating the inertial fluid model. Initial testing of this concept has proved successful; the Eulerian transport option mitigates the issues
encountered when transferring plasma directly between the MHD fluid and fully kinetic PIC descriptions described in section 5.6.2 of the previous chapter. Additionally, as the Eulerian remap is cell centred, the MHD advection routine [103] can be coupled directly to the two-fluid plasma to consistently transfer mass and energy between the different plasma descriptions. This model would offer significant reductions in the computational overhead for these higher density plasma systems, compared to a pure kinetic PIC model, as the plasma frequency would not need to be resolved in the densest MHD plasma.
Chapter 7

Conclusions

In this thesis we have addressed the issue of current loss in the Z DPHC and inner MITL using detailed 3D PIC simulations, coupled to circuit models of the wire array Z-pinch load and PF circuit and radial lines, of the evolution of electrode plasma and charged particle sheaths formed during the high voltage discharge. We focussed on the Z and not the refurbished ZR convolute, mainly because we had access to a relevant circuit model of Z, which was complicated for ZR due to a change in how the water lines coupled to the vacuum insulator stack [2]. However, as the convolute electrode geometry did not change dramatically during the refurbishment, we expect our results for Z to be generally applicable to the ZR configuration.

Assuming negligible plasma expansion, a SCL electron sheath was predicted to form from the cathode plasma in the radial lines with electron Larmor radii of less than the a-k gap spacing, such that the sheath was magnetically insulated here. Magnetic insulation was lost in the convolute where electrons could impact the anode across the magnetic nulls formed by the current addition path and on the downstream sides of the anode posts. However, this electron flow current loss was not sufficient to reproduce the measured 10% current loss at peak current, for the large diameter Aluminium wire-array load modelled in the simulations [2,16]. This under prediction of the peak current loss compared to experiment, was consistent with published LSP [16] and Quicksilver [14] simulations, as well as circuit models including only an electron flow current loss element.
For the relatively dense and low temperature plasma formed in the Z DPHC, the grid cell length, $\Delta x$, was much larger than the electron Debye length, $\lambda_e$; energy conserving force interpolation was found to be sufficient to mitigate numerical heating and the simulated electron temperature remained below 10eV, consistent with typical experimental measurements [17, 27]. Modelling Coulomb collisions in the weakly coupled limit using a binary algorithm and injecting a fully ionised Hydrogen plasma from the cathode electrode, at a rate of $0.0075\text{mln}s^{-1}$ and temperature of 3eV, the simulated current loss at peak current, was increased to $\sim 2\text{MA}$, consistent with the 10% losses measured in experiment [16]. Coupled with spectroscopic measurements made of a Hydrogen plasma in the ZR DPHC [17] and equivalent results from LSP simulations [16], it was concluded that the formation and evolution of a plasma from the cathode electrode was responsible for the high measured loss currents at these times. However, our model over predicted the early time current loss ($< 10\text{MA}$) by up to 1MA, compared to the experimental measurements [2] and the LSP predictions [16]. Here, the current loss was closer to the result from SCL emission only simulations. As such, our SCL emission and plasma simulations bounded the experimental loss. It was therefore concluded that an additional free parameter was required in the plasma creation model; specifically, the delay between the start of SCL electron emission and plasma injection from the cathode electrode. This was physically justified by considering the finite expansion velocity of the plasma across the source cell, where to establish the plasma in the simulation it had to be loaded throughout this cell. With realistic delays, consistent with expected plasma expansion velocities of between 1 and $3\text{cm}\mu\text{s}^{-1}$ [17, 27], we could match the measured current loss at both early time and peak current.

In terms of minimising the current loss in the DPHC, in order to maximise the power delivered to the load, our simulation results suggest that this would be a difficult task. The main enhancement of the current loss compared to the electron flow current only simulations, came from plasma penetrating the downstream side of the anode posts; the effective a-k gap was reduced from 1cm to $\sim 2\text{mm}$, enhancing the number of electrons able to cross from the plasma to the anode post across this gap. This penetration came partly from plasma being transported along field lines from the upstream inner edge of the cathode hole, which collected on the downstream side of the posts and partly
from plasma that had expanded into the central null from the downstream cathode being transported into this gap. It is therefore difficult to envision a convolute topology modification, involving posts and holes that would mitigate this. Increasing the a-k gap sizes is limited by maintaining a low inductance to achieve fast current rise times for Z-pinch experiments. Cut-away convolute geometries have been fielded on ZR, where the magnetic null (the positions of the nulls was shown in Figure 4.6 in chapter 4) was extended by increasing the size of the bottom hole, by removing part of the upstream level B and C cathode. Although the total inductance was not altered significantly, neither was the current loss reduced compared to the baseline design; this result was consistent with PIC simulations predicting a similar level of plasma penetration on the downstream side of the anode posts [15].

Considering our simulation results, we therefore conclude that a more radical change in the convolute geometry is required. The Z DPHC design was based on that of the lower current Saturn (8MA) machine [10]; experiments on Saturn also exhibited \( \sim 15\% \) current losses in the convolute [52]. Considering that the relatively small changes made in the DPHC electrode geometry going from Z to ZR (larger a-k gaps to account for the higher peak voltage and increased slopes in the radial lines for better diagnostic access at the load) resulted in an increase of the peak current loss from \( \sim 10\% \) to up to 20\%, this conclusion is particularly applicable to the design of future, higher-power facilities, such as the next generation of petawatt (PW) class Z-pinch driver, ZX [122].

Current designs for this next generation machine, replace the Marx bank and water line pulse forming circuit with Linear Transformer Drivers (LTDs), but the vacuum section remains practically unchanged [122]. Although the post-hole configuration is the most mature design, alternative designs for the convolute have been proposed. For example the Clam Shell MITL (CSMITL) is described in [123]. Here, the magnetic nulls are moved to larger radius where the cathode electric field is kept below the threshold for particle emission. Additionally, the magnetic field topology is designed to avoid plasma from the cathode moving along field lines to highly stressed gaps. This design has been fielded on Saturn and delivered more power to a high impedance load, than the equivalent post-hole convolute [123]. A less mature convolute design has also been proposed by Jennings, where each level of the radial lines is connected to the inner MITL by a series of posts, arranged in a spoke pattern. As such, apart from where the
connection to the inner MITL is made, the magnetic nulls are confined between the posts and a high magnetic field is maintained on the post to confine the plasma and electron sheath. An investigation of these designs, using either the simulation tools developed in this thesis or similar models, should therefore be undertaken as future work.

In [2,3], an additional, undiagnosed multi-mega ampere current loss was inferred to be occurring within the inner MITL for a series of compact wire array Z-pinch experiments. The loss was found to be dependent on the inner MITL electrode geometry and was largest for the right-angled bend design used in the DPHC simulations presented in this thesis. Due to the relative poor spatial resolutions, no particle creation was allowed within the inner MITL in these simulations. However, electrons transported from the convolute by their drift motions formed a sheath on the anode electrode. Coupled with plasma transported from the convolute filling the inner MITL, a peak electron loss current of 120kA between the convolute and load currents was found in the simulation at peak current. We were unable to reproduce this loss in higher resolution 2D simulations of the inner MITL only, were plasma was injected from the cathode electrode. We therefore concluded that further coupled convolute-inner MITL simulations were required to constrain the inner MITL loss. Here, the spatial resolution within the inner MITL could be improved whilst maintaining a practical resolution in the convolute, for example by using variable grid spacing. In addition, coupled PIC convolute and MHD load simulations, using our hybrid PIC-MHD model, were discussed; the 0D load boundary condition was replaced with a shell of MHD plasma as the resolution was not sufficient to resolve the individual wires. Kinetic electron and ions were transported through the inner MITL into the load region by their drift motions. Again, we suggest that higher resolution versions of these simulations would be of interest to both investigate the impact of a more realistic implosion (by resolving the wires in the MHD load) on the convolute plasma and charged particle sheath evolution and to investigate the coupling of plasma from the inner MITL with the load. This could again be practically achieved using variable grid spacing. In this thesis we exclusively modelled large diameter wire array loads; in order to constrain the inner MITL model, it would be beneficial to model the compact wire array loads considered in [2,3]. Due to the smaller initial radius, these loads will be more stressing on the PIC model, due to both a smaller minimum cell length (which sets the Courant limit) and larger peak magnetic
field strengths (which set the maximum cyclotron frequency). Combined with the additional code modifications required for variable grid spacing, this was therefore left as further work.

The computational overhead of the fully kinetic PIC DPHC plasma simulations was large; this prevented a thorough investigation of the effect on the simulated current loss of the cathode plasma injection rate, initial temperature and ion species. In addition, the convergence of the simulated current loss with the grid cell size could not be established. This was concluded to be of particular importance for the convolute plasma, due to the large discrepancy between the thermal kinetic energy (~10eV) and the electric potential energy in the line electric field (~1MeV). Here, we found that the plasma transport and therefore the simulated current loss were relative insensitive to the initial temperature between 1 and 10eV (the typical measured range), but were sensitive to the order of the electric field interpolation.

The long run times followed from the requirement of the time step to resolve the electron cyclotron frequency; this was required to accurately model the gyro-orbits and resulting drift motions in the crossed electric and magnetic fields and not for stability. As such, the time step could be safely increased, as the plasma frequency (determined by the highest plasma density) was on the order of the Courant time step. However, this would result in inaccurate drift motions and therefore inaccurate electron sheath dynamics, which were found to be of critical importance for simulating the current loss. Additionally, the high magnetisation in the plasma meant that resolving the electron cyclotron orbits was also important for accurately modelling the magnetic field transport in the plasma [56]. Moving to implicit algorithms, where larger time steps could be taken whilst maintaining stability, would therefore still be inaccurate. We therefore concluded that resolving the electron cyclotron frequency was essential for accurately simulating the convolute.

Assuming sufficient collisionality in the plasma, the computational overhead could be reduced by treating part of the plasma with a fluid description. However, this was found not to be accurate for the lower density plasma and charged particle sheaths formed in the convolute. As such, we concluded that a hybrid fluid-PIC model was required to simulate the current loss. To this end, we implemented our PIC code in the MHD code, Gorgon. The MHD code was modified by including an ad-hoc correction to
the plasma resistivity in the lower density cells and reintroducing the Hall term into the
generalised Ohm’s law, the neglect of which was no longer accurate for the convolute plasma. Stable simulations of the Z DPHC, treating the cathode plasma as an MHD fluid, were achieved. Here, the run time was substantially reduced from approximately one month for the fully kinetic PIC model, to less than 24 hours for the MHD model. However, the plasma penetration into the a-k gap was significantly under predicted compared to the fully kinetic PIC simulations, even where the PdV work term had heated the plasma to unphysical temperatures. As such, it was concluded that the single fluid MHD model was not applicable to simulating the Z DPHC plasma.

Some of the issues encountered when applying the MHD model to the convolute plasma, could be mitigated by extending our PIC code to include an inertial two-fluid plasma description. Treating both the electron and ion components of the plasma as a fluid was found to be problematic; a more robust model was to treat part of the convolute plasma electron population as an inertial fluid, whilst treating the whole ion population kinetically. A kinetic treatment of the ions was also justified by a consideration of the ion self-thermalisation time, compared to the time scales on which the plasma evolved. To achieve any significant reduction in the computational overhead compared to the fully kinetic PIC model, it was necessary to use an Eulerian transport scheme for the electron fluid [94]: coupled with a high fluid to kinetic transition energy required to maintain a significant fraction of the plasma electrons in the fluid description, the hybrid model over predicted the current loss compared to the fully kinetic result, due to more diffusive plasma evolution in the radial lines. As for the MHD model, it was therefore concluded that the inertial PIC fluid model was not applicable to simulating the Z DPHC plasma.

However, the fluid plasma approximation will be more accurate at higher plasma densities; the hybrid models considered in this thesis could therefore be more successfully applied to the ZR DPHC and future high-power facilities. Here, we suggest a three component hybrid model, comprising an MHD description of the densest part of the plasma, transitioning to a fully kinetic PIC description of the lower density plasma and charged particle sheaths, through an inertial two-fluid plasma description. Here, the Eulerian transport scheme in the inertial two-fluid model can be coupled directly to the MHD advection routines for consistent mass and energy exchange and the fully kinetic PIC plasma can be transitioned conservatively to the two-fluid description; it was found
that this step could not be easily achieved going directly from the kinetic PIC to MHD description. The run time saving of this model would be significant compared to a fully kinetic PIC model, due to the reduction in the number of kinetic macroparticles and the fact that the plasma frequency would not need to be resolved in the densest part of the plasma, described by an MHD fluid. In this way the use of implicit algorithms for stability could also be avoided. Current addition is and will continue to be an important part of achieving fast rise times and high peak currents on future pulsed power machines. Accurate modelling of the formation and evolution of electrode plasma and charged particle sheaths will be vital for the design of efficient pulsed power systems. Initial tests of our three component hybrid model have been promising; applying the hybrid and fully kinetic models to simulating the ZR DPHC and new designs will be the focus of future work.
References


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