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Drift Orbits and Neoclassical Transport in the H-1NF Heliac

A thesis submitted for the degree of Doctor of Philosophy of the Australian National University

Sean Alexander Dettrick

September 9, 1997
The work in this thesis is entirely my own, produced with some guidance from my supervisors. Any material taken from other references is explicitly acknowledged as such.

Sean Alexander Dettrick
Abstract

This thesis is concerned with neoclassical transport in the H-1NF heliac, and contains an examination of drift-orbit geometries, a description of a neoclassical Monte Carlo transport code, and a description of a method to use that code to self-consistently calculate ambipolar radial electric fields.

We set out to study the contributions to neoclassical transport in H-1NF, by first describing the topology and the abundance of collisionless, trapped particle orbits in the presence of radial electric fields. We give an overview of the trapped orbit geometries in H-1NF, and develop a method to numerically classify the trapped particle orbits. On average, the trapped particle fraction in H-1NF is 40%, with approximately 5%, 15%, and 20% of the orbits in the deeply trapped, helically trapped, and toroidally trapped states, respectively. A condensed version of this component of the thesis has been submitted to Nuclear Fusion.

The orbit studies provide a background for the development of a neoclassical Monte Carlo transport code, MCMuPPeT (for Monte Carlo, Multi Processing Plasma Transport). Using the code, we compare several Monte Carlo transport diagnostics, taken from the literature. Confinement times and diffusion coefficients are calculated for plasma conditions which will be achievable in H-1NF after the National Facility upgrade.

Since the electric field can dominate in the determination of the transport, we develop an iterative method to self-consistently calculate the ambipolar radial electric field, using the Monte Carlo code. The method is applied
to the Argon plasma conditions observed in H-1NF, in the experimentally observed Improved Confinement Mode (ICM). To help interpret the results, the ambipolar electric fields were calculated in the same conditions using a well-known analytic model which was geometrically-fitted to H-1NF for our purposes. Qualitative agreement was found between both of the neoclassical models and the experimental results; the electric fields predicted in the ICM conditions are typically twice as large as those predicted in the conditions before the transition. The two models were also used to look for the neoclassically predicted transition from negative to positive radial electric field. Positive radial electric fields were observed, at long mean free path, in Hydrogen plasma conditions which will be achievable in H-1NF after the National Facility upgrade.

We have also developed methods to optimise the Monte Carlo code for both parallel and vector computing environments. Two Message Passing algorithms that we use to parallelise the MC code are presented in the appendix.
Acknowledgements

This work would not have been possible without the help of many people. I would like to thank Henry Gardner for his good humour, for help, encouragement, advice, and for his cautious criticism. Bob Dewar also made a great contribution, and provided the central idea behind the orbit categorisation scheme of chapter 2. Scott Painter generously provided his original Monte Carlo code, as well as some useful ideas on what to do with it, and I would like to thank him for his continued interest, long after he had found greener pastures.

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Notation

SI units are used throughout this thesis, with the exception being that energies and temperatures are measured in electron volts. The following is a list of some of the more common symbols used.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Units</th>
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<tbody>
<tr>
<td>( a_p )</td>
<td>mean plasma radius</td>
<td>m</td>
</tr>
<tr>
<td>( B )</td>
<td>magnetic field strength</td>
<td>T</td>
</tr>
<tr>
<td>( \chi )</td>
<td>Straight field line coordinates (SFLC)</td>
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<tr>
<td>( \chi_i )</td>
<td>ion thermal diffusivity</td>
<td>eV m(^2)s(^{-1})</td>
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<td>( E )</td>
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</tr>
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<td>( \varepsilon_h )</td>
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</tr>
<tr>
<td>( \varepsilon_t )</td>
<td>toroidal ripple</td>
<td></td>
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<tr>
<td>( g )</td>
<td>poloidal current</td>
<td>( 2 \times 10^{-7} ) A</td>
</tr>
<tr>
<td>( \Gamma_a )</td>
<td>radial particle flux of species ( a )</td>
<td>m(^{-2})s(^{-1})</td>
</tr>
<tr>
<td>( I )</td>
<td>toroidal current</td>
<td>( 2 \times 10^{-7} ) A</td>
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<td>( \iota )</td>
<td>rotational transform</td>
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</tr>
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<td>( J )</td>
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<td></td>
</tr>
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<td>( K )</td>
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<tr>
<td>( K_{|} )</td>
<td>parallel kinetic energy, ( m v_{</td>
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<tr>
<td>$\psi$</td>
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</tr>
<tr>
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<td>temperature</td>
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<td>90° scattering time, $1/\nu_p$</td>
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<td>confinement time</td>
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Chapter 1

Introduction

This chapter begins with a gentle review of some of the key issues regarding neoclassical transport in stellarators, and ends with an outline of the rest of the thesis. We do not attempt an exhaustive literature review here, because there are already several good reviews of stellarator physics [1, 2, 3, 4] and neoclassical transport [5, 6, 7, 8, 9, 10, 11, 12]. Instead, this chapter provides background to the work in chapters 2, 3 and 4, and attempts to provide an underlying thread to the more technical discussions which occur there. More focused literature reviews appear later, at the beginning of each chapter.

1.1 Stellarators

Stellarators differ from tokamaks in that the poloidal magnetic field component required for good confinement is provided by external coils, rather than by currents flowing inside the plasma. This has the advantage that stellarators do not require continual ramping of the current in an external transformer in order to maintain a large toroidal plasma current, so they are more naturally suited to steady state operation. Also, because large currents do not flow in the plasma, the kink, tearing, and rippling modes are absent, as are the current-driven disruptions which can terminate a toka-
mak discharge [13]. The externally maintained helical magnetic field also permits explicit control of the magnetic configuration as the plasma beta increases [4]. However, confinement can be highly degraded in stellarators, especially in reactor relevant collisionality regimes, because the helical-field coils destroy the axisymmetry which exists in ideal tokamaks. On the other hand, it is fortunate that this lack of symmetry increases the number of free parameters that can be varied to optimise stellarator geometry with respect to equilibrium, stability, and transport.

The H-1 flexible heliac [14, 15, 16] was designed to explore MHD equilibrium and stability over a broad range of magnetic configurations. It is a 3 field period, modular coil, helical axis stellarator, with a major radius of 1m and an aspect ratio ranging between 5 and 10. The most common operating regime at present is a 40–80eV Argon discharge, in a background field of up to 0.1 tesla. After the first phase of the National Facility (NF) upgrade [17], due by the end of 1998, H-1NF will be able to operate at 0.5 tesla, with a 200eV, \( n = 1 \times 10^{18} \text{m}^{-3} \) plasma. When the final phase of the upgrade is complete, by 2002, H-1NF is expected to operate at 1 tesla, with temperatures of up to 500eV, and densities of up to \( 5 \times 10^{18} \text{m}^{-3} \). A description of H-1NF’s magnetic geometry is contained in chapter 2.

In this thesis, we are concerned with neoclassical transport in the H-1NF, so in this section we briefly review orbit dynamics and the (neoclassical) transport optimisation of stellarators.

1.1.1 Orbit dynamics

Tokamaks have a finite rotational transform \( \iota \), and the field strength is approximately inversely proportional to the major radius, \( B \sim 1/R \), so particle orbits wind about the torus and experience a varying magnetic field strength. As a result, the conservation of both the magnetic moment \( \mu \) (the first adiabatic invariant) and the total particle energy \( \mathcal{E} = m v_{\parallel}^2/2 + \mu B + qV \), implies
1.1. Stellarators

that there will be some particles which experience bounce motion — they are reflected by regions where the magnetic field strength is greater than $\mathcal{E}/\mathcal{\mu}$ (neglecting the electrostatic potential $V$). These orbits are called "bounce" or "trapped" or "banana" orbits. The term "trapped" comes historically from magnetic mirror physics, where transport along the field line was the main source of plasma loss, and particles which were reflected by $B$ maxima were confined. (In toroidal systems, the converse is true, and the "trapped" particles have the worst confinement characteristics.) The term "banana orbit" arises because, when the orbits are projected onto a plane of constant toroidal angle $\phi$, they are closed, and, in an ideal tokamak, are shaped like bananas [18, 19]. The bananas are closed in this projection because the canonical angular momentum is conserved. In an idealised "straight" stellarator, where the canonical helical momentum is conserved, the bananas likewise appear closed when projected onto a symmetry plane. In both cases, the banana center is free to drift in the direction of symmetry. Radial banana widths scale with the gyroradius (i.e. with $\sim 1/B$) so transport processes which are due to the finite banana width can be reduced by increasing the magnetic field strength.

In a toroidal stellarator, the external helical magnetic field breaks axisymmetry, so there is one less constant of the motion than in axisymmetric (tokamak) or helically symmetric (idealised, straight stellarator) systems. The passing orbits in toroidal stellarators remain qualitatively similar in behaviour to those in a tokamak, but the trapped orbits are no longer simply closed, and the banana centers drift in three dimensions. The banana-center trajectory may eventually intersect the confinement boundary (and be lost), or it may, sometimes, be closed after a number of smaller "open banana" transits, in which case the orbit is called a "superbanana." In the adiabatic limit, there still remains an approximate invariant of the trapped particle motion, called the "second adiabatic invariant", or "longitudinal adiabatic
invariant”, $J$. In this limit, the banana orbits are almost-closed, and $J$ is related to the area in phase-space, interior to the almost-closed orbit locus. In adiabatic conditions, both the closed and the unclosed trajectories of the banana-centers are confined to isosurfaces in $J$, called drift surfaces. The geometry of these surfaces is not a function of the magnetic field strength, but is a function of the field geometry only. Therefore, unlike banana transport, any transport which arises because of the shape of the drift surfaces cannot be reduced by simply increasing the magnetic field strength. On the other hand, the drift surface geometry is a function of the radial electric field strength, and it occurs that the radial electric field can be the main determinant of the shapes of the drift surfaces. It can localise particles in the radial direction, in arbitrary magnetic geometry, so the detrimental effects of nonaxisymmetry on particle transport can be ameliorated.

1.1.2 Transport optimisation

Neoclassical transport optimisation of stellarators can be pursued in several ways. Most of the published work has focused on optimising the magnetic field structure. This has been done by modifying the poloidal profiles of the helical ripple, $\varepsilon_h$ [20, 6, 21], by designing “quasihelical” systems which are approximately helically symmetric in magnetic coordinates [22, 23], and by attempting to realise approximate “omnigeneity” [21, 24]. Omnigeneity is the condition that radial drifts are zero in the system [25, 26]; a condition that has been shown to be impracticable in stellarators [27, 28, 29]. Approximate omnigeneity (also called “global omnigeneity” [26] and “near-isodynamicality” [29]) which may be realisable, is the condition that the bounce-averaged radial drift be zero on each flux surface. Another approach to transport optimisation is to exploit the transport scalings in databases such as in reference [11] or in analytic models such as those in references [18, 30, 31, 32, 33, 34], and to optimise the energy confinement time with respect
1.2. Neoclassical transport

to size, geometry, and field strength parameters. It is also important to ensure the integrity of the nested flux surfaces by designing magnetic configurations which minimise the resonant plasma currents which occur at finite $\beta$ [35, 36, 33].

As well as optimising transport using the magnetic fields, it may be possible to optimise neoclassical stellarator transport by controlling the radial electric field, using the heat and particle sources. This has been considered by some authors using simple models for the magnetic field field [37, 38, 39], but methods for calculating the radial electric field in real magnetic configurations are still being refined. One new computational method for achieving this is presented in chapter 4 of this thesis.

1.2 Neoclassical transport

Neoclassical stellarator transport is normally treated as a helical perturbation to neoclassical tokamak transport. The transport coefficients are represented as a sum of an axisymmetric component, due mainly to the toroidally trapped particles, and a nonaxisymmetric component, due to the helically trapped particles. The trapped particles make the main contributions to transport, even when the drift surfaces are well closed, because they have larger radial orbit widths than the passing particles. There are four transport scaling regimes due to the helically trapped particles. The first three apply when the radial electric field magnitude is small ($|E_r r/T| \ll \varepsilon_h$)\footnote{We use units of eV for temperature, and Vm$^{-1}$ for electric fields throughout.}. The fourth is a modification due to large electric fields ($|E_r r/T| \gg \varepsilon_h$).

1.2.1 Zero electric field

To illustrate a description of the neoclassical transport scalings, we plot in figure 1.1a stellarator diffusion coefficient, $D$, as a function of the normalised
mean free path \([40]\), \(L_* = L_{\text{mfp}} / L_c\). Here \(L_{\text{mfp}}\) is the collisional mean free path (and \(L_{\text{mfp}} \sim 1/\nu\)), and \(L_c\) is half the connection length, \(L_c = \pi R_0 / \ell\) (where \(R_0\) is the major radius and \(\ell\) is the rotational transform). In the figure, the red curves are ion diffusion coefficients, the green curve is the electron diffusion coefficient, and the black curve is the diffusion coefficient, of either species, in a tokamak. To create this graph, the nonaxisymmetric contribution to diffusion was calculated using the analytic interpolation model due to Shaing \([41]\) (described in chapter 4) and the axisymmetric (tokamak) contribution was calculated using a model from reference \([42]\).

Beginning in the short mean free path regime, and progressing to the very long mean free path regime (from right to left in figure 1.1) the first three scaling regimes are as follows. In the Pfirsch-Schlüter regime, when the mean free path is less than the bounce length, \(L_b \approx \pi R_0 / N\) (where \(N\) is the number of toroidal field periods), the transport scales like tokamak transport, i.e. \(D \sim \nu\). When the mean free path exceeds the bounce length (i.e. in the "banana" or "ripple" or "1/\(\nu\)" regime), the helically trapped particles have more time to move along their drift surfaces before being scattered out of the trapping state, so as the collision frequency decreases, the diffusive step length, \(\Delta\), increases. That is, \(\Delta \sim 1/\nu\), and since \(D \sim \Delta^2 \nu\), we find that \(D \sim 1/\nu\). The so-called "plateau" regime (where the transport genuinely plateaus in a tokamak, but where it is actually in a trough in a stellarator) is between the Pfirsch-Schlüter and 1/\(\nu\) regimes. When the mean free path is increased still further, the particles reach their maximum diffusive step length, the superbanana width, so \(\Delta\) no longer scales with 1/\(\nu\), and the transport again begins to decrease as \(\nu\) decreases. In this "superbanana regime," transport is dominated by collisionless losses as particles in the loss cone (i.e. certain trapped particles) move along their drift surfaces. Diffusion in velocity space acts as a source term to keep the loss cone replenished. Collisionless, chaotic scattering of particles off the background field ripple
1.2. Neoclassical transport

Figure 1.1: Ion (red) and electron (green) diffusion coefficients in a stellarator. The solid curves have no electric field, and the red dashed curve is the ion diffusion coefficient evaluated with a thermal electric field. The black curve is the axisymmetric (tokamak) contribution, and the coloured curves are the sum of the axisymmetric and nonaxisymmetric contributions.

also contributes to transport in this regime [43]. In between this regime and the $1/\nu$ regime is the “superbanana plateau.” The electrons (the green curve) behave in the same way as the ions, but their mean free path is $(m_i/m_e)^{1/2}$ times shorter, so their transitions between regimes occur at longer ion mean free path.

This “textbook description” of stellarator transport regimes is based on the assumption that the banana width is small compared to the plasma radius. In particular, the $1/\nu$ scaling assumes an isotropic Maxwellian, but, if the radial drift of trapped particles is fast (i.e. $\tau_{\text{drift}} < \tau_9$) because of a
larger banana width, then a Maxwellian cannot be maintained [44]. Diffusion in velocity space occurs to fill the loss cone, and, in this way, the $\nu$ scaling can set in before the $1/\nu$ scaling if $a_p/\rho$ is not large.

1.2.2 Radial electric fields

When a significant radial electric field is present (i.e. when $|E_r r/T| \gg \epsilon_h$) the transition between trapped and untrapped particles begins to dominate the diffusion processes, and the transport scales as $\nu^{1/2}$ in the long mean free path regime [45]. The confinement is thus improved, as can be seen from the dashed red line in figure 1.1.

The transport coefficients of each species are quite sensitive to the electric field, when they are in the long mean free path regimes. It is therefore important to know the radial electric field when calculating transport coefficients, so that the relevant neoclassical predictions can be obtained. The neoclassical radial electric field is also important because it has been implicated in the L-H transition in stellarators [46, 47, 48, 49, 50], and because it gives rise to a parallel current in nonaxisymmetric systems [51]. The calculation of radial electric fields in stellarators is the subject of chapter 4.

1.2.3 Computation of transport coefficients

The drift kinetic equation (DKE) is obtained by gyroaveraging the Fokker-Planck kinetic equation. The diffusion coefficients in figure 1.1 are based on solutions of the banana-kinetic equation (the “BKE” is the bounce averaged DKE) in certain limiting cases, for an idealised stellarator. For realistic stellarators it is not generally possible to exactly solve the DKE or the BKE, so numerical methods are used to calculate transport coefficients.

To date, there have been two main approaches to this problem. One approach is to use programs, sometimes referred to as “Fokker-Planck codes,”
1.2. Neoclassical transport

which solve the BKE or the DKE directly to obtain the transport coefficients. One, due to Mynick and Hitchon [20], solved the BKE on each flux surface, using a finite difference method. This was appropriate for magnetic configurations with only one type of localised particle. For more complicated geometries, a Drift Kinetic Equation Solver (DKES) was developed by Hirschman et al. [52], which solves the drift kinetic equation on each flux surface using a Fourier-Legendre series expansion. In both codes, collisions are modelled using a pitch-angle scattering operator, and collisional energy scattering is neglected. A separate approach to the computation is to use Monte Carlo codes, which follow the drift trajectories of a population of test particles, and calculate transport coefficients from the evolution of functionals of the test particle distribution. There have been several developments of this method, and both pitch-angle [53, 44, 54] and energy scattering [55, 56, 42] have been considered in the calculation of the transport coefficients.

In the long mean free path regimes, the computer time required for Monte Carlo calculations scales approximately with $1/\nu$, which makes them expensive in reactor-relevant regimes. Some Monte Carlo codes have greatly improved efficiency, because they follow a distribution of bounce averaged orbits, instead of drift orbits [57]. This requires careful treatment of the trapping/detrapping transition layers in phase space, which is difficult for a complicated geometry such as the H-1NF heliac. The DKES code has the advantage that the computer time required is independent of the collision frequency. However, implicit in the scheme is the assumption that the radial orbit width is small, and it has been shown recently [58] that finite drift-orbit width effects can change both the magnitude and the scaling of neoclassical transport coefficients.

In this thesis, we develop a drift-orbit Monte Carlo code based on one which has already been used [54] to calculate transport coefficients in H-1NF. This choice is a compromise between computing efficiency, and the accurate
Chapter 1. Introduction

treatment of drift orbit geometry. The original version of this code was specifically designed to run on a massively parallel CM-2 supercomputer [59]. Since then, efforts have been made to parallelise the calculation using more general models of computer parallelism. The parallelisation algorithms we have developed for this purpose are described in the appendix. The Monte Carlo model is described in chapter 3, where it is used to calculate transport coefficients in H-1NF.

1.3 Thesis outline

This thesis addresses neoclassical confinement in the H-1NF heliac, including the effects of realistic drift-orbit geometry, and realistic (ambipolar) radial electric fields.

In chapter 2, we develop methods to understand orbits in helical axis systems, and apply them to H-1NF. We discuss in detail the trapped particle populations and the trapped orbit geometries in the presence of electric fields, using drift surfaces to illustrate our arguments. The results are analysed with a view to understanding the neoclassical transport features which can be expected in H-1NF.

This is intended to form a conceptual background to the material in chapter 3, where a Monte Carlo code is developed to calculate neoclassical transport coefficients in H-1NF. The Monte Carlo model is described in some detail, and a comparison is made of the transport coefficients which are obtained using several different methods which appear in the literature. Emphasis is placed on simulating transport in conditions which will be realisable in H-1NF in the near future — 200eV Hydrogen plasmas, in a 1 T background field. We interpret the differences in the results that can be obtained, and make conclusions about the features of neoclassical transport in H-1NF. Most of these results were obtained using a parallelised Monte Carlo
1.3. Thesis outline

transport code, McMuPPeT (for Monte Carlo, Multi Processing, Plasma Transport.) The parallel algorithms which were developed for this implementation are described in appendix A.

In chapter 4, we develop a method to calculate the ambipolar radial electric field using the Monte Carlo code. This is motivated by the need to assist with the interpretation of experiments, and to contribute to the transport optimisation of future stellarator designs. The method is applied to conditions in H-1NF, where an Improved Confinement Mode (ICM) has been observed experimentally [49, 50]. In the cases studied, the Monte Carlo results agree well with the experimental results, suggesting that the transition to ICM may be explainable with neoclassical theory. The Monte Carlo method is also used to calculate ambipolar radial electric fields in the neoclassical conditions which will be obtainable after the National Facility upgrade, and we observe a transition from the ion to the electron root. The ambipolar fields from the Monte Carlo code are compared with those calculated using a well known analytic model.

Conclusions are presented in chapter 5.
Chapter 1. Introduction
Chapter 2

Drift Orbits in H-1NF

In this chapter we describe collisionless drift orbit topologies in the H-1NF heliac [14]. We compare the effects of the radial electric field and the magnetic configuration on orbit topologies.

The trapped particle population is divided into a number of subclasses of orbit using a scheme based on the number of maxima in the parallel kinetic energy between bounce points, $N_{C_{||}}$. The effect of the radial electric fields and the magnetic configuration on the trapped particle populations in H-1NF is studied, and is analysed from a transport perspective.

2.1 Introduction

The work described here has been inspired by earlier studies of collisionless orbit topologies in tokamaks and conventional stellarators [60, 19, 61, 62, 63, 64] which described the dominant classes of guiding center orbits of trapped particles as well as the transitions between them and the circulating orbits. Such studies are helpful in gaining a qualitative feeling for the neoclassical transport behaviour of these fusion experiments even in the absence of full Monte Carlo simulations.
2.1.1 Review

In 1967 Gibson and Taylor [60] showed that in a conventional $l = 3$ stellarator the trapped particle population is composed of "localized" particles, trapped in the local helical well, and "blocked" particles, which are not localized, but which nevertheless experience bounce motion. They worked in the absence of electric fields, and pointed out that, since the passing and blocked orbits have drift motions averaged over many field periods, the "effective field" that they experience may be represented by an axisymmetric geometry. In 1968 Furth and Rosenbluth [19] gave a general description of trapping in quasistatic magnetic and electric fields. They showed that, when there is no conserved canonical angular or helical momentum (i.e. no ignorable coordinate) which would give rise to closed bananas, the longitudinal adiabatic invariant $J$ can be used to describe orbits. Using $J$ they demonstrated that the locus of a superbanana orbit can be shifted close to the magnetic axis by a radial electric field which will allow the particle to experience a potential drop of magnitude $eV > kT\tilde{B}/B$ during its orbit (where $\tilde{B}$ is the magnetic field variation experienced over the orbit.)

In 1971, Dobrott and Greene [61] calculated the probability of transitions between 4 trapping states (passing, blocked, and localised in the $l = 1$ and $l = 3$ ripples) that occur in a large-aspect-ratio stellarator with $l = 1$ and $l = 3$ helical windings. The work was performed in the absence of electric fields. Nearly 20 years later, Cary, Hedrick and Tolliver [63] derived a new longitudinal adiabatic invariant, $J^*$, and relaxed Dobrott and Greene's assumption of small aspect ratio, to show orbit topologies and calculate transition probabilities, in the presence of electric fields, for stellarators which conform to the limit of small rotational transform per field period, $\epsilon/N \ll 1$, and to $\epsilon\epsilon_t/N\epsilon_h \ll 1$.

In 1995, Rome [64] used Cary's second adiabatic invariant to extend previous tokamak work [62] by giving an extensive overview of orbit topologies,
2.1. Introduction

in the presence of electric fields, in a “conventional” stellarator, the Advanced Toroidal Facility (ATF). As in Cary’s work, the drift surfaces were calculated by identifying them with isosurfaces of $J^*$. Rome also used the $J^*$ technique to consider the drift surface topologies which would be expected in different heating scenarios in the ATF torsatron.

2.1.2 Chapter Outline

In this chapter, we study orbits and particle trapping in the presence of electric fields in the H-1NF heliac, which is a “non-conventional” stellarator in the sense that it has large rotational transform per field period, low shear and a helical magnetic axis. The low aspect ratio and strong coupling of helical and toroidal curvatures in H-1NF means that the magnetic configuration is not well approximated by either the axi-symmetric or (quasi-) helically symmetric limits. Furthermore, the presence of multiple wells and saddles in the magnetic field strength on each flux surface gives rise to a number of classes of trapped orbits which have different topological features. We describe this hierarchy of trapped orbit classes in this chapter.

In addition to the H-1NF heliac, there are a number of helical axis stellarator experiments being planned or built, or that are in operation at the present time [65, 66, 67, 68]. The comparison of the experimental results of all these machines with each other and with numerical simulations will be an important step to an eventual synthesis of the stellarator approaches to fusion. Two objectives of this chapter are, firstly, to show that the computational techniques described here are useful and robust and, secondly, to document the collisionless orbit behaviour of the H-1NF so that it can be compared with other machines. The third main objective is to provide a detailed background to help interpret the Monte Carlo transport calculations performed in previous work [54] and later in this thesis, in chapters 3 and 4.

Before describing the results of our computations, we outline, in Sec-
Chapter 2. Drift Orbits in H-1NF

tion 2.2, our methodology and plotting conventions. In Section 2.3, we describe the qualitative features of the H-1NF magnetic field strength and of the dominant trapped particle orbits. In Sections 2.4 and 2.5 we present drift surfaces in H-1NF in the absence and presence of electric fields, respectively. The results of the studies of orbit populations, in Section 2.7, are followed by the conclusions in Section 2.9.

2.2 Background to the Computational Studies

In subsequent sections we will describe calculations of collisionless guiding center orbits for trapped (bouncing) particles in representative magnetic configurations of the H-1NF heliac. Here we wish to briefly comment on the model assumptions and numerical considerations behind these calculations.

2.2.1 Guiding center calculations

The use of Boozer coordinates [53, 69] for calculating guiding center orbits in curl-free stellarator magnetic fields has been a standard procedure for some time. The equations of motion can be written,

\[
\frac{d\psi}{dt} = -F \frac{\partial B}{\partial \theta_0}, \quad (2.1)
\]

\[
\frac{d\theta_0}{dt} = \frac{\partial V}{\partial \psi} + F \frac{\partial B}{\partial \psi}, \quad (2.2)
\]

\[
\frac{d\chi}{dt} = \frac{qB^2}{m} \rho_\parallel, \quad (2.3)
\]

\[
\frac{d\rho_\parallel}{dt} = -F \frac{\partial B}{\partial \chi}, \quad (2.4)
\]

where \( F = \mu/q + qB\rho_\parallel^2/m \), the parallel gyroradius is \( \rho_\parallel = \eta mv/qB \), and \( \eta = v_\parallel/v \) is a pitch-angle parameter, and \( m, q, v \) and \( \mu \) are the mass, charge, velocity and magnetic moment of the particle. We are using MKSA units.
2.2. Background to the Computational Studies

with electron volts to that $B$ is the field strength in tesla and $V$ is the electrostatic potential in electron volts. The spatial coordinates $(\psi, \theta_0, \chi)$ are such that $2\pi\psi$ is the toroidal magnetic flux within a magnetic surface, $\chi$ is a coordinate along a field line (proportional to the magnetic potential of a curl free field) and $\theta_0 = \theta - \omega \phi$ is a rotating helical angle which is constant on a given field line.

The choice of numerical methods for integrating the guiding center orbits is, necessarily, dependent on the application. A Monte Carlo transport study at medium to high collisionalities might use faster integration methods (possibly using fixed step lengths in preference to adaptive routines) than one at very low collisionality. A serious study of collisionless orbit topologies needs to have very good resolution about the tips of the banana orbits to guard against artificial trapping and detrapping due to numerical errors, and Rome [64] has advocated the use of symplectic integrators for this task. We chose to use a more standard "off the shelf" numerical routine for the bulk of the present study, and most of the H-1NF orbit trajectories described below were calculated by integrating Equations 2.1 to 2.4 using the variable order, variable-step-size, NAG algorithm D02CJF [70] with tolerance limits usually set at $10^{-8}$. We benchmarked our results against those of a symplectic integrator (a three stage, fourth order Runge Kutta symplectic integrator [71]) for cold ion orbits: each integrator was tuned by decreasing the step size until a measure of the qualitative features of a long ($\sim$ 100 toroidal transits) orbit became conserved. Using the resulting tolerances, the NAG integrator was 10-25 times faster than the symplectic integrator. Significant differences in the results were only observed in situations that were manifestly chaotic such as the high energy ion orbits shown in figure 2.21 below. Thus we found that our non-symplectic integrator was relatively fast and accurate enough for most purposes and note that convergence studies by changing the error tolerance can indicate situations where it may be advisable to switch to
symplectic integration.

### 2.2.2 Plotting conventions

The results presented in the rest of this chapter are plotted in terms of Boozer magnetic coordinates described above. The contours of the magnetic field strength in figures 2.1, 2.2 and 2.6 are plotted for surfaces of constant $\psi$ and with the poloidal, $\theta$, angle and the toroidal, $\phi$, angle on the $x$ and $y$ axes. These plots display a covering space [72] for the magnetic field of the H-1NF. Both $\theta$ and $\phi$ are $2\pi$ periodic, though $\phi$ is actually $2\pi/3$ periodic because of the three toroidal field periods.

The particle orbits in this chapter are shown for particular $\phi$ cross-sections of the toroidal H-1NF for which the remaining coordinates form a polar grid with the normalised average flux surface radius $r = \sqrt{\psi/\psi_{\text{ref}}}$ as the radial coordinate. Most of these figures display cross-sections of toroidal orbits as they intersect the $\phi$ plane, but, in one case, the entire toroidal orbits are projected onto that plane. Most of these figures use the poloidal angle $\theta$ as the azimuthal coordinate but in one case the helical angle $\theta_0$ is also used.

### 2.2.3 Model Configurations

The coupling between toroidal and helical curvatures in the tight-aspect-ratio H-1NF heliac results in magnetic configurations which are far from possessing any continuous symmetry. For this reason, the series expansion of the magnetic field strength in Boozer coordinates needs to have many more terms than is the case for conventional stellarators (or for optimised helical axis stellarators). For our orbit studies below, we have chosen model magnetic fields for three representative H-1NF configurations which have been used for stability studies in the past: the “standard” case, a “high-transform case” [73] and a “low-transform” case [15]. The low-transform
2.2. Background to the Computational Studies

case has a magnetic hill in the vacuum configuration; the others have a magnetic well. The $|B|$ contours of the three configurations studied here are plotted in figure 2.1 in a covering space [72] in Boozer coordinates, at half the plasma radius, where they have similar features: in each case the landscape is dominated by a narrow diagonal ridge of high field strength (due to the proximity of the central ring conductor to the inner edge of the plasma) and a deep, double-lobed well with twin minima on the outboard side of the device. The differences between the three configurations become more obvious when the $|B|$ contours are plotted at the last closed flux surface (figure 2.2) — in particular there is a significant variation in the shape of the diagonal high-field feature, which has a local maximum at $\theta = 0$ in the standard configuration, and a saddle at the same point in the other configurations. These standard, high-transform, and low-transform configurations are close to cases (a), (e) and (d), respectively, in reference [54].

The model magnetic fields are calculated by a vacuum run of the VMEC equilibrium code [74]. After transforming to Boozer coordinates and interpolating across flux surfaces a series representation for the field strength is obtained,

$$B(\psi, \theta, \phi) = \sum_{m,n} B_{mn}(\psi) \cos(m\theta - n\phi), \quad (2.5)$$

with

$$B_{mn}(\psi) = \psi^{\frac{|m|}{2}} \sum_{p=0}^{3} B_{mnp}\psi^p. \quad (2.6)$$

In comparison with reference [64] the series for the field strength were truncated to remove the toroidal field coil ripple (36 coils around the complete torus) so that 14 terms were used in the series altogether (rather than the 16 terms used by reference [64]). The neglect of this ripple component (with a magnitude of $B_{36}/B_{00} \sim 1.5\%$ at $r = a_p$, $B_{36}/B_{00} \sim 0.2\%$ at $r = a_p/2$) means that we neglected some localised trapped orbits near the edge of the flux surfaces but simplified the construction of our empirical signature, $N_{K\parallel}$,
for the important classes of trapped orbits discussed in Sec. 2.7 below.

The additional simplification of a curl-free vacuum magnetic field for these orbit studies, rather than a finite pressure field, is reasonable for the H-1NF heliac because of its small Shafranov shift at moderate pressures.

We also assumed a model electric potential of the form \( V(\psi) = V_0(1 - \psi/\psi_{cfs}) \), where \( \psi_{cfs} \) is the toroidal flux enclosed by the last closed flux surface. A particle's total energy can thus be written \( \mathcal{E} = K_\parallel + \mu B + qV \), where \( K_\parallel = mv_\parallel^2/2 \). Where comparisons are made between the central potential, \( V_0 \), and a particle (usually ion) temperature, it is understood that a central temperature is being compared with the magnitude of \( V_0 \).

### 2.3 Magnetic geometry and \( N_{K_\parallel} \)

It is clear from the contour plots of section 2.2.3 that there are many local minima in the field strength of H-1NF that can act as magnetic traps for particles with a low enough \(|v_\parallel/v|\) fraction. The multiple \( B \) minima that a particle experiences in H-1NF can be appreciated by comparing the magnetic field strength along a field line with a conventional stellarator. In figure 2.3(a) we plot the field strength, at half the plasma radius, in the H-1NF standard configuration, using equations 2.5 and 2.6 to evaluate the field. For comparison, we show in figure 2.3(b) the field strength along a field line for an idealised \( l = 2 \) stellarator which has similar field parameters to H-1NF (with \( m = 3, \varepsilon_{ta} = 0.1, \varepsilon_{ha} = 0.3, \) and \( \iota = 1.156 \).) The field strength for the ideal stellarator is given by \( B = B_0(1 - \varepsilon_t \cos \theta - \varepsilon_h \cos(l\theta - m\phi)) \). The H-1NF heliac has a more complicated field structure, with many local wells of varying depth along the field line. H-1NF’s irregularity is due mainly to the helical
shape of the plasma column — strong local maxima occur in the field at the points where it winds about the inner side of the ring conductor, and deep (double-lobed) wells appear on the outboard side. In comparison, the ideal stellarator field is much more regular, and it is possible to predict "by eye" the existence of two classes of trapped orbit; the locally trapped, which are confined within a single ripple well, and the locally passing, which pass over several ripple wells but bounce in the long-range modulation. The number of possible trapping states is not so clear in H-1NF. For this reason we develop, in the rest of this section, a method to classify the varieties of trapped orbit which occur in H-1NF.

In the adiabatic limit, deeply trapped orbits have a phase-space signature which is very similar to the periodic oscillations of a pendulum — the orbits are roughly circular when $v/\sqrt{v}$ is plotted as a function of distance along the field line (see figure 2.4.) The existence of multiple ripples in the field gives rise to a hierarchy of closed (in the adiabatic limit) orbits in phase space, some of which are also shown in figure 2.4. A separatrix lies between each category of closed phase-space orbits (the separatrices are not shown here.) Each level of the hierarchy of orbits may be distinguished by the number of maxima in the parallel kinetic energy which occur between bounce points. For example, the two locally trapped orbits in figure 2.4 have one maximum in $\mathcal{K}_\parallel$ between bounce points, and the next members out in the hierarchy, which encircle these ones, have two maxima in $\mathcal{K}_\parallel$ between bounce points. An orbit with 10 maxima in $\mathcal{K}_\parallel$ is also shown, which is close to the separatrix. Some orbits (not shown here) with 4 maxima in $\mathcal{K}_\parallel$ between bounces will exist within the left and right "arms" of the orbit which has 10 maxima. It turns out that the number of maxima in parallel kinetic energy between bounce points is a useful tool for the categorisation of orbits in this way. We call this quantity $N_{\mathcal{K}_\parallel}$.

In the adiabatic limit, the bounce-orbit center remains stationary, and
as a result, \( N_{\kappa_{||}} \) is constant. However, when we relax the constraint of adiabaticity, orbits may undergo collisionless transitions between trapping states, because at different positions along the drift trajectories, the relative energies of the different trapping states can change [61]. When an orbit undergoes a collisionless transition between trapping states, it is well known that two things occur: the orbit crosses a separatrix in phase space, and at the same time there is a bifurcation in the longitudinal adiabatic invariant, \( J \) [61, 64, 63]. This is illustrated for an orbit in H-1NF in figure 2.5. Here a deeply trapped orbit, with \( N_{\kappa_{||}} = 1 \), drifts until the energy of the separatrix drops below that of the particle, and it makes an instant transition to the \( N_{\kappa_{||}} = 2 \) state. There is an associated transition in the longitudinal adiabatic invariant, which is plotted along the back right panel. The transition is an increase in \( J \), since \( J \) approximately represents the cross-sectional area in phase-space which is enclosed by the trapped orbit [61]. Such transitions in \( J \) occur when an orbit changes drift surfaces, because the drift surfaces are isosurfaces in \( J \). The \( N_{\kappa_{||}} \) categorisation tool is useful because it detects these transitions between drift surfaces, and it also distinguishes between a hierarchy of geometrically distinct trapped orbit classes.

Before going on to look at the drift orbits, we note that the \( N_{\kappa_{||}} \) categorisation scheme works effectively as long as the \( n = 36 \) components of the magnetic field (due to the modular nature of the toroidal field coils) are ignored. In the next section, we will look at typical examples of the main types of trapped orbit in H-1NF, and will show (in table 2.1) the \( N_{\kappa_{||}} \) number for each.
2.3. Magnetic geometry and $N_{\kappa_4}$

Figure 2.1: Contour plots of $|B|$, evaluated at half the plasma radius and plotted in Boozer coordinates, for three configurations of H-1NF, (a) Standard configuration, $\iota = 1.12$, (b) high transform, $\iota = 1.30$, and (c), low transform, $\iota = 0.89$. The thick contour lines are where $B = 1.15T$, and the contours are 0.05T apart. Both the toroidal and poloidal angles are $2\pi$-periodic. The dashed lines are field lines.
Figure 2.2: Contour plots of $|B|$, evaluated at the last closed flux surface (the plasma radius) and plotted in Boozer coordinates, for three configurations of H-1NF, (a) Standard configuration, $\kappa = 1.16$, (b) high transform, $\kappa = 1.31$, and (c), low transform, $\kappa = 0.97$. 
Figure 2.3: Comparison of the magnetic field, evaluated along a field line, for the H-1NF standard configuration (top) and an "ideal" stellarator with similar parameters (bottom.)
Figure 2.4: The magnetic field strength, evaluated along a field line (top,) and the result: phase space trajectories of particles trapped between field maxima (bottom.)
2.3. Magnetic geometry and $N_{K_\parallel}$

Figure 2.5: A near-closed ($v_{\parallel}/v, \chi$) phase-space orbit which displays several collisionless crossings of separatrices, due to drift in the poloidal direction. The longitudinal adiabatic invariant, $J$, is plotted on the back right panel.
2.4 Drift orbits with no electric field

We begin with a qualitative comparison of the main types of trapping that occur in the magnetic ripple of H-1NF, and we correlate each of these classes with values of $N_{\kappa_\parallel}$. We then give an overview of the drift surfaces in H-1NF, which occur in the absence of electric fields. The effect of electric fields on the drift surfaces is treated in section 2.5.

2.4.1 Drift orbits

The four orbits shown in figure 2.6, plotted in a covering space in Boozer coordinates, are examples of trapped proton orbits in the standard configuration of H-1NF. The regions of grey shading in the background of this plot are where $\partial B/\partial \theta_0 > 0$, i.e. where the particles experience an inward drift (toward the magnetic axis). The white regions are where the drift is outward and the thick dashed line is a magnetic field line. Each of the orbits shown has the same kinetic energy, $\mathcal{K}_i = 100$ eV, and the average magnetic field is 1 tesla. The same orbits are shown projected onto a cross-section of constant toroidal angle in figure 2.7, and their phase space trajectories are shown in figure 2.8.

The orbits labelled A and B are helically trapped, and as can be seen from figure 2.7, they are classic examples of unclosed banana orbits, and are poorly confined if the radial electric field is weak, since they can spend many bounce periods in a region where $\partial B/\partial \theta_0 < 0$. (A strong electric field will rectify this, by inducing a poloidal drift which ensures that they do not spend many bounce periods with a fixed sign of $\partial B/\partial \theta_0$.) These types of orbits are largely responsible for the direct orbit losses which occur in H-1NF. Figure 2.8 shows that the A and B orbits have different values of $N_{\kappa_\parallel}$, having values 1 and 2 respectively.

The orbits labelled C and D are the closest analogues to the trapped
2.4. Drift orbits with no electric field

particle orbits in (axisymmetric) tokamaks; they are almost closed in the radial direction because they sample regions with differing signs of $\partial B / \partial \theta_0$. Because of this they are “almost-closed” bananas (see figure 2.7) but, in contrast to the bananas found in tokamaks, their banana centers are at $\theta = \pi$ instead of $\theta = 0$. These “toroidally trapped” C and D orbits are the first two members of a hierarchy of orbits which originate on the right hand side of the high-field ridge and bounce off the left hand side of its image at a subsequent field period (C orbits bounce after one period, D orbits bounce after two periods and so on). The C and D orbits shown have $N_{\kappa_{\|}} = 4$ and 6 respectively. Of the trapped orbits, the long C and D type orbits make the least contribution to direct (collisionless) losses.

From this point on, we identify the A, B, C, etc classes of drift orbit with the values of $N_{\kappa_{\|}}$ listed in table 2.1. It will become clear in the coloured drift surface plots of the following section that the alphabetical labelling system distinguishes between several classes of orbit with different geometries. It will also become clear that the numerical orbit signature, $N_{\kappa_{\|}}$, reliably distinguishes between these geometrically distinct orbits.

<table>
<thead>
<tr>
<th>Class</th>
<th>$N_{\kappa_{|}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1</td>
</tr>
<tr>
<td>B</td>
<td>2</td>
</tr>
<tr>
<td>C</td>
<td>3 or 4</td>
</tr>
<tr>
<td>D</td>
<td>5 or 6</td>
</tr>
<tr>
<td>E</td>
<td>7 or 8</td>
</tr>
<tr>
<td>F</td>
<td>9 or 10</td>
</tr>
</tbody>
</table>

Table 2.1: Number of maxima in parallel kinetic energy per bounce section for the orbit classes of Sec. 2.4.
Figure 2.6: The position of several bounce orbits in the H-1NF magnetic field. Typical contours of $|B|$ are shown in the background. The grey regions are where the radial drift is inward, and the dashed line is a magnetic field line.
2.4. *Drift orbits with no electric field*

Figure 2.7: The toroidal projections (onto a plane of constant $\phi$) of the four orbits in figure 2.6.
Figure 2.8: The phase-space trajectories of the four orbits in figures 2.6 and 2.7.
2.4. Drift orbits with no electric field

2.4.2 Drift surfaces

In this section we present toroidal cross-sections of H-1NF drift surfaces in the absence of radial electric fields. Firstly, the drift surfaces of the most-deeply-trapped orbits are calculated using the \( \min B \) method, for the three magnetic configurations of section 2.2.3. We then survey the drift surfaces of the other classes of trapped orbit in the standard configuration, by taking toroidal cross-sections of cold ion orbits. These plots are presented using the Boozer coordinate conventions of section 2.2.2. To help with the visualisation of the surfaces, some of them are then presented in real coordinates. Finally, we compare toroidal cross-sections of the helically trapped drift surfaces for the three magnetic configurations, before going on to look at the effect of the radial electric field in section 2.5.

a) The \( \min B \) surfaces

The most-deeply-trapped orbits, which have \( \mathcal{K}_{\parallel} = 0 \) and \( J = 0 \), are expected to lie on the \( \min B \) contours [75, 64]. These orbits are the limiting case of the deeply-trapped orbits (the class A orbits), which are characterised by low \( J \) and \( N_{\mathcal{K}_{\parallel}} = 1 \), and they mostly do not intersect the \( \phi = 0 \) plane.

In H-1NF the helical ripple has a double lobed well in each field period, so if the \( \min B \) curves are plotted conventionally (by varying \( \phi \) over a field period and plotting the resulting contours of \( \min B \) in the \( (\psi, \theta) \) plane [64]) they will exhibit an up-down symmetry which is not present in projections of the deeply trapped orbits onto the same plane. Therefore we find \( \min B \) contours by varying \( \phi \) over half a field period, \([0, \pi/3]\), only (spanning only one lobe minimum.) The resulting contours, plotted in figure 2.9 for the three configurations studied, reflect the topologies of half of the (type A) deeply trapped orbits in the absence of electric fields. The complementary family of (type A) deeply trapped orbits, occurring in the other lobe minimum, looks identical but is inverted in the horizontal axis. In the 3 configurations
studied in this paper, the A-type orbits are not confined at all when $E_r = 0$, except for a small fraction in the magnetic hill configuration. Compared to a conventional stellarator such as the ATF [64], the resulting confinement of deeply trapped orbits in H-1NF, in the absence of radial electric fields, is extremely poor.

b) Cold ion orbits

The topologies of the other classes of trapped orbits are best studied using drift surfaces. Unlike Rome, we do not use isosurfaces in $J^*$ to calculate the drift surfaces of these orbits, because the $\epsilon/N \ll 1$ assumption, used in the derivation of the original $J^*$, is invalid in H-1NF. Instead we use cold ion orbits to trace out the surfaces; when the orbits are cold, the motion is adiabatic (i.e. drifts transverse to the field lines are very slow) and so the second adiabatic invariant, $J = \oint mv_{||}dl$, is conserved for the bounce orbits. In the rest of this chapter, toroidal cross sections of drift surfaces are drawn by plotting the puncture points of cold ion orbits where they cross through the $\phi = 0$ and $\phi = \pi/3$ planes. The colours which appear in the drift surface graphs (in figures 2.10–2.19) are indexed to the value of $N_{x_4}$, which was measured while the code calculated the orbits.

To get an overview of the full spectrum of (zero electric field) drift surfaces in H-1NF, we plot toroidal cross-sections of drift surfaces in this manner, for several phase-space cross-sections which are specified by a normalized magnetic moment, $\hat{\mu} = \mu B_0/\mathcal{E}$. We have normalized the magnetic moment in this way because the drift surface geometries are expected to be independent of the field strength and particle energy. In each single graph, the total energy $\mathcal{E}$ of each of the particle orbits is kept the same, so that the resulting drift surfaces do not intersect. The resulting $\phi = 0$ (toroidal) cross-sections are shown in figure 2.10, and the $\phi = \pi/3$ (toroidal) cross-sections of the same drift surfaces are shown in figure 2.11. There are eight graphs in each figure.
2.4. Drift orbits with no electric field

corresponding to $\hat{\mu} = 1.05, 1.0, 0.95, 0.9, 0.85, 0.8, 0.75$ and 0.70, ranging from deeply trapped ($\hat{\mu} = 1.05$) to marginally trapped ($\hat{\mu} = 0.8$) to passing ($\hat{\mu} < 0.7$). The maximum and minimum values that $\hat{\mu}$ can take are $B_0/B$ and 0, respectively.

Each of the lines shown in figures 2.10 and 2.11 is composed of many puncture points, very close together. There is one such puncture point recorded (in each figure) between each bounce of each orbit. The colours of the puncture points represent the number of maxima in the parallel kinetic energy, $N_{K_\parallel}$ which occur between each bounce. The large blank sections, in which there are no orbits, are regions where orbits cannot exist with that value of $\hat{\mu}$, because the local magnetic field is too high. So, most of the trapped orbits occur at around $\theta = \phi = 0$, which is quite consistent with what one would expect from the background magnetic field structure shown in figure 2.6: there are very few trapped orbits which pass through $\phi = \pi/3$ (the top three panels of figure 2.11 are completely blank) because this is the region where the field strength is at its maximum. Also, the red orbits (the helically trapped, class B orbits) begin at the top of the figure, and move in a downward direction on the plots.

Figures 2.10 and 2.11 show that, like the deeply-trapped orbits, the helically trapped orbits are unclosed, and in some places are even perpendicular to the flux surfaces, so H-1NF will have a high level of direct losses in the absence of electric fields. The higher classes of trapped orbits, such as the class C orbits (with $N_{K_\parallel} = 3$ and 4) are also not well confined, but they do not intersect the flux surfaces (which are concentric circles in these plots) at such obtuse angles. The passing orbits, characterised by $N_{K_\parallel} = 0$, are well confined as expected, since they are approximately concentric with the flux surfaces.
c) Trapped orbit drift surfaces

We show later (see figure 2.22) that the dominant classes of trapped orbit are the B and C types. Therefore we concentrate on these types of orbit by exclusively looking at the $\mu = 0.9$ (mainly B-type) and $\mu = 0.85$ (mainly C-type) cases in the rest of this section. To begin, we take a look at the B and C drift surfaces, in real coordinates, before seeing what they look like, again in Boozer coordinates, in the other two magnetic configurations.

To view the drift surfaces in real coordinates, we take toroidal cross-sections of the drift orbits, by recording the puncture points of the orbits at the $\phi = 0$, $\pi/6$, $\pi/3$, and $5\pi/6$ planes (i.e. at four quarters of one field period.) The resulting curves (composed of puncture points) are then mapped into real coordinates. The $\mu = 0.9$ result is presented in figure 2.12 and the $\mu = 0.85$ result is in figure 2.13. The square in the middle of each figure represents the 10.5cm thick central ring conductor, and the major axis is to the left. Each of the figures show that the helically trapped drift surfaces rotate slowly as they wind about the central ring conductor. That is, the normal vector to the red drift surfaces only rotates by about 90° in one 360° rotation about the ring conductor. The blue/grey class C orbits display a similar behaviour. It is can also be seen that the regions where trapping is excluded (ie the blank regions) are where the field strength is high, due to proximity to the central ring conductor.

Now we revert to Boozer coordinates, and compare the $\mu = 0.9$ and $\mu = 0.85$ drift surfaces for the three magnetic configurations. Figure 2.14 shows the $\mu = 0.9$ drift surfaces, from left to right, for the low-transform configuration, the standard configuration, and the high-transform configuration, at $\phi = 0$ (top row) and $\phi = \pi/3$ (bottom row.) There is only a slight variation in the shapes of the drift surfaces in Boozer coordinates. However, there is a significant variation in drift surface type which occurs at a given point. This is due to the differing values of the local field strength in the
2.4. *Drift orbits with no electric field*

different configurations — the high-transform configuration is most similar to the standard configuration, and the low-transform configuration, which has the least variation in the field strength, has fewer trapped particles (at $\tilde{\mu} = 0.9$) close to the magnetic axis. The excluded region at $\phi = \pi/3$ is much smaller for the low transform case because the field ripple is smaller. Passing orbits appear near the magnetic axis in the low-transform case for the same reason. The $\hat{\mu} = 0.85$ drift surfaces in figure 2.15 reinforce this interpretation, but here it appears that the low-transform configuration tends to have fewer C-type (blue/grey) orbits because there is less variation in $\max_\phi B$ in the poloidal direction, so orbits are mainly either helically trapped or passing. A more detailed analysis of orbit class populations is carried out in section 2.7 below.

d) *Summary*

In summary, the drift surfaces of the trapped orbits in all three configurations studied are unclosed in the absence of electric fields. Thus, in H-1NF there are no closed superbananas in the conventional sense. The passing orbits have very favourable drift surface geometries. The change in magnetic geometry has little influence over the drift surface geometries, but it does seem to have some influence over the relative abundances of the different classes of orbit.
Chapter 2. Drift Orbits in H-1NF

Figure 2.9: Contour plots of $\min_{\phi} B$ for the three configurations, (a) standard, (b) high transform and (c) low transform. $\phi$ was only varied over half a field period, in the increasing direction from $\phi = 0$. In each of the plots, the thick line corresponds to 1 tesla and the contours are separated by 0.02 tesla and the value of $\min_{\phi} B$ increases from right to left. In (a), some projections of deeply trapped orbits are superposed.
2.4. Drift orbits with no electric field

Figure 2.10: Phase space scan at $\phi = 0$ and with zero electric field, for the H-1NF standard configuration. The total energy of every orbit in these plots is the same. Also, in each particular frame, $\mu = B_0 \mu / E$ is held constant. From left to right and from top to bottom, $\mu = 1.05, 1.0, 0.95, 0.9, 0.85, 0.8, 0.75, 0.70$. Colours denote the number of maxima in parallel kinetic energy, $N_{k||}$ between each bounce.
Figure 2.11: Phase space scan at $\phi = \pi/3$ and with zero electric field, for the H-1NF standard configuration. The total energy of every orbit in these plots is the same. Also, in each particular frame, $\mu = B_0\mu/E$ is held constant. From left to right and from top to bottom, $\mu = 1.05, 1.0, 0.95, 0.9, 0.85, 0.8, 0.75, 0.70$. 


2.4. Drift orbits with no electric field

Figure 2.12: Toroidal cross sections of $\mu = 0.9$ drift surfaces in real coordinates, for the standard configuration, at (a) $\phi = 0$, (b) $\pi/6$, (c) $\pi/3$, and (d) $5\pi/6$. The horizontal coordinate is the major radius, and the vertical coordinate is the $z$-axis.
Figure 2.13: Toroidal cross sections of $\hat{\mu} = 0.85$ drift surfaces in real coordinates, for the standard configuration, at (a) $\phi = 0$, (b) $\pi/6$, (c) $\pi/3$, and (d) $5\pi/6$. 
2.4. Drift orbits with no electric field

Figure 2.14: Drift surface cross sections taken at $\phi = 0$ (top) and $\phi = \pi/3$ (bottom) for the low transform case (left), the standard configuration (middle) and the high transform configuration (right). The section of phase space represented here is specified by $\mu B_0/\mathcal{E} = 0.9$. 
Figure 2.15: As in figure 2.14, but here the section of phase space is specified by $\mu B_0/E = 0.85$. 
2.5 Drift surfaces and the electric field

In the absence of electric fields, the poloidal drift is driven by the $\partial B/\partial \psi$ magnetic field gradient term in equation 2.2. When radial electric fields are introduced, a further poloidal drift term arises, which can greatly exceed that due to the magnetic field gradient, so the drift surface topologies can be significantly modified. In fact, the introduction of a radial electric field has three significant effects: (a) poloidal rotation, (b) an electrostatic trapping/detrapping effect which occurs as the particle drifts radially, and (c) electrostatic confinement. The latter two effects are due to the change in a particle's kinetic energy as it drifts radially in a background electrostatic potential gradient.

To examine the impact of these effects on the trapped particle population, we present in figures 2.16 and 2.17 the $\mu = 0.9$ drift surfaces, in the presence of 9 electric fields. The $\mu = 0.9$ surfaces are used because they are mainly composed of helically trapped orbits, which have the worst shape, from a transport perspective, in the absence of electric fields. In each case the electrostatic potential is parabolic in the average minor radius,

$$V = V_0(0.25 - r^2/a_p^2),$$

and the 9 electric fields are specified by $V_0 = -1, -0.5, -0.2, -0.1, 0, 0.1, 0.2, 0.5, \text{ and } 1$. This potential profile was chosen to ensure that the particle kinetic energy at $a_p/2$ is the same in each case. This works because $E$ and $\mu$ are both fixed in all of the graphs. Keeping $\mathcal{K}(a_p/2)$ constant ensures that we can observe, at least at $a_p/2$, the effect (labelled (a) above) of the potential gradient on the drift surface geometry; i.e. it allows us to distinguish between the geometry change due to $\partial V/\partial \psi$ from the trapping change due to $V(\psi)$. As in all of the previous plots, the drift surfaces are those of ions — electron drift surfaces are not plotted, but their behaviour can be inferred from the ion surfaces, by reversing the sign of $V_0$. 


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The results are as follows. Firstly, comparing the $V_0 = -0.1$ drift surfaces with the $V_0 = 0$ drift surfaces, we see that effect on the drift surface curvature, due to this small potential gradient, is already comparable to the $\partial B/\partial \psi$ influence on the curvature. This is consistent with well known results in neoclassical transport, where it is generally expected that the “resonant” electric field (where the poloidal drifts due to the magnetic and electric forces cancel) is small compared to a thermal potential gradient.

Now consider the $V_0 = -1$ (ion root) case. The drift surfaces of trapped orbits at $r = a_p/2$ have much smaller radial widths due to the enhanced poloidal rotation. This is because the minimum energy surfaces which the orbits lie on become dominated by the electrostatic potential, the gradient of which is entirely in the radial direction. The electrostatic trapping/detrapping effect can also be seen: if we consider a trapped particle at $a_p/2$ which has some inward drift, the decrease in $V$ as $r$ decreases means that the particle kinetic energy must increase to conserve energy. Since $\mu$ is also constant and (as we have just seen) the magnetic field gradient term is small, most of the extra kinetic energy will be in the parallel direction. As a result, the orbit becomes “more passing”, until it reaches the interior region, where its kinetic energy exceeds $\mu B_{\text{max}}(r)$, and it becomes a passing particle (black orbits). Conversely, if it drifts outward in radius, the kinetic energy decreases rapidly until the conservation of $\mu$ and $E$ requires that $K$ vanishes. Thus there is a large (white) excluded region beyond $r \approx 0.6a_p$. The passing particles at the centre are well confined, and the trapped particles near $a_p/2$ are electrostatically confined, in that the conservation of energy forces them to remain within a certain potential isosurface.

At the opposite extreme, when $V_0 = 1$ (the electron root) the reverse trapping/detrapping behaviour occurs, and the passing (high $K$) region occurs at the exterior of the plasma. In some sense, the trapped orbits which exist at $a_p/2$ are “held in” by the passing orbits. The energy-excluded region is
close to the axis this time. Again, the trapped orbit geometries are superior to those in the $V_0 = 0$ case.

As the sequence of $V_0$ values progresses between -1 and 1 in figure 2.16, we observe the change in curvature of the trapped drift surfaces, from good ($V_0 = -1$) to bad ($V_0 \approx 0$) to good again ($V_0 = 1$). As an example, the tangent to the red surfaces, evaluated at $(r, \theta) = (a_p/2, \pi/4)$, rotates by approximately $180^\circ$ as $V_0$ changes from $-1$ to $1$. Simultaneously, the forbidden region contracts, and shifts to the left side of the plots, until at $V_0 = 0.2$ it is enclosed by trapped orbits. By the time we reach $V_0 = 1$, the forbidden region has shifted to the center of the plasma.

In the $\phi = \pi/3$ cross sections (figure 2.17) the same general behavior is observed, but this time the forbidden region appears first on the right hand side of the plots, and moves inward from there. As in figures 2.10 and 2.11, the forbidden region is bigger in the $\phi = \pi/3$ cross sections than in the $\phi = 0$ cross sections because the field magnitude is greater there. Again, at some points on the $\phi = \pi/3$ cross sections (e.g. at $(\theta, r) = 3\pi/2, a_p/2$) the tangent line to the red surfaces rotates by approximately $180^\circ$ in the progression from $V_0 = -1$ to $V_0 = 1$.

Our final observations regarding figures 2.16 and 2.17 come from a comparison with figure 2.14. It is clear from all of the figures that the effect of the magnetic configuration on the drift surfaces is only comparable to the effect of the electric fields which have $|V_0| \approx 0.1$. Theory has predicted [20, 41, 38, 37, 76], and experiment has verified [49, 77, 78, 79, 46, 80], that electric fields in stellarators are expected to be an order of magnitude greater than this in ordinary circumstances. The radial electric field will therefore have the dominant effect on transport, so we treat it in more detail later in this thesis, in chapter 4.

Before closing this discussion of drift surfaces, we again orient ourselves in real space. Figures 2.18 and 2.19 show the drift surfaces, in real coordinates,
which correspond respectively to the $V_0 = -1$ and $V_0 = 1$ cases for $\hat{\mu} = 0.9$. These plots indicate that the behaviour we have described above, regarding the presence of electric fields, extends over the whole torus. Figure 2.18 also shows a new feature: close to the excluded region at $\phi = \pi/6$ and $\phi = 5\pi/6$ (sections b and d,) there are some light green ($N_{K_\parallel} = 1$) orbits. These are the deeply trapped orbits which we began our discussion of drift surfaces with in section 2.4.2, and they too have become closed by the radial electric field.

In summary, we have shown that the details of the radial electric field are more important than the details of the magnetic configuration, for thermal particles. For high energy fusion products such as alpha particles, this will not necessarily be the case, because their total energy will be large compared to the electrostatic potential variation caused by a “thermal” radial electric field, so the drift surfaces that they follow could be unclosed in a stellarator with a geometry like that of H-1NF.

When a small negative electric field is present (e.g. in the $V_0 = -0.2$ case in figure 2.16) the red (helically trapped) drift surfaces can become closed, like the closed superbananas that occur in conventional stellarators. When a thermal electric field of either sign is present, the orbits become more localised in the radial direction. In the electron root, trapped particle populations tend to be excluded from the center of the plasma, and any significant motion in the radial direction will be curtailed by a transition to the passing state. In the ion root, the situation is reversed; inward radial motion is limited by transitions to the passing state, and outward radial motion is prevented by electrostatic confinement. In both cases, trapped particle drift surfaces adopt favourable shapes, from a transport perspective, because the electrostatic potential mainly determines the minimum energy surfaces which the particles follow.
2.6 Drift surfaces and finite orbit widths

The drift surfaces described above are dependent on the local conservation (i.e. conservation between transitions) of the longitudinal adiabatic invariant. At 1 eV in a 1 tesla background field, \( J \) has been found to be locally conserved to within less than 0.01\% By way of comparison with more realistic operating conditions, figure 2.20 shows projections of proton drift orbits, at temperatures up to 1 keV, onto a \( \chi = \) const. plane, with \( \theta_0 \) acting as the poloidal angle of the plot (again \( V_0 = 0 \) \( \hat{\mu} = 0.9 \)). Since \( \theta_0 = \theta \) when \( \phi = 0 \), they can be compared with the \( \phi = 0 \) (and \( \hat{\mu} = 0.9 \)) cross sections in figure 2.10. As the orbit widths increase in figure 2.20, the deviation about the drift surfaces increases, but the trajectory of the banana center continues to follow the drift surface. For each temperature, the deviation is higher when the orbit is toroidally trapped than when it is helically trapped. A comparison with the puncture plot of figure 2.21 (which has been obtained under the same conditions as figure 2.20 by following orbits for up to 1000 transits of the complete torus and plotting intercepts with the \( \phi = 0 \) plane) shows that orbits which continually undergo transitions between the B and C type orbits can be confined, at high temperatures, even in the absence of electric fields. The "iteration" of the "mapping" between the B and C orbit types has a number of periodic orbits associated with it (at the centres of the closed curves in 2.21(c) and (d)). These periodic orbits are surrounded by islands (the closed curves) which appear to be separated by a chaotic region. This qualitative result has been verified by comparison with a symplectic integrator.

The presence of a collisionless (partial) confinement region for the high energy trapped particles may have important implications for the efficiency of ECH heating in H-1NF. Very high energy (\( E \sim 10 T_e \)) electrons are produced by ECH heating, which excites the perpendicular velocity of electrons on the
resonant surfaces, so the electrons will tend to be directly lost along the drift surfaces, in what has become known as "electron pumping". The high loss rates degrade the heating efficiency, and can degrade overall confinement by making the electric field more positive. In H-1NF, the position of the resonance layer can be selected via control of the magnetic field strength, and the positioning of mirrors which direct the microwave radiation from the gyrotron. For example, the resonance layer could be positioned at point 1 or point 2 in figure 2.21. If it were at point 1, then electron pumping would take place in the usual sense, along the type B drift surfaces, but, if it were at point 2, then electron losses would be diminished by collisionless detrapping into the type C (toroidally trapped) state. We estimate that this process would double the confinement time of electrons heated at point 2, compared to electrons heated at point 1, with a resulting improvement in the heating efficiency and the overall particle confinement. It would be relatively straightforward to test this experimentally.
Figure 2.16: Electric field scan at $\phi = 0$, for the $\hat{\mu} = 0.9$ section of phase space, in the H-1NF standard configuration. The kinetic energy is the same at $a_p/2$ in each plot.
Figure 2.17: Electric field scan at $\phi = \pi/3$, for the $\mu = 0.9$ section of phase space, in the H-1NF standard configuration. The kinetic energy is the same at $a_p/2$ in each plot.
Figure 2.18: Toroidal cross sections of $\mu = 0.9$ drift surfaces in real coordinates, with an electric field specified by $V_0 = -1$. The plots are for the standard H-1NF configuration, at (a) $\phi = 0$, (b) $\pi/6$, (c) $\pi/3$, and (d) $5\pi/6$. 
Figure 2.19: Toroidal cross sections of $\mu = 0.9$ drift surfaces in real coordinates, with an electric field specified by $V_0 = 1$. The plots are for the standard H-1NF configuration, at (a) $\phi = 0$, (b) $\pi/6$, (c) $\pi/3$, and (d) $5\pi/6$. 
Figure 2.20: Drift orbits in the standard configuration, projected onto the $\chi = 0$ plane, and plotted using the *rotating* poloidal angle (*i.e.* $\theta_0$) as the azimuthal coordinate. For each case, $\mu B_0/E = 0.9, V_0 = 0$ and $B_0 = 1T$. (a) $T_i = 1$ eV, (b) $T_i = 10$ eV, (c) $T_i = 100$ eV, and (d) $T_i = 1000$ eV.
Figure 2.21: Effect of particle kinetic energy on the drift surfaces. Proton orbit cross sections are shown at $\phi = 0$ for the $\mu B_0/E = 0.9$ case, at temperatures of (a) $T_i = 1$ eV, (b) $T_i = 10$ eV, (c) $T_i = 100$ eV, and (d) $T_i = 1000$ eV. To demonstrate the global features of the motion, 100 orbits were initialised on a “spoked wheel” pattern for each case.
2.7 Orbit populations

In this section, we use the value of $N_{K_{\parallel}}$ to study the populations of (i.e., the fractions of phase-space occupied by) the various orbit classes. We study the distribution of orbits on a flux surface, and in the toroidal cross section, using the assumption of an isotropic velocity distribution. An isotropic velocity distribution is uniformly distributed in the pitch angle parameter, $\eta = v_{\parallel}/v$.

2.7.1 Effect of configuration and electric field

We have computed $N_{K_{\parallel}}$ in order to study the distribution of orbits on a flux surface, assuming an initially isotropic velocity distribution. For this purpose, $10^6$ particle orbits were initialised uniformly through $(\theta, \phi, v_{\parallel}/v)$ space at half the plasma radius in the standard configuration. The orbits were propagated both forward and backward in time to their first bounce points and $N_{K_{\parallel}}$ was recorded for each. The resulting populations, shown in figure 2.22, show that at $T_i = 100$ eV and $V_0 = 0$, approximately 60%, 5%, 15%, and 20% of orbits are in the passing, locally trapped (A), helically trapped (B), and toroidally trapped (C and so on) classes respectively. Therefore the total trapped particle fraction, at half the plasma radius and in the absence of electric fields, is about 40% in the H-1NF standard configuration. The relative population densities of the trapped particle classes will change depending on temperature, electric field, and magnetic configuration. The dependence on electric field and magnetic configuration is shown in figures 2.22-2.25.

Figure 2.22 shows that, over a wide range of electric fields, the low-transform configuration has the least number of C, D and E type orbits, and the highest numbers of passing orbits, deeply trapped, and helically trapped orbits. This result was foreshadowed by our discussion of figures 2.14 and 2.15 in section 2.4.2: in the low-transform configuration, orbits are mostly (~ 85% when $V_0 = 0$) passing, or helically trapped. The total trapped particle frac-
tion is 40%. The standard configuration and the high-transform configuration have very similar behaviour with respect to trapping fractions. They both have a 45% total trapped particle fraction, which is mainly composed of C-type orbits (15–20%) and helically trapped orbits (10–15%). The preponderance of C type orbits in these configurations is largely due to the higher rotational transform. It ensures that orbits are more skewed with respect to the $\theta = const$ lines, so there is a narrower window in $\theta$ which particles trapped in the ripple well will occupy. Figure 2.23 compares the flux-surface-averaged radial orbit widths which occur in the three configurations.

In figures 2.24 and 2.25 the effect of finite orbit widths is shown for the standard configuration. Increasing orbit width tends to redistribute the relative trapping fractions, with a marked decrease in type B orbits when the electric field is high, a slight increase in type A orbits overall, and an increase in the numbers of orbits with higher $N_{K_i}$ values. Figure 2.25 shows that the orbit width increases with $\sqrt{T}$, as expected, with some variation created by the electric field. The electric field has the biggest impact on orbit widths when the orbit width is large.

We note that, whereas it is widely known that $E_r$ improves the topology of helically trapped orbits, we have shown here that it also reduces their numbers relative to the toroidally trapped orbits.

### 2.7.2 Effect of local geometry

In order to understand the geometric dependence on the radial electric field, we have plotted local orbit populations and local average orbit widths, in the $\phi = 0$ cross section of the standard configuration in figures 2.26 and 2.27. Figure 2.26 shows the spatial dependence of the populations of the dominant trapped particle types for no electric field, with electric fields of thermal magnitude, and with a strong (ion root) electric field. These populations were arrived at using the same counting method as used for figure 2.22, again
under the assumption of an initially isotropic velocity distribution. In this case, 1300 mesh points were distributed in the $\phi = 0$ plane, and 200 orbits were initialized at each point, uniformly distributed in $\eta$. Figure 2.27 was produced by recording the radial excursion of each of these orbits between their bounce points, and averaging this excursion according to the number of particles in each trapping class on each mesh point.

A comparison of figures 2.26 and 2.27 indicates that the geometrical dependence of the population densities are best correlated with the radial orbit widths for the longer toroidally-trapped (D and E) orbits. Also, the effect on the widths and populations of the positive and negative electric fields is very similar. There is a concentration of the population of the C orbits at the outboard side of the cross-sections but this is shifted inward for the high-field case. It is interesting to note that a potential of thermal magnitude almost completely eliminates the E orbits (but this trend does not continue at higher potentials, i.e. there is a specific potential for which the contribution, and width, of the E orbits is a minimum). The fields of thermal magnitude have a substantial effect on the orbit widths, but the transport "hotspots" in the $\theta \sim \pi/2$ and $\theta \sim -\pi/2$ regions persist. When the electric field becomes strong, almost all geometric dependence of the orbit widths is removed. In a fusion reactor this feature could be significant because of the importance of the heat load distribution on the vessel wall. In the H-1NF heliac, this information can be used to help guide the positioning of plasma detector plates for experimental transport studies.

### 2.8 Discussion

As with the ATF [64], the H-1NF heliac is an experimental facility which has been designed to explore MHD equilibrium and stability rather than to optimise transport in the absence of equilibrium electric fields. The drift
Figure 2.22: Fractions of the total particle population occupied by the six main classes of orbit (passing, A class, B class, etc,) as a function of electric field. The results are shown for the three magnetic configurations: low transform (dotted lines,) standard configuration (solid lines,) and high transform (dashed lines.)
Figure 2.23: Average radial orbit widths of the six main classes of orbit (passing, A class, B class, etc,) as a function of electric field. The results are shown for the three magnetic configurations: low transform (dotted lines,) standard configuration (solid lines,) and high transform (dashed lines.)
Figure 2.24: Fractions of the total particle population occupied by the six main classes of orbit (passing, A class, B class, etc.) as a function of electric field. Four cases are shown for each orbit class, corresponding to the temperatures 1eV (thickest lines,) 10eV, 100eV, and 1000eV (thinnest lines.)
2.8. Discussion

Figure 2.25: Average radial orbit widths of the six main classes of orbit (passing, A class, B class, etc.) as a function of electric field. Four cases are shown for each orbit class, corresponding to the temperatures 1eV (thickest lines,) 10eV, 100eV, and 1000eV (thinnest lines.)
Figure 2.26: Percentile orbit populations at (a) $V_0 = 1$, (b) $V_0 = 0$, (c) $V_0 = -1$ and (d) $V_0 = -3.5$. 
Figure 2.27: Local orbit widths at (a) $V_0 = 1$, (b) $V_0 = 0$, (c) $V_0 = -1$ and (d) $V_0 = -3.5$. The width is measured between bounce points, and is normalized to the plasma minor radius.
surfaces of deeply trapped particles, in the absence of electric fields, are generally unclosed, leading to a level of direct particle losses which is worse than in torsatrons. This is significant in H-1NF, because it is observed experimentally that the electric field takes some time to establish itself, and within the first 3ms of a discharge, it may be effectively zero [81]. The large direct ion losses which can be expected to occur in this period would establish a negative radial electric field. The unclosed drift surface geometry also has implications for ECH heating experiments in H-1NF, as described above in section 2.6.

For thermal particles, electric fields of thermal magnitude improve greatly the geometry of the trapped orbits. Recent experimental results [49] have consistently measured radial electric fields in H-1NF of thermal magnitude or greater. Further optimisation of the magnetic field of the H-1NF to improve particle confinement could take the direction of the three field period Modular Helias-like heliac which has been shown to have an energy confinement time near 2 seconds under reactor conditions [36]. The techniques used in this study are robust enough to successfully treat H-1NF, which has a complicated magnetic field structure, so they should be effective in the study of trapped particle orbits in other helical axis stellarators. A review of the coloured drift surface plots in this chapter will reveal that the classification number, \( N_{K_E} \), derived from the phase space signature of each class of trapped orbit, reliably distinguishes between drift surfaces with different geometries. This empirical orbit classification method could be extended to determine the collisionless detrapping probabilities required [43] to analytically model transport due to collisionless trapping and detrapping in the long mean free path regime.
2.9 Conclusion

In this chapter, we have set out to describe the dominant trapped particle orbits in the H-1NF heliac and to understand some of the predictions of Monte Carlo studies (in the next chapter of this thesis and in reference [54]) in terms of these orbits.

We have shown that there is a hierarchy of trapped orbit types which occur in the magnetic ripple in H-1NF, ranging from the deeply trapped (with $\mu \approx 1$) to the marginally trapped ($\mu \approx 0.85$) to the passing ($\mu < 0.7$). Of these, the toroidally trapped (C and D) types can be "almost-closed" bananas (as in figure 2.7) when there is no electric field, but the deeply trapped (A type) and helically trapped (B type) orbits will not be "almost-closed" bananas, regardless of the radial electric field. Except when the electric field is small and negative (as in the $V_0 = -0.2$ case in figure 2.16) closed superbananas are usually absent. Nevertheless, there are still some orbits which remain collisionlessly confined by repeatedly making transitions between some of the trapping states. We speculate that it may be possible to use this feature to improve the efficiency of ECH heating in H-1NF, by positioning the resonant surface in the middle of the collisionless (partial) confinement region.

In adiabatic conditions, the drift orbits lie on drift surfaces, which have been identified [61, 63, 64] with isosurfaces of the longitudinal adiabatic invariant, $J$. In H-1NF, transport due to direct losses can be high, because the deeply-trapped and helically-trapped particles, which together make up 15–25% of an isotropic distribution, have unclosed drift surfaces when the radial electric field is small. A thermal radial electric field of either sign will greatly reduce such transport by improving the drift surface geometries, and by confining particles within a certain electric potential isosurface. The latter effect is accomplished by a positive radial electric field via orbit detrapping.
(converting trapped particles to passing particles), and by a negative radial electric field via energy exclusion. The radial electric field will be a more important determinant of the transport than the magnetic configuration will, except for the very high energy particles.

Using the value of $N_{Ki}$, we can quite effectively distinguish between the trapping states (which have different geometries), when the modular coil ripple is not included in the Fourier series representation of the magnetic field strength. The method has been used to show that the total trapped particle fraction varies from 40 to 45% in H-1NF, in the three configurations studied. The radial electric field has a significant effect on the way the trapped particles are distributed between the trapping states which we have defined; for example, it can heavily deplete the E-class state in some conditions.
Chapter 3

Monte Carlo transport coefficient calculations

In this chapter, we describe a Monte Carlo code which has been developed to study neoclassical transport in H-1NF. The matter in this chapter extends previous work [54] which has been done on the Monte Carlo calculation of diffusion coefficients in H-1, and emphasis is placed on Monte Carlo transport diagnostics and on computing considerations.

3.1 Review

The first Monte Carlo transport studies were done by Potok, Politzer and Lidsky [55] and by Boozer and Kuo-Petravic [53]. These were followed by Mynick [82], by Wobig [44], by Lotz and collaborators [83, 84, 56, 40], by Fowler, Rome and Lyon [42], by Betancourt and Garabedian [85], and, with application to H-1NF, by Painter and Gardner [59, 54]. Monte Carlo methods have also been developed to calculate the bootstrap current [86] and to simulate ICRF minority heating [87].
3.1.1 Transport coefficients

Monte Carlo transport codes follow many particles along their orbits, for several collision times, and calculate transport coefficients from the spatial evolution of the test particle distribution. The technique is computationally intensive because of the multiple timescales which exist in toroidal confinement systems. The CPU time requirements are reduced by the use of gyroaveraged orbits, and some codes further improve their efficiency by following the bounce averaged orbits. In H-1NF however, the second adiabatic invariant is not well conserved in normal experimental conditions, and so we use the gyroaveraged, rather than the bounce averaged, equations of motion.

The Monte Carlo procedure is also problematic because of difficulties involved in the computation of the transport coefficients. The first [55, 53, 82] Monte Carlo studies calculated diffusion coefficients. However, in the long mean free path regime, the transport is dominated by direct losses along the drift surfaces, sustained by diffusion in velocity space, which replenishes the loss cone. In these conditions, it has become accepted in the literature [42, 56, 88, 89, 44, 40, 90] that diffusion coefficients are not well defined. Two more general confinement time calculations have been proposed, based respectively on an asymptotic test particle loss rate [84] and on the decay rate of a functional of the test particle distribution [90]. We use both of these techniques later in this chapter, and compare their results with $D$ measurements. Details of the methods are given in sections 3.4.1, 3.4.2 and 3.4.3 below.

3.1.2 Collisions

Many works [53, 44, 83, 59, 54] use pitch angle scattering in a monoenergetic test particle distribution. In addition, an energy relaxation is usually applied to the distribution when electric fields are present, so that the confinement
3.1. Review

is not spuriously dominated by electrostatic confinement. Results regarding several different monoenergetic distribution energies may be convolved with a Maxwellian distribution [54, 40] to obtain total diffusion coefficients. Alternatively, a Maxwellian test particle distribution may be simulated, using both pitch angle and energy scattering [53, 55, 42, 91, 40]. The use of energy scattering does not have a significant effect on the results, but it increases the required computing time by an order of magnitude [40].

3.1.3 Transport scalings

Monte Carlo simulations have been used to study transport over wide ranges of collisionality. Universally, the predicted $\nu$ scaling of $D$ at low collisionality has been verified, but in the intermediate mean free path regime, where the $1/\nu$ scaling can sometimes be expected, there has been some variation in the results. Some controversy began with the results of Potok et. al. [55], who found that the predicted $1/\nu$ scaling of $\chi_i$, due to ripple trapping, did not occur, in a toratron in the reactor regime. Instead, $\chi_i$ remained approximately equal to the neoclassical plateau value as collisionality decreased. Mynick [82] criticised their results, arguing that Potok et. al. used simulation times which were too short, but, more importantly, Wobig [44] went on to explain that a $1/\nu$ scaling could not be expected, because Potok’s simulations were performed in a regime of large radial orbit width, where the loss cone would prevent an isotropic velocity distribution from being maintained. Wobig noted that the absence of an isotropic velocity distribution undermines the original argument for the existence of the $1/\nu$ regime. Since then, several authors [83, 84, 54] have presented results where the $1/\nu$ scaling was either not evident, or was greatly suppressed by either finite orbit widths or a radial electric field. The expected transport scalings in the tokamak plateau regime have not been contradicted, but at higher collisionality, Solano et al. [94] found, using the DKES code, that the transport scaling predicted by
analytic theory can be violated; in particular, the diffusion coefficient in a stellarator can drop below that of a tokamak, well within the Pfirsh-Schlüter regime. This has not, apparently, been observed in Monte Carlo studies, perhaps because the results have generally [84, 56, 42, 53, 54] not extended to collision frequencies much higher than the tokamak-plateau collision frequency. The confinement improvement was only observed by Solano et al. in the presence of strong ($|e\Phi/kT| > 1$), negative, radial electric fields. We consider the short mean free path regime later in this chapter, and we find results which agree qualitatively with those of Solano et al.

3.1.4 Monte Carlo studies of H-1NF

In 1993, Painter and Gardner [54] calculated diffusion coefficients in H-1, using a Monte Carlo code [59], over wide ranges of radial electric field, gyroradius, particle energy, and magnetic configuration. They fitted Shaing's model-based interpolation formula for the diffusion coefficient [41] to the Monte Carlo results, in the standard configuration, by varying the geometric parameters of the formula. The resulting analytic model, which is described in detail in chapter 4, was found to closely reproduce the Monte Carlo results in the wide range of conditions which were studied. In the present chapter, we develop more fully the Monte Carlo model used by Painter and Gardner, adding energy scattering [53], equations of motion for finite beta [42], new transport diagnostics [88, 40, 56], and optimising the code for both parallel and vector computing environments.

\[\text{A similar effect can be seen in the results of reference [55], where it was not remarked upon.}\]
3.2 The MCMuPPeT Code

The MCMuPPeT code (for Monte Carlo, Multi-Processing Plasma Transport) developed in this thesis is based on a parallelised Monte Carlo code [59] which has previously been used to calculate diffusion coefficients in H-1NF [54]. The code has a new name because it has been extensively rewritten using Message Passing techniques, so that it now fits within the Multiple Program, Multiple Data model of computer parallelism (the original code was parallelised using the Single Instruction, Multiple Data model.) The details of the parallelisation methods are described in the appendix. In this section we present the equations of motion followed by the test particles, and the models for the collisional processes. The transport diagnostics which have been implemented are described later, in section 3.4.

3.2.1 Equations of Motion

The code uses a gyroaveraged form for the drift velocity [53]

\[ v_d = v_\parallel \frac{B}{B} + \frac{mc}{eB}(v_\parallel^2 + \frac{1}{2}v_\perp^2) \frac{B \times \nabla B}{B^2} + c \frac{B \times \nabla \phi}{B^2} \]

This is expressed in the Boozer straight-field-line coordinates (SFLC), for which the field satisfies

\[ B = \nabla \chi = \nabla \theta_0 \times \nabla \psi. \]

The radial coordinate \( \psi \) is a flux surface label which corresponds to \( 2\pi \) times the enclosed toroidal flux. The poloidal coordinate \( \theta_0 \) labels a field line on the surface and \( \chi \) is proportional to the distance along the magnetic field line. We refer to this coordinate system, which does not have periodic angles, as "rotating SFLC coordinates," because the position of \( \theta_0 = 0 \) follows the field line as it winds about the flux surface. We also use a periodic system of SFLC coordinates, which has the same radial coordinate, but with poloidal...
Chapter 3. Monte Carlo transport coefficient calculations

and toroidal angles equal to $\theta = \theta_0 + \epsilon \phi$ and $\phi = (\chi - I \theta)/g$ respectively. Here $g = RB_\phi$ and $I = rB_\psi$ [53] are $2 \times 10^{-7}$ times the poloidal current (in ampere) outside a flux surface and $2 \times 10^{-7}$ times the toroidal current inside a flux surface, respectively [42]. In straight-field-line coordinates, the equations of motion can be expressed in terms of the magnetic field strength $B$ rather than the full $B$ vector. For the Monte Carlo calculations, we use the Fourier series representation of the magnetic field given in equations 2.5 and 2.6 of chapter 2. To model the electric field, we use the electrostatic potential profile, given in equation 2.7 of chapter 2, which is parabolic in the average radius. The use of the SFLC implies the assumption of nested flux surfaces.

One of the modifications from the original Monte Carlo code [59] has been to incorporate equations of motion which are valid for both vacuum and finite-beta fields. These equations, due to Boozer, can be found in reference [42]:

$$\dot{\psi} = \frac{\hat{P}_\theta g - \hat{P}_\phi I}{\gamma}, \quad (3.1)$$

$$\dot{\theta} = \left( \frac{\delta}{\partial \theta} \frac{\partial B}{\partial \psi} + e \frac{\partial V}{\partial \psi} + \frac{e^2 B^2}{m} \frac{\partial \rho_\parallel}{\partial \theta} \right) \frac{\partial \psi}{\partial \theta} - \frac{e^2 B^2}{m} \frac{\partial \rho_\parallel}{\partial \phi}, \quad (3.2)$$

$$\dot{\phi} = \left( \frac{\delta}{\partial \phi} \frac{\partial B}{\partial \psi} + e \frac{\partial V}{\partial \psi} + \frac{e^2 B^2}{m} \frac{\partial \rho_\parallel}{\partial \phi} \right) \frac{\partial \psi}{\partial \phi} + \frac{e^2 B^2}{m} \frac{\partial \rho_\parallel}{\partial \phi}, \quad (3.3)$$

$$\dot{\rho}_\parallel = \left[ -(\rho_\parallel g' - \epsilon) \hat{P}_\theta + (\rho_\parallel I' + 1) \hat{P}_\phi \right]/\gamma, \quad (3.4)$$

where $\rho_\parallel = m v_\parallel/eB$ is the parallel gyroradius, the dots denote time derivatives, and the primes denote derivatives with respect to $\psi$. The functions $\gamma$ and $\delta$ are defined by

$$\gamma = e[g(\rho_\parallel I' + 1) - I(\rho_\parallel g' - \epsilon)], \quad (3.5)$$

$$\delta = e^2 \rho_\parallel^2 B/m + \mu, \quad (3.6)$$

where $\mu = m v_\parallel^2/2B$, and the canonical momenta are

$$\hat{P}_\theta = -\delta \frac{\partial B}{\partial \theta}, \quad (3.7)$$
3.2. The MCMuPPeT Code

\[ \dot{P}_\phi = -\delta \frac{\partial B}{\partial \phi}. \quad (3.8) \]

Finally,

\[ \frac{\partial \psi}{\partial P_\theta} = \frac{\gamma}{\gamma}, \quad (3.9) \]
\[ \frac{\partial P_{\parallel}}{\partial P_\theta} = -\frac{\rho_{\parallel} g - t}{\gamma}, \quad (3.10) \]
\[ \frac{\partial \psi}{\partial P_\phi} = -\frac{I}{\gamma}, \quad (3.11) \]
\[ \frac{\partial P_{\parallel}}{\partial P_\phi} = \frac{I' \rho_{\parallel} + 1}{\gamma}. \quad (3.12) \]

In the zero-beta case, when \( I = 0 \) and \( g' = 0 \), equations 3.1–3.4 reduce to the equations of motion used in chapter 2 and references [53] and [54].

3.2.2 Collision operators

To model the pitch angle and energy scattering processes, the equations of motion for the pitch angle parameter \( \eta = v_{\parallel}/v \) and the energy \( E \) are formulated as stochastic differential equations, which are integrated using a weak, 2nd order stochastic predictor-corrector method due to Platen [93]. This method was described, for pitch angle scattering, by Painter [59]. It was tested against conventional integrators and found to produce the correct results, with significant computing speedups in some conditions.

To formulate the equations of motion in terms of stochastic differential equations, the stochastic (collision) process in each coordinate is decomposed into a drag (or drift) term, \( a \), and a dispersion (or diffusion) term, \( b \). The drag terms are associated with the mean changes in pitch angle and energy of each particle due to collisions. The dispersion terms are related to the standard deviations of the change in pitch angle and energy due to collisions. Following Platen, the drag and dispersion terms in \( \eta \) are defined as

\[ a(\eta_0) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{-1}^{1} (\eta - \eta_0) f(\eta, t + \Delta t|\eta_0, t) d\eta, \quad (3.13) \]
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and

\[ b^2(\eta_0) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{-1}^{1} (\eta - \eta_0)^2 f(\eta, t + \Delta t|\eta_0, t) d\eta, \quad (3.14) \]

where \( f(\eta, t + \Delta t|\eta_0, t) \) is the probability of transition from \( \eta_0 \) to \( \eta \) in a time \( \Delta t \) for a test particle. That is, \( f \) is the probability distribution function for a test particle at time \( t + \Delta t \), given that it was at \( \eta_0 \) at the earlier time \( t \). The drag and dispersion terms in \( E \) are defined analogously. Following Painter, the probability distribution function is expanded in a Taylor series,

\[ f(x, t + \Delta t|x_0, t) = \delta(x - x_0) + \frac{\partial f}{\partial t} \Delta t + O((\Delta t)^2), \quad (3.15) \]

where the delta function is involved because each test particle is treated separately, and each test particle is both monoenergetic and mono-directional. The time derivatives of the distribution functions are evaluated using the Lorentzian scattering operators from Boozer\[53]\:

\[ \frac{\partial f(\eta)}{\partial t} = \nu_p \frac{1}{2} (1 - \eta^2) \frac{\partial f}{\partial \eta} \quad (3.16) \]

and

\[ \frac{\partial f(v)}{\partial t} = \frac{1}{v^2} \frac{\partial}{\partial v} \left[ v^2 \nu_e \left( v f(v) + \frac{T}{m} \frac{\partial f(v)}{\partial v} \right) \right]. \quad (3.17) \]

The latter expression involves a distribution in velocities, which must be converted to one involving a distribution in energies:

\[ \frac{\partial f(E)}{\partial t} = \frac{\partial}{\partial E} \left[ (2E - T) \nu_e f(E) + 2 \nu_e T E \frac{\partial f(E)}{\partial E} \right] \quad (3.18) \]

Substituting equation 3.16 into 3.15, and integrating the resulting equation 3.14 by parts, we obtain the drag coefficient,

\[ a(\eta) = -\nu_p \eta. \quad (3.19) \]

Again substituting equation 3.16 into 3.15, but this time integrating equation 3.14 by parts, we obtain the dispersion coefficient,

\[ b(\eta) = \sqrt{\nu_p (1 - \eta^2)}. \quad (3.20) \]
3.2. The MCMuPPeT Code

In terms of the parallel gyroradius $\rho_\parallel$, the drag and dispersion terms become

$$a(\rho_\parallel) = -\nu_p \rho_\parallel$$

(3.21)

and

$$b(\rho_\parallel) = \sqrt{\nu_p \frac{m v}{e B} (1 - \eta^2)}$$

(3.22)

respectively. The effects of the drag and dispersion coefficients compete, with the drag term acting mainly on the passing particles, scattering them into a more deeply trapped state, and the dispersion term acting mainly on the trapped particles, scattering them into the passing state. The combination of the terms tends to make the velocity distribution isotropic.

For the energy coordinate, the analogous substitutions are made using equation 3.18 instead of 3.16, and we arrive at the drag and dispersion terms

$$a(\mathcal{E}) = -2\nu_\mathcal{E} \left( \mathcal{E} - \frac{3}{2}T - \frac{\mathcal{E} T}{\nu_\mathcal{E}} \frac{\partial \nu_\mathcal{E}}{\partial \mathcal{E}} \right)$$

(3.23)

and

$$b(\mathcal{E}) = 2\sqrt{\mathcal{E} T \nu_\mathcal{E}},$$

(3.24)

which are equivalent to the Monte Carlo operators in reference [53]. The drag coefficient tends to relax the distribution toward the thermal energy, while the dispersion coefficient tends to “thermalise” the energy distribution. Under the influence of these two terms only, the distribution will eventually arrive at a Maxwellian, of temperature $T$.

3.2.3 Stochastic differential equations

To complete the stochastic differential equation formulation using Platen’s prescription, the collisional drag and dispersion coefficients are combined with equations 3.1-3.4 above:

$$d\psi = \left[ (\dot{\psi}_g - \dot{\psi}_I) / \gamma \right] dt,$$

(3.25)

\footnote{We note that $\eta^2 = (eB/mv)^2 \rho_\parallel^2$.}
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\[ d\theta = \left[ \left( \frac{\partial B}{\partial \psi} + e \frac{\partial V}{\partial \psi} \right) \frac{\partial \psi}{\partial \theta} + \frac{e^2 B^2}{m} \frac{\partial \rho_{||}}{\partial \theta} \right] dt, \]  \hspace{1cm} (3.26)

\[ d\phi = \left[ \left( \frac{\partial B}{\partial \psi} + e \frac{\partial V}{\partial \psi} \right) \frac{\partial \psi}{\partial \phi} + \frac{e^2 B^2}{m} \frac{\partial \rho_{||}}{\partial \phi} \right] dt, \]  \hspace{1cm} (3.27)

\[ d\rho_{||} = \left[ -\left( \rho_{||} \dot{v} - \dot{I}_f \right) \dot{P}_{\theta} + \left( \rho_{||} \dot{I} + 1 \right) \dot{P}_{\phi} \right] / \gamma - \nu_{\rho} \rho_{||} \right] \right] dt 
+ \sqrt{\nu_{\rho}^2 \frac{m v}{e B} (1 - \eta^2)} dW_1, \]  \hspace{1cm} (3.28)

where the \( dW_1 \) are stochastic analogues [95] of the time increments \( dt \):

\[ dW_1 = \begin{cases} 
-\sqrt{3} dt, & 0 \leq p < 1/6 \\
\sqrt{3} dt, & 1/6 \leq p < 1/3 \\
0, & 1/3 \leq p < 1,
\end{cases} \]

where \( p \in [0, 1) \) is a random number.

When only pitch angle scattering is used in the code, which is the usual case, the test particle energy is relaxed with the same time constant as is used in the pitch angle scattering [56],

\[ d\mathcal{E} = \nu_{\rho} (\mathcal{K}_0 - \mathcal{K}) dt, \]  \hspace{1cm} (3.29)

where \( \mathcal{K}_0 \) is the initial kinetic energy for each particle. This is to stop collisionless, electrostatic confinement from dominating the transport which is measured in the code. When energy scattering is included, the increment in the energy coordinate is

\[ d\mathcal{E} = -2 \nu_{\mathcal{E}} (\mathcal{E} - \frac{3}{2} T - \frac{\mathcal{E} T}{\nu_{\mathcal{E}}} \frac{\partial \nu_{\mathcal{E}}}{\partial \mathcal{E}}) dt + 2 \sqrt{\mathcal{E} T \nu_{\mathcal{E}}} dW_2, \]  \hspace{1cm} (3.30)

where \( dW_2 \) is defined [95] by

\[ dW_2 = \begin{cases} 
-dt, & 0 \leq p < 1/2 \\
dt, & 1/2 \leq p < 1
\end{cases} \]

where \( p \in [0, 1) \) is a random number.

Usually, energy scattering is not used, because it increases the simulation times by up to an order of magnitude, without significantly effecting the results [40].
3.2.4 Collision frequencies

We use the pitch angle scattering frequency $\nu_p$ from Trubnikov [96], which appears in the NRL plasma formulare [97] as the relaxation rate for transverse diffusion,

$$\nu_p^{ab} = 2\nu_0^{ab} \left( 1 - \frac{1}{2x^{ab}} \right) \Psi(x^{ab}) + \frac{d\Psi}{dx^{ab}}.$$  \hspace{1cm} (3.31)

Here the superscript $ab$ denotes a quantity which applies to a particle of species $a$ streaming through a background composed of species $b$. The variable $x^{ab} = m_b K_a/m_a T_b$ is the normalised kinetic energy ($K_a$ is the kinetic energy of the particle of species $a$), and should not be confused with the normalised velocity, $x = (K/T)^{1/2}$ which is used by Boozer [53] and Lotz et al. [40]. To avoid confusion we use $v_n$ to denote the normalised velocity from here on.

The characteristic scattering frequency $\nu_0^{ab}$ appears in the NRL formulare as

$$\nu_0^{ab} = 4\pi e_a^2 e_b^2 \lambda_{ab} n_b / m_a^2 v_b^3.$$  

The function $\Psi$ is defined by

$$\Psi(z) = \frac{2}{\sqrt{\pi}} \int_0^z t^{1/2} e^{-t} dt.$$  

In practice we evaluate $\Psi$ and $d\Psi/dx^{ab}$ from the relation

$$\Psi(x^{ab}) = \Phi(v_n) - v_n \frac{d\Phi}{dv_n},$$

where $\Phi$ is the error function,

$$\Phi(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt.$$  

The Coulomb logarithm, $\lambda_{ab} = \log_e \Lambda_{ab}$ ranges from 13.3 for a 60eV Argon plasma, to 14.2 for a 200eV Hydrogen plasma in the H-1NF heliac. For the ion test particles streaming through a background of ions, it is [97]

$$\lambda_{ii} \simeq 6.5 - \log_e (Z^2 \sqrt{n / T^3}).$$
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with $T$ in eV and $n$ in $10^{20} \text{m}^{-3}$. For ions streaming through electrons, or electrons streaming through either species, it is

$$\lambda_{ab} = 7.9 + \log_e(T/\sqrt{n}),$$

in the same units.

For the energy scattering frequency $\nu_e$, we use Boozer's expression [53]. Written in the same notation as that used by the NRL formulary, it is:

$$\nu_e = 2\nu_0^a \Psi(x^{ab}).$$

3.3 Normalisations

In this thesis we employ the mean free path and loss rate normalisations introduced by Lotz and Nührenberg [40, 56]. The collisional mean free path and the diffusion coefficients and loss rates are normalised using the values that they take in the plateau regime in a tokamak.

Directly following Lotz and Nührenberg, we write the normalised mean free path, $L_*$, as

$$L_* = \frac{L_{\text{mfp}}}{L_c}, \quad (3.32)$$

where $L_{\text{mfp}} = v\tau_{90}$, and $L_c = \pi R_0 / \epsilon$, which is half of the connection length. The dimensionless diffusion coefficient, $D_*$, is

$$D_* = \frac{D}{D_p} \quad (3.33)$$

where $D_p$ is the tokamak plateau value

$$D_p = 0.64 \frac{\rho^2 v}{t^2 L_c} = 0.64 \frac{\rho^2 v}{\epsilon \pi R_0}. \quad (3.34)$$

Here, $v$ is the particle velocity and $\rho = mv/eB_0$ is the formal gyroradius, where $B_0$ is the magnetic field strength at $R_0$.

A normalised loss rate, $S_* = S/S_p$, is calculated using the analogous plateau loss rate, $S_p$, which is derived from the relationship between the
3.4 Monte Carlo transport diagnostics

diffusion coefficient and the confinement time in a cylindrical plasma column [45]:

\[ S_p = D_p \left( \frac{2.4}{a_p} \right)^2. \]  

(3.35)

In the Monte Carlo code, the loss rate \( S \) is calculated from the inverse of the confinement time, \( 1/\tau \). Three methods of calculating \( \tau \) are given in the next section.

The advantage of these normalisations is that they permit a straightforward comparison between the mean free path and a scale length of the magnetic system, and they similarly allow straightforward comparisons between the loss rates in an arbitrary toroidal system, and those expected in a tokamak of similar dimensions.

3.4 Monte Carlo transport diagnostics

In this section we describe a MC diffusion coefficient method, and the confinement time methods due to Lotz and Garabedian.

3.4.1 The Diffusion Coefficient, \( D \)

Classically, the diffusion coefficient can be estimated from \( D \sim \Delta^2/2\tau \), where \( \Delta \) is the step length of the diffusive process, and \( \tau \) is the time between random walk steps. In the “plateau” regime of neoclassical transport, \( \Delta \) is approximately the average banana width, \( \Delta_b \), and \( \tau \approx \tau_{90} \), the 90 degree scattering time.

It is generally considered [44, 45, 40] that, in the stellarator long mean free path regime, transport is dominated by direct losses along the drift surfaces, with diffusion in velocity space acting to replenish the loss cone. The presence of direct losses makes the usual [42, 53] methods of calculating diffusion coefficients questionable. To correctly incorporate the effect of lost
particles, we use a diffusion coefficient estimator due to Painter [59], which was derived by solving the diffusion equation for $D$, in the presence of an arbitrary distribution function, with zero boundary conditions which simulate particle losses from a region.

**Method**

In Monte Carlo codes, $D$ is measured from the average rate of change, during the simulation, of the radial variance of the test particle distribution. If $\tau_{\text{orb}}$ is the time a particle takes to make a toroidal orbit, and $\tau_{\text{conf}}$ is the confinement time, then the simulation time, $\tau_{\text{sim}}$, should satisfy

$$\tau_{\text{orb}} \cdot \tau_{90} < \tau_{\text{sim}} < \tau_{\text{conf}},$$

(3.36)

to ensure that the effects of the magnetic geometry and the collisional processes are properly incorporated, and that most of the test particles are retained in the calculation. We use a diffusion coefficient estimator which combines Painter’s [59] method with that of Fowler *et al.*[42], in such a way that it has three distinguishing features:

1. simulations begin with a “quiet start” [42]

2. test particles which are lost during the simulation are included in the statistical calculation of $D$ [59]

3. when a test particle is lost, it is replaced by “cloning” one of the confined particles. Each particle has a statistical weight, $w_i$, which is split between the clones when a particle is duplicated [59].

The first two of these are physically motivated, and the third is used to improve code vectorisation. The quiet start is to ensure that the resulting diffusion coefficient is not effected by the initial, rapid, spreading of the test particle distribution into the orbit width. To this end, the test particles
are integrated collisionlessly, for several toroidal orbits, before the collision operator is switched on, and before any diffusion statistics are collected. The second feature is designed to include in the diffusion statistics the particles which diffuse the fastest. The third feature improves code vectorisation by keeping the number of test particles constant in the simulation, even when particles are lost. It also improves the statistics, by increasing the number of test particles used in the simulation, without changing the integrated test-particle weight.

In summary, the calculation proceeds as follows:

1. all test particles are initialized at \( r_0 = 0.5 \), with statistical weight \( w_i = 1 \)

2. the particles are propagated collisionlessly for several toroidal orbits, and the resulting positions, \( r_{1i} \) are recorded

3. collisions are switched on, and the particles are propagated for a time, \( \tau_{\text{sim}} \), which obeys condition 3.36 above. The time, \( t_i \), that each particle spends in this phase of the simulation is recorded.

Here, the index \( i \) runs over the test particles, and \( r = (\psi/\psi_{\text{cfs}})^{1/2} \). If a test particle crosses \( r = 1 \), then it is “lost”; \( t_i \) and \( w_i \) are recorded, and the particle is replaced in the simulation by cloning one of the remaining test particles. The duplicated particle, \( j \), is chosen at random, and the two clones continue in the simulation with statistical weights \( w_j/2 \).

The diffusion coefficient estimator is

\[
D = \frac{a_p^2}{2} \sum_i \frac{[w_i(r_{2i} - r_2)^2 - (r_{1i} - r_1)^2]}{\sum_i w_i t_i},
\]

where the overbar denotes the average over the test particle distribution, and the index \( i \) runs over all test particles, including those which were lost. The \( r_{1i} \) are the positions of the particles at the end of the quiet start phase (at
Chapter 3. Monte Carlo transport coefficient calculations

the beginning of the collisional phase), and the \( r_{2i} \) are the positions when the diffusion coefficient is calculated. For confined particles, \( t_i = \tau_{\text{sim}} \), and for lost particles, \( t_i \) is the time when \( r = 1 \) was crossed. If \( \sigma^2 \) is the variance of the test particle distribution, then equation 3.37 has the form \( (\sigma^2_2 - \sigma^2_1)/(t_2 - t_1) \), which makes it the average rate of change of \( \sigma^2 \) in the time \( t_2 - t_1 \).

Painter derived equation 3.37, without the \( (r_{1i} - \tau_1)^2 \) quiet start term, by solving the diffusion equation with zero boundary conditions to simulate the loss of test particles. When the quiet start is introduced, equation 3.37 is still obtained, by a similar derivation. The resulting diffusion coefficient estimator provides useful results across two limiting regimes; when direct losses are negligible, the usual diffusion coefficient is obtained, but when direct losses dominate, \( D \) is a loss rate.

When energy scattering is incorporated in the code, a thermal diffusivity [55] can be calculated in an analogous way, by replacing \( w_i \) with \( w_i \mathcal{K}_i \) in equation 3.37. This thermal diffusivity is used to help determine the electron flux in chapter 4.

Direct Losses

We assert that the above diffusion coefficient estimator deals with lost test particles correctly. To illustrate, we look at the evolution of the variance in equation 3.37, in three representative cases. The top-left plot in figure 3.1 shows the variance, in the plateau regime, when it is expected that the transport is diffusive. The total variance and the variance of the confined particle distribution are both approximately linear in time, and the \( D \) calculation converges. Even though only about 5% of the particles were lost, they still make a contribution to \( D \) which is about the same as that made by the confined particles. At the opposite extreme of collisionality, the middle row of figure 3.1 shows a simulation performed at \( L_* = 1000 \), with no radial electric field, so the helically trapped particles are directly lost. In this case, the con-
3.4. Monte Carlo transport diagnostics

tribution of the confined particles to the variance (the numerator) can just be seen above the time axis. Most of the particles are lost in the simulation time, and the lost particle contribution dominates the variance completely. Nevertheless, $D$ converges even though the variance is not linear in time — in this limit, our $D$ is really a loss-rate estimator. In a less extreme condition, when a thermal-sized radial electric field (specified by $V_0 = -1$) is imposed in the long mean free path, the behaviour of the numerator changes greatly. The variance is still dominated by the fast, lost particles, but it is now linear in time (bottom row of figure 3.1). Again, $D$ converges, this time to something which is more like a diffusion coefficient.

Sensitivity to region width

In chapter 4 it will become necessary to calculate radial profiles of the electron diffusion coefficient, in order to arrive at radial profiles of the particle flux. To see if this is possible, we investigate the relationship between $D$ and the radial width of the region in which it is calculated.

In figure 3.2 we show monoenergetic diffusion coefficients which were calculated in the plateau regime of a tokamak for several known banana widths. The region width was varied artificially, and lost particles were treated as described above. We conclude from the result that the region width must be greater than ten times the average radial orbit width, for a local $D$ to be well defined. In the conditions of chapter 4, the electron orbit width meets this requirement comfortably, so in that chapter we calculate the radial flux profile from $D(r)$. In the same conditions, the ion orbit width does not meet the requirement; in chapter 4 we develop a separate technique to cater for the ion flux.

\[ \tau_{\text{conf}} \approx 7\tau_9 \]

\[ \tau_{\text{conf}} \approx 7\tau_9 \]

\[ \tau_{\text{conf}} \approx 7\tau_9 \]
Figure 3.1: Variance (left column) and resulting diffusion coefficient (right column) as a function of simulation time, for three conditions: $L_\ast = 1$, $V_0 = 0$ (top), $L_\ast = 1000$, $V_0 = 0$ (middle), and $L_\ast = 1000$, $V_0 = -1$ (bottom). The portion of the variance due to the lost particles (dashed lines), and the confined particles (thin solid lines) are shown, as well as the total variance (thick solid lines).
3.4. Monte Carlo transport diagnostics

Figure 3.2: Dependence of diffusion coefficient on width of diffusion region. Width is normalized using the banana width.
3.4.2 Lotz's confinement time, $\tau_L$

Lotz and Nuhrenberg [56, 40] introduced a method of calculating a confinement time, which is similar to a method originally used by Wobig [44]. The confinement time which is arrived at, $\tau_L$, is equivalent to the decay constant of the slowest mode of decay of the test particle distribution.

The test particles are propagated in the background fields as before, but lost particles are replaced by sampling from a source term which has the same shape as the test particle distribution function. This is accomplished by duplicating one of the confined test particles, and using the duplicate to replace the lost test particle in the simulation. To uniformly sample the confined test particle distribution, the index of the test particle to be duplicated is calculated from the cyclic relationship

$$n_{\text{dup}}^i = (n_{\text{dup}}^{i-1} + k_{\text{cyc}}) \mod N,$$

where the last particle duplicated had index $n_{\text{dup}}^{i-1}$, $N$ is the number of test particles in the simulation, and $k_{\text{cyc}}$ is relative prime to $N$. The procedure continues until a steady state is achieved, at which point the inverse of the MC replenishment rate is the confinement time, $\tau_L$.

The resulting confinement time depends on the shape of the asymptotic radial test particle distribution. For example, in a tokamak, where the particle flux is determined by $\Gamma = -D\partial n/\partial r$, the value of $\tau_L$ depends on the radial electric field, because radial electric fields (of thermal magnitude) effect the asymptotic radial test particle distribution [56]. By contrast, the diffusion coefficient is independent of the radial electric field in a tokamak.

Because Lotz's method does not rely on a diffusive model it is more appropriate in stellarator measurements where there are unclosed drift surfaces, and it is general enough to handle superbanana transport. However, in the unusual case where $\tau_{90} \sim \tau_{\text{conf}}$ (for example in some regimes of present interest in the H-1NF heliac), the asymptotic distribution that the method
3.4. Monte Carlo transport diagnostics

relies on becomes localised about the magnetic axis. The confinement time then measured can be expected to be an overestimate since it represents the average confinement time of particles emitted from a thin filament source at the magnetic axis. Another drawback of the method is that in short mean free path ($L_\ast < 1$) regimes, the method can be very computationally intensive. The method is suitable for computer parallelisation, and all of the $\tau_L$ results which we present in this thesis are obtained using the “dynamic queue” parallel computing algorithm described in appendix A.

3.4.3 Garabedian’s confinement time, $\tau_G$

Garabedian [98, 88, 99] has also introduced a method for calculating a confinement time. The method involves the calculation of the exponential decay constant, $\tau_G$, of a functional, $H(t) \sim \exp(-t/\tau_G)$, of the test particle distribution:

$$H(t) = \frac{1}{N} \sum_j (1 - s_{0k}) \cos \left( \frac{\pi}{2} \frac{s_{1j} - s_{0k}}{1 - s_{0k}s_{1j}} \right),$$

(3.38)

where $s = (\psi/\psi_{cgs})^{1/2}$, and $N$ is the total number of test particles. The $N$ test particles are initialized simultaneously on 8 flux surfaces (with $N/8$ particles per surface), which have radial positions $s_{0k}$, and the $s_{1j}(t)$ are the later positions of the test particles. The summed functions in equation 3.38 describe a series of smooth peaks, with maxima at the points $s_{0k}$; they are depicted in figure 3.3. Particles are removed from the simulation when they cross $s = 1$.

3.4.4 Exponential decay time, $\tau_e$

To put the confinement time calculations into some perspective, we also calculate the exponential decay constant of the particle distribution, directly. For this purpose, $N_0$ test particles are initialised with a parabolic radial
distribution in the plasma, and they are propagated, with no particle source terms, until there are \( N_0/e \) test particles left. During this time, we record the logarithm of the number of confined test particles, \( \log N(t) \). When \( \log N(t) \) is linear in time, the time-gradient is the exponential decay constant, \( \tau_e \).

### 3.5 Computing approaches

The computing time required for a Monte Carlo calculation is a function of the magnetic geometry which is being simulated, since to obtain an accurate result, the test particle distribution must adequately sample both the field geometry and the velocity phase space regions over the course of its trajectory. To ensure that the sampling is adequate, we use a large number of test particles \( (N_p \sim 10^3) \) for the \( D, \tau_G, \) and \( \tau_e \) methods described above, and follow the test particle orbits for a period, \( \tau_{\text{sim}} \), which is typically \( 3 \max(\tau_{90}, \tau_{\text{orb}}) \). Because \( N_p \) is large and the test particles do not interact,
the code is suitable for vectorisation on vector supercomputers, such as the Fujitsu VPP-300 (which has a vector length, $N_{\text{vec}}$, of 512, 1024, or 2048, depending on the implementation). The $\tau_L$ method, on the other hand, requires much longer simulation times $\tau_{\text{sim}} \gg 10$ to arrive at the asymptotic test particle distribution, so a smaller test particle population ($N_p \sim 100$) is sufficient to collect the Monte Carlo information. The method is therefore inefficient on machines like the VPP-300, since $N_p \ll N_{\text{vec}}$, but it can be made efficient on scalar-parallel supercomputers, such as the SGI PowerChallenge (SGI-PC), on which (because it is scalar) the computing time, per test particle, is mainly independent of the number of test particles.

To implement the code on the two different types of computer, we have developed two driving subroutines, one for single processor computers with a long vector, such as the VPP-300\textsuperscript{†}, and the other parallelised, for multiprocessor computers like the SGI-PC. The single PE routine was straightforward to implement, but the parallel code was more complicated, because we chose to write it in such a way that it is highly portable (that is, it can be run on most parallel computers with minimal alteration). For optimal portability, the parallel code was written using the Message Passing Interface, and an algorithm was designed to perform the message-passing transactions required by the particle source term in the Lotz method. We call this algorithm the "dynamic queue" algorithm, and we describe it in detail in appendix A. Another parallel algorithm is also described in the appendix — based on a "bank-queue" model, it was developed to parallelise the $D$, $\tau_G$, and $\tau_e$ methods. In this chapter, the $\tau_L$ results were computed using the parallel dynamic-queue routine, and the other results were computed using the (vectorized) single-PE driving routine.

\textsuperscript{†}The VPP-300 is actually a vector parallel computer, but each of its 13 processing elements is sufficiently powerful (with $\sim 4$GFlop peak speed) to be treated like a separate, single PE supercomputer.
3.6 Results

In this section, we present results produced using the above Monte Carlo code, for a tokamak test case and for the H-1NF. The tokamak case is used to benchmark the four transport diagnostics, and the message-passing code is benchmarked using an H-1NF field. Comparisons of the four transport diagnostics are made in the H-1NF field, where, unlike the tokamak case, there is not general agreement. The comparisons are made possible by the normalised diffusion coefficient, $D_* = D/D_p$, and the normalised loss rate, $S_* = S/S_p = 1/\tau S_p$, where $\tau$ is the decay time. Throughout this section, the H-1NF results were calculated for a 200eV Hydrogen plasma, in a 1T field, in the standard magnetic configuration.

3.6.1 Tokamak benchmark

To benchmark the code against an analytic model, we calculated the diffusion coefficient and the three decay times described above, for the same tokamak test case that was studied by Fowler, Rome, and Lyon [42]. We use their analytic model for the tokamak diffusion coefficient, which is derived from the general expressions of Hinton and Hazeltine [10]. The test case parameters were $B = 2T$, $R_0 = 2m$, $a_p = 0.2m$, $i = 0.5$, and $T_i = T_e = 1000eV$. The mean free path was varied via the density, and the radial electric field was zero for each calculation. In figure 3.4, Monte Carlo results are calculated using both monoenergetic ($E/T_i = 1.5$) test particle distributions ($\triangle$, $+$, $\times$, and $\bullet$) and maxwellian distributions ($\square$ and $\ast$). As has been found previously [40], the monoenergetic and maxwellian results closely coincide. We use Lotz's normalisation scheme (section 3.3) to compare the diffusion coefficients with the inverse of the confinement times. The Monte Carlo results all agree to within statistical error, and they have fair agreement with the analytic model, displaying deviations which are consistent with those found by other
Figure 3.4: Comparison of normalised tokamak loss rates, calculated from $D$ (\(\Delta\), monoenergetic, and \(\Box\), maxwellian) from $1/\tau_L$ (+, monoenergetic, and \(*\), maxwellian), from $1/\tau_C$ (\(\times\), monoenergetic) and from $1/\tau_e$ (\(\bullet\), monoenergetic). The solid curve is the analytic result, and the dashed line represents the loss rate at which $\tau_{90} = \tau_{\text{conf}}$. 
authors [40, 42]. The agreement between the MC results is due to the fact that tokamak banana orbits are closed, so the transport is diffusive, even at long mean free path, with the flux given by $\Gamma = -D\partial n/\partial r$. The Lotz result agrees with the $D$ result because the radial electric field was zero.

### 3.6.2 MCMuPPeT benchmark

The tokamak $\tau_L$ results in figure 3.4 were obtained using the dynamic-queue parallelism algorithm described in appendix A. The results indicate that the method works well, but to apply a more stringent test, we perform a second benchmark of the method, in conditions where the message passing burden is high due to a large number of lost particles. In figure 3.5, the dynamic-queue code (run on the SGI-PC) is compared with the single PE code (run on the VPP-300), for a 200eV Hydrogen plasma, in a 1T field in the H-1NF standard configuration. A zero electric field is used, so there are many direct losses along the drift surfaces, to the extent that $\tau_{\text{conf}} < \tau_{90}$ when $L_* \geq 150$. Agreement between the two codes is good, over 4–5 orders of magnitude in the collisionality.

### 3.6.3 Comparison between $\tau$ methods

We have seen, in the tokamak benchmark above, that the three decay time calculations obtain very similar results in a tokamak, with zero electric field. We are interested in comparing the results that the methods obtain in the H-1NF, for two reasons; for physical insight, and also, to arrive at the most computationally efficient method. To this end, we show in figure 3.6 the loss rates which are obtained using the three methods, with three electric fields, specified by $V_0 = -1$, $V_0 = 0$, and $V_0 = 1$. The $\tau_L$ results were produced using the MPMD driver routine, and the $\tau_G$ and $\tau_e$ results, using the single PE driver.
Figure 3.5: Benchmark of the MCMuPPeT code, in the H-1NF, at zero electric field. Here the MPI code (+) is compared to the single PE code (○).
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In figure 3.6 there is good agreement between the $\tau_G$ method ($\times$) and $\tau_L$ method (+), when the electric field is zero (blue curves) and/or when the mean free path is long (lmfp, where $L_\ast \gtrsim 30$). In the short and intermediate mean free path regimes (smfp and imfp, where $L_\ast \lesssim 30$), the agreement breaks down when thermal-sized electric fields are present (red and green curves). We interpret this as follows: in the intermediate mfp regime, the transport is mainly diffusive, so the loss rate is a function of the density gradient. In Lotz’s method, the asymptotic test particle density gradient is a function of the electric field [56], but in Garabedian’s method, the effective density gradient is independent of $E_r$, since it is determined by the envelope of the function $H(t)$, in equation 3.38. Therefore the results differ in the intermediate mfp regime. This interpretation is supported by the fact that the $\tau_G$ results are independent of $E_r$ at $L_\ast \approx 1$, where a diffusion coefficient is expected to be independent of $E_r$. In the lmfp regime ($L_\ast \gtrsim 30$), the loss rate is not determined by the density gradient, rather, by direct losses, so the $\tau_G$ and $\tau_L$ results are in agreement.

The figure also demonstrates that the $\tau_e$ method (•) has fair agreement with the $\tau_L$ method (+) throughout. This agreement is at its best when $\tau_{\text{conf}} \gg \tau_{90}$ (red and green curves) because the collisions have time to replenish the loss cone before it is significantly depleted. The (decaying) test particle distribution in the $\tau_e$ method is therefore in a state which is close to the asymptotic state arrived at using Lotz’s technique. An exception to this good agreement is the lowermost red $\tau_e$ point in the figure. This anomalous disagreement was caused by a limitation on the CPU time, which brings us to the disadvantage of the $\tau_e$ calculation method: the required computing times are long. The method is inefficient (poorly vectorised) because the logarithm of the number of confined particles does not become linear in time (so that $\tau_e$ cannot begin to be calculated) until a significant fraction of the test particles are lost. Furthermore, $\log N_p$ sometimes does not even become
linear, so $\tau_e$, which is the time-gradient of log $N_p$, is not always well defined.

### 3.6.4 Comparison between $\tau_G$ and $D$

We use the normalisation in section 3.3 to compare the $D$ and $1/\tau_G$ results for the same conditions as in the previous section. The results are in figure 3.7, where two extra curves (black) represent the results for a tokamak of similar dimensions as H-1NF, with $R_0 = g/B_0 = 1.231$ m and $a_p = (2\psi_{\text{lfs}}/B_0)^{1/2} = 0.124$ m. Here $B_0$ is the average field strength, equivalent to $B_{mn} = B_{000}$ in the Fourier representation for the magnetic field given by equations 2.5 and 2.6.

As before, there is good agreement between the two methods in the tokamak case, where transport is diffusive. In the H-1NF cases, the results display the same tendencies, but the magnitudes differ. Best agreement is found at $L* \approx 1$, where diffusive transport dominates. The different magnitudes do not necessarily imply that either of the methods are flawed — rather, it can be explained using the fact that the $S*$ normalisation method is based around the consideration of diffusion in a straight cylinder, rather than in a helical toroid.

### 3.6.5 $D$ at short mean free path

The diffusion coefficient is often considered to be insensitive to the electric field at short mean free path, with many authors assuming that the stellarator diffusion coefficient will become equal to the tokamak diffusion coefficient, when $L* \ll 1$. Examples which contradict this assumption have been found using the DKES code [94] and another Monte Carlo code [55]. To look for this effect in H-1NF, we have extended our $D$ results into the smfp regime, in figure 3.8. Only negative electric fields (this time $V_0 = 0, -1, \text{ and } -2$) were simulated, since positive ambipolar fields are only expected in the Imfp
Figure 3.6: Normalised loss rates in H-1NF, calculated using Lotz's technique (+), Garabedian's technique (x), and the direct loss rate (●), for three electric fields, specified by \( V_0 = -1 \) (red), \( V_0 = 0 \) (blue) and \( V_0 = 1 \) (green). The diagonal dashed line represents the loss rate at which \( \tau_{90} = \tau_{\text{conf}} \). Throughout, \( T_i = 200 \text{eV} \) and \( B_0 = 1 \text{T} \).
3.6. Results

Figure 3.7: Normalised loss rates in H-1NF, calculated using Garabedian's technique (×) and the diffusion coefficient (△), for three electric fields, specified by $V_0 = -1$ (red), $V_0 = 0$ (blue) and $V_0 = 1$ (green). The black results correspond to a tokamak of similar dimensions. The diagonal dashed line represents the loss rate at which $\tau_{90} = \tau_{\text{conf}}$. Throughout, $T_i = 200\text{eV}$ and $B_0 = 1\text{T}$. 
regime. The results show qualitative agreement with the results in references [94] and [55], and with the predictions of fluid theory [100].

The dependence of $D$ on $E_r$ in the smfp regime can be explained within the Monte Carlo framework, since, when $L_* \ll 1$, the usual notions of passing and trapped orbits lose their meaning, so the transport is determined by an effective time-average over many short-lived orbit states. In such a scenario, the transport can be expected to depend on the average value of $v_r/v$ ($v_r$ is the radial component of the drift velocity), which is diminished by large radial electric fields.

3.6.6 Computing considerations

For the $D$ and $\tau_G$ methods, we use 1024 test particles on the VPP-300, with the simulation time determined by $\tau_{\text{sim}} = 3 \max(\tau_{90}, \tau_{\text{orb}})$, so that condition 3.36 is met where possible. An adaptive timestep length is used for the integration, so it is not obvious how the CPU time will scale with collisionality — we plot it in figure 3.9, where we see that the CPU time scales unfavourably in the lmfp regime. In this graph, the CPU time is presented in arbitrary coordinates, so there is no meaningful comparison between the CPU times on the VPP (bold curve) and the CPU times on the SGI-PC (thin curves).

For the $\tau_L$ method, the simulation continues until an asymptotic state is obtained. It is not practical to monitor this manually, so simulations (with $N_p \approx 200$ test particles) are performed until $5N_p$ test particles have been lost from the system and replaced. We have found that this condition consistently produces an asymptotic state, and in figure 3.9 we use this rule to provide a basis for comparison of the CPU times required, for different plasma conditions (thin curves). We find that the CPU time is most favourable in the long mean free path regime (where the $D$ and $\tau_G$ methods have poor CPU scaling), and when the electric field is small or positive. The CPU times are
3.6. Results

Figure 3.8: Normalised diffusion coefficients in H-1NF, at short mean free path, for electric fields specified by $V_0 = 0$ (dark blue), $V_0 = -1$ (red) and $V_0 = -2$ (light blue). The black results correspond to a tokamak of similar dimensions. The diagonal dashed line represents the loss rate at which $\tau_90 = \tau_{\text{conf}}$. Throughout, $T_i = 200\text{eV}$ and $B_0 = 1\text{T}$. 
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Figure 3.9: Computing time versus mean free path, for the diffusion coefficient method (thick solid curve) and the Lotz method. Four cases are shown for the Lotz method: a tokamak (dotted line), H-1NF with no electric field (thin solid line), H-1NF with $V_0 = -1$ (dash-dotted line), and H-1NF with $V_0 = 1$ (dashed line).

reduced for the Lotz method by initializing the radial test particle distribution with a guess at the eventual asymptotic state: a (typically) parabolic radial distribution of test particles is generated, using a Von Neumann rejection technique [101] designed for sampling from non-rectangular random number distributions.

The single-PE version of the code achieves approximately 98% vectorisation on the VPP-300.
3.7 Discussion

We have compared the results of three methods for the calculation of the confinement time, and have found good agreement in the long-mean-free-path regime in H-1NF. In the intermediate mfp regime, we find fair agreement between $\tau_e$ and $\tau_L$, and poor agreement between $\tau_L$ and $\tau_G$. We attribute this to the role that the density gradient plays in determining the loss rate, when the transport is mainly diffusive. Of the three methods, we prefer the one due to Lotz, since it simultaneously generates an equilibrium loss rate and an asymptotic test particle distribution function [40, 56]. Also, Lotz's method has favourable CPU scaling in the lmfp regime.

One advantage of calculating the confinement time is that this is the quantity which is most readily measured in experiment [102], so direct comparison between simulations and experiment is possible. In contrast, comparison of a computed diffusion coefficient with experimental results usually requires some intermediate theoretical interpretation. The diffusion coefficient method has the advantage that it is computationally efficient in the intermediate and short mean-free-path regimes, and also it calculates a transport coefficient which is not influenced by the density profile, except by the collision frequency. As a result, $D$ is more appropriate for the fitting of analytic models to the MC results, as was done by Painter and Gardner[54]. Such analytic models are important for studies of transport, because they are capable of closely reproducing the Monte Carlo results, over a wide range of physical conditions, in a very small fraction of the MC computing time. In this chapter, we have verified a previous result of the DKES code in TJ-II [94], that the diffusion coefficient is sensitive to strong radial electric fields in the high collision frequency regime. One implication of this is that the model fitting performed by Painter and Gardner may need to be reevaluated in this regime. Before going into this though, it is important to analyse
Chapter 3. Monte Carlo transport coefficient calculations

the Monte Carlo $D$ result in more detail, since there is a possibility that the anomalous results which we observe may be due to a defect in the collision operator. In particular, the pitch-angle scattering model used here does not conserve momentum. Presumably, a defect in the collision operator would make the greatest difference in the high collision frequency regime, which is where our anomalous result has been observed. One way to investigate this possible cause for the result would be to implement Tessarotto's momentum-conserving collision operator [103] in the code, and see if it anulls the sensitivity of $D$ to the radial electric field, at high collision frequencies. This investigation is beyond the scope of the present work.

In this chapter, we have described and benchmarked a Monte Carlo transport code, and used it to compare some of the Monte Carlo transport diagnostic techniques which can be found in the literature. We have not performed a detailed transport study in H-1NF, rather, our objective has been to come to a better understanding of the Monte Carlo model. This chapter provides a background for the next chapter, where the Monte Carlo code is used to self-consistently calculate ambipolar radial electric fields in H-1.
Chapter 4

Neoclassical ambipolar radial electric fields in H-1NF

In this chapter, we describe a Monte Carlo method which has been developed to calculate the ambipolar radial electric fields in the H-1NF. Throughout the chapter, the Monte Carlo results are compared to those obtained with a fitted version of an analytic model due to Shaing.

The Monte Carlo method and the fitted analytic model are applied to the H-1NF plasma conditions bordering the experimentally observed transition to the Improved Confinement Mode (ICM). We do not simulate the bifurcation itself, but calculate the equilibrium ambipolar electric fields before and after the transition, using density and temperature profiles similar to those found in experiment. We conclude that these feature of the transition to ICM are consistent with neoclassical theory.

The last part of the chapter concerns a different bifurcation, the ion–electron root transition, which has been predicted in stellarators. Again the bifurcation itself is not simulated; instead, $E_r$ is calculated over a range of collisionalities. Both the ion and electron roots are found to occur within a small collisionality window, in this range.
Chapter 4. Neoclassical ambipolar radial electric fields in H-1NF

In section 4.1 we introduce the ambipolarity equation, and we review the literature in section 4.2. A well known analytic model is fitted to H-1NF in section 4.3, and the Monte Carlo code is described in section 4.4. To introduce the results section, the experimental ICM conditions are reviewed in section 4.5. Analytic ICM results are presented and discussed in section 4.6, Monte Carlo ICM results are presented and discussed in section 4.7, and the Monte Carlo and analytic results, for the ion–electron root transition, are presented and discussed in section 4.8. Conclusions are drawn in section 4.9.

Some additional experimental results regarding the Improved Confinement Mode became available after this chapter was written. Section 4.10 is an addendum, which briefly addresses the issue of the comparison between model ambipolar fields and experimentally measured electric field profiles.

4.1 Introduction

In nonaxisymmetric systems, both ion and electron fluxes can be a strong function of $E_r$. Because of this, the fluxes predicted by neoclassical theory are not intrinsically ambipolar, but they can be made ambipolar by finding an electric field for which their radial currents cancel. The confinement calculated with and without an ambipolar radial electric field can differ by an order of magnitude or more, and so accurate determination of the ambipolar field is required to find the relevant predictions of neoclassical transport theory for a given situation.

Solution of the ambipolarity equation has become an established method for determining the radial electric field. This equation comes from the flux surface average of the charge balance equation in the steady state [38]:

$$\sum_a Z_a \Gamma_a^{ma} = 0. \quad (4.1)$$

Here the $a$ indices label the various plasma species, $Z_a$ represents the electric charge on the species (so that $Z_e = -1$ for electrons,) and $\Gamma_a^{ma}$ is the
4.1. Introduction

nonambipolar radial flux of species \(a\). The total radial flux for each species, \(\Gamma_{a}^{\text{tot}}\), is usually represented as the sum of a nonambipolar part, due to nonaxisymmetry in the system, and an intrinsically ambipolar part, \(\Gamma_{a}^{\text{tok}}\), which is the neoclassical flux which would be expected in a tokamak with the same dimensions as the system.\(^1\)

Since in some situations the radial electric field has a much stronger effect on the geometry of drift surfaces than the magnetic field structure does, it is important to include the calculation of ambipolar radial electric fields in stellarator transport-optimisation studies. This is another motivation for us to develop a technique to calculate the neoclassical ambipolar radial electric field using a model which includes the detailed orbit geometry.

It has been shown by Garabedian [98] that it is also possible to find ambipolar fluxes with a Monte Carlo code [90, 91], by allowing the electric field to have a component within the flux surface. Garabedian demonstrated that, for an electrostatic potential determined by a single radial coefficient, and by just a few surface-varying components, ambipolar fluxes can be induced when small \((eV/kT \sim 5\%)\) surface-varying components are resonant with the magnetic field structure. In collision frequencies where ion fluxes usually dominate, the method works by degrading the electron confinement until it is the same as the ion confinement. The resulting increase in electron flux goes some of the way to bridge the gap between conventional neoclassical electron transport predictions, and anomalous electron transport observations. Notwithstanding this important result, in this chapter we work exclusively with potentials which are constant on a flux surface, because it seems that no Monte Carlo method for calculating the radial profile of the radial electric field has so far been developed elsewhere.

\(^1\)This amounts to treating each stellarator as a helical perturbation upon a tokamak. There is some evidence [82, 55] to suggest that it may be more productive to consider a stellarator as a toroidally perturbed straight helix.
4.2 Review

4.2.1 Zero dimensional ambipolarity

Solution of the bounce averaged drift kinetic equation to first order in the deviation of the particle from the flux surface yields a local relationship between the radial electric field and the radial particle flux for each species [38]. The relationship is local in the sense that the flux depends on the electric field at a point, but it does not depend on the gradient of the electric field. In this situation, the ambipolarity equation can be solved to find $E_r$, and simultaneously, the neoclassical nonambipolar flux can be obtained.

In 1983, Mynick and Hitchon [104] used analytic formulae [18, 105] for the ion and electron fluxes to calculate zero dimensional, ambipolar radial electric fields. They showed that when the ions are in the $\nu$ regime and the electrons are in the $1/\nu$ regime (and $T_i = T_e$) the curves of radial flux versus electric potential have quite different shapes for ions compared to electrons, and the ion and electron flux curves may intersect at up to three "ambipolar" roots. Two of the roots are positive, that is $E_r > 0$, and the other is negative, $E_r < 0$. Using a model based on an interpolation between the low collisionality results of Galeev and Sagdeev, Shaing [41] investigated the thermodynamic stability of these roots and found that the smaller positive root is unstable, while the negative root and the larger positive root are both stable. The negative or "ion" root is the most common, because it occurs in collisionality regimes where the ion flux would tend to dominate the electron flux in the absence of electric fields. The stable positive root (the "electron" root) only occurs at very low collisionalities, where the electron flux would tend to exceed the ion flux. Between these two regimes there is a bifurcation region, where both roots may occur. Appendix 2 of Painter and Lyon [106] contains a characterisation of the collisionality regimes in which the various ambipolarity roots may occur.
4.2. Review

In situations where both the ion and electron roots are possible, the electron root has superior confinement characteristics, because it occurs at a higher value of $|E_r|$. This has inspired efforts to control the transition from a negative to a positive root. It has been shown theoretically [20] and experimentally [107] that a transition to the electron root can be induced by heating the electrons using ECH.

4.2.2 1 Dimensional ambipolarity

The ambipolarity equation has also been solved [38, 108, 109, 78, 39], using analytic models for the fluxes, to calculate radial profiles of the radial electric field. This is somewhat problematic, because the collisionality changes across the plasma radius, so in some regions the $E_r$ solution may be multivalued. It is therefore possible to arrive at discontinuous, nonphysical, radial electric field profiles [110, 111].

To overcome this, Hastings [111] has solved the bounce averaged drift kinetic equation to higher order in the orbit deviation from the flux surface. This allows differential terms in the electric field to appear, which can be represented as a radial electric field diffusion coefficient, $D_E$. Using $D_E$ to preclude the possibility of discontinuous field profiles, Hastings et al [38] have solved the ambipolarity equation to arrive at radial electric fields in the Advanced Toroidal Facility (ATF), using Shaing's model for the fluxes. In this model, the helical ripple is a function of radius only: $\varepsilon_h(r_n) = \varepsilon_{ha}r_n^2$. Hastings et al also included an “Alcator scaling” anomalous transport model ($D_{an} \sim 1/n_e$). Momentum and power-balance equations were used to model the time evolution of the radial electric field, including bifurcation from the ion to the electron root. The existence of a radial electric field diffusion coefficient, $D_E$, provides a mechanism for root control in the whole plasma using just the plasma edge conditions, since, for instance, a positive radial electric field which is established at the edge will diffuse inwards to the axis [107].
Lyon et al. [108] have also included self consistent temperature, density and radial electric field profiles in a reactor study, using the power balance code COLTRANE [112], which incorporates the transport models due to reference [38]. The COLTRANE code includes the effects of heat sources, alpha-particle heating, radiation terms, and arbitrary particle fuelling sources. In this paper Lyon et al. studied the optimization of stellarator transport using the self-consistent electric fields, as well as the magnetic fields. No positive radial electric fields were found.

Sanuki et al. [109, 78, 39] calculated ambipolar electric fields for the Compact Helical Stellarator (CHS), using a more sophisticated magnetic field model. The helical ripple used was still a function of the radius only, and the flux model used was that due to Kovrizhnykh [6]. In addition, models were used to include the effects of charge exchange, fast ion orbit loss, Neutral Beam Injection, and the “alcator” anomalous transport scaling [78]. Both positive and negative roots were found. The solutions were found to be quite sensitive to the neutral particle density profile, and once the correct neutral density profile was used, good agreement with experiment was found.

Fokker-Planck codes, which permit an accurate representation of the magnetic field, have also been used to calculate the ambipolar field. D’Haeseleer et al. used the FLOCS code [113], which is an enhanced version of the bounce averaged Fokker-Planck code, FPSTEL, developed by Mynick and Hitchon [20]. They calculated an electric field, in a reactor-grade stellarator, on a single flux surface. Going further still, radial profiles of the electric field have been calculated in W7-AS by Baldzuhn [79], using the DKES code [52]. Good agreement with experiment was found.

The Fokker-Planck codes are superior to the analytic models mentioned above, because they calculate transport in arbitrary (toroidal) magnetic fields, but, they also use the assumption that the orbit deviation from flux surfaces is small. Apropos of this, it has been shown recently that finite drift-
4.3 An analytic model for the ambipolar field

Orbit width effects (not to be confused with finite Larmor radius effects) can significantly affect the magnitude and the scaling of neoclassical transport estimates [58]. For this reason, it is quite timely and appropriate, especially in view of the large drift orbit widths in H-1NF, to develop a Monte Carlo method for the calculation of ambipolar electric fields. Before we present our Monte Carlo method though, we describe an analytic model which we have used to help understand the results.

4.3 An analytic model for the ambipolar field

The analytic model used for this calculation is a slightly modified version of the neoclassical transport model which appears in references [41] and [38]. The expression for the nonambipolar flux/gradient relationship is:

\[
\Gamma^{na}_a = -D^{na}_a \frac{\partial n_a}{\partial r} - D^{na}_a n_a \frac{Z_a e \partial V}{T_a \partial r} - \left( \chi^{na}_a - \frac{3}{2} D^{na}_a \right) \frac{n_a \partial T_a}{T_a \partial r},
\]

where

\[
D^{na}_a = \int_b^\infty dxx \frac{3}{2} e^{-x} D^a_{na}(x)
\]

and

\[
\chi^{na}_a = \int_b^\infty dxx \frac{3}{2} e^{-x} x D^a_{na}(x)
\]

and

\[
D^a_{na}(x) = \sqrt{\varepsilon_h^2 \nu^2},
\]

where \(x = \kappa/T_a\), \(\nu(x)\) is the collision frequency, \(V_d\) is the radial drift velocity, \(\varepsilon_h\) is the local helical ripple, and \(\varepsilon_t\) is the local inverse aspect ratio (local toroidal ripple). The lower terminal of the integrals in equations 4.3 and 4.4 is different in references [41] and [38], and is listed as \(b = (\nu^h R_0/\nu^h m \varepsilon_h^{3/2})^{1/2}\) and \(b = 0\) in these papers respectively (here \(m\) is the number of toroidal field periods.) We use the former definition because it is more strictly correct [114]: \(x > b\) is the ripple trapping condition, and \(D^{na}_a\) and \(\chi^{na}_a\) are the
nonaxisymmetric contributions to the diffusion. The contribution due to the
toroidal geometry is described by an analytic tokamak model [42].

The effect of the electric field and the magnetic geometry on $D_{a}^{n}(x)$ are
described by the function $\omega^2$:

$$\omega^2 = C_{1/\nu}\tilde{\nu}^2 + \omega_d^2 + \omega_{sb}^2 + \omega_{sbp}^2,$$

where

$$\begin{align*}
\omega_d^2 &= C_{\nu}(\omega_E + \omega_{VB})^2 \\
\omega_{sb}^2 &= C_{sb}\omega_{VB}^2 \\
\omega_{sbp}^2 &= C_{sbp}\omega_{VB}\nu
\end{align*}$$

and

$$\begin{align*}
\tilde{\nu} &= \nu/\varepsilon_h \\
\omega_E &= \frac{1}{a^2_r B r} \frac{\partial V}{\partial r} \\
V_d &= -\frac{T}{a_p Ze B r} x \\
\omega_{VB} &= C_{VB} V_d,
\end{align*}$$

where $C_{VB}$ is a coefficient representing the $\nabla B$ drift, and $C_{1/\nu}, C_{\nu}, C_{sb},$ and $C_{sbp}$ are geometric coefficients corresponding to the $1/\nu$, the $\nu$, the superbanana, and the superbanana plateau regimes of neoclassical transport.

### 4.3.1 Fitting the model to H-1NF

The geometric parameters in this model have previously [54] been tailored
for the H-1NF heliac by fitting the analytic model results to monoenergetic
diffusion coefficient results which were calculated using a Monte Carlo trans­
port code [59]. The resulting geometric coefficients were $\varepsilon_h = 0.35, C_{1/\nu} = 5,$ $C_{\nu} = 0.8, C_{sb} = 70, C_{sbp} = 70$ and $C_{VB} = 0.20.$
4.3. An analytic model for the ambipolar field

The resulting analytic model closely reproduced the Monte Carlo diffusion coefficients over a range of electric fields, particle energies, and gyroradii, but the Monte Carlo results were only computed at half the plasma radius, and, for the ambipolarity solution, we require a model which applies across the full plasma radius. Therefore we have extrapolated the geometric coefficients of reference [54] using the radial profile of the actual helical ripple in the H-1NF standard configuration. To calculate the helical ripple, we use

$$\varepsilon_R(r, \theta) = \frac{\max B - \min B}{B_{\text{avg}}} \quad \text{and}$$

$$\varepsilon_h(r) = \max_{\theta} \varepsilon_R(r, \theta) - \min_{\theta} \varepsilon_R(r, \theta).$$

The local ripple, $\varepsilon_R$, and the helical ripple, $\varepsilon_h$ are represented in figures 4.1(a) and (b). As can be seen from 4.1(b), the $\varepsilon_h$ which is calculated in this way is very close to the value which was obtained from the Monte Carlo results by Painter and Gardner, at half the plasma radius.

Using the same functional dependence of the $C$'s on the toroidal and helical ripples as in references [41] and [38], and calibrating the geometric
coefficients in this model using the $r = a_p/2$ values obtained by reference [54], we arrive at the extrapolated geometric coefficients:

\[
\begin{align*}
C_{1/\nu} &= 0.74 \varepsilon_h/\varepsilon_t \\
C_{\nu} &= 0.8 \\
C_{sb} &= 180 \left(\varepsilon_t/\varepsilon_h\right)^{1/2} \\
C_{sbp} &= 3.5/\varepsilon_t \\
C_{\nabla B} &= 0.04 \partial\varepsilon_h/\partial r
\end{align*}
\]

(4.14) (4.15) (4.16) (4.17) (4.18)

Using these geometric coefficients and equation 4.2, we have found roots to the ambipolarity equation using the bisection method, in a variety of conditions in H-1NF.

### 4.3.2 Ion/electron root behaviour

To begin, we provide a brief comparison of the $E_r$ behaviour in H-1NF with that in a "model" stellarator. For the purpose of this comparison, and to check that our model produces the correct results, we have used it to reproduce Figure B.1 of Painter and Lyon [106]. The result, shown in figure 4.2(a) represents the ambipolarity roots for three torsatron-like reactor environments, plotted in a normalised coordinate system due to Painter and Lyon. The normalised electric field is $E_{\text{norm}} = -(1/T)(dV/dr_n)$, where $V$ is the electrostatic potential and $r_n$ is the normalised radius, and the normalised temperature is

\[
T_{\text{norm}} = T\left(\frac{40}{3C_eC_i} \frac{\varepsilon_t\varepsilon_h}{B^2a_p^4n^2}\right)^{1/3},
\]

where $T_e = T_i = T$, $C_e = \nu_e T^{3/2}/n$, $C_i = \nu_i T^{3/2}/n$, $\nu_e = \nu_{ee} + \nu_{ei}$ and $\nu_i = \nu_{ii}$.

In this graph there are four curves, three of which overlap. These three curves correspond to 3 ATF-like scenarios: (1) $R_0 = 2m$ $a_p = 0.25m$, $B_0 = 2T$, $\varepsilon_h = 0.2$, and $n_0 = 2 \times 10^{19}$ m$^{-3}$; (2) $R_0 = 10m$ $a_p = 2m$, $B_0 = 7T$, $\varepsilon_h = 0.2$, and $n_0 = 2 \times 10^{20}$ m$^{-3}$; and (3), which is the same as (2), but
Figure 4.2: (a) Reproduction of Figure B.1, from Appendix B of Painter and Lyon [106]. There are three coincident curves here corresponding to 3 ATF-like reactors, and one curve (the thin dotted curve) corresponding to the H-1NF geometry coefficients 4.14–4.18. They are all calculated using a normalised radius $r_n = 0.75$. (b) Comparison of ATF geometry and H-1NF geometry at $r_n = 0.25$. 
Chapter 4. Neoclassical ambipolar radial electric fields in H-1NF

with \( n_0 = 2 \times 10^{19} \) m\(^{-3}\). In each case, the radial profile of the helical ripple is parabolic (\( \varepsilon_h = \varepsilon_{ha} r_n^2 \)) as are the temperature and density profiles, and the calculation is performed at \( r_n = 0.75 \). The coincidence of the 3 curves indicates the utility of the normalisation. The results agree with those presented by Painter and Lyon, so our implementation is correct. The fourth curve, the thin dotted one, was calculated for H-1NF, at \( B_0 = 1 \)T and \( n_0 = 10^{-18} \) m\(^{-3}\), and \( r_n = 0.75 \), using the modified geometric parameters, 4.14–4.18 above.

In the H-1NF case, the magnitudes of the expected electric fields are smaller than the torsatron case by a few normalised units. This suggests that ambipolar confinement will always be better in a torsatron geometry because the electric field will dominate the magnetic geometry in the determination of transport. However, the bifurcation to the positive root may occur at a lower normalised temperature (shorter mean free path) in H-1NF than in the ATF geometry. Since positive electric fields are associated with improved confinement, the confinement in H-1NF may compete with that in an ATF geometry, in a small “window” about \( T_{\text{norm}} = -0.35 \).

Another significant feature is the shift of the position of the “point” on the curve in figure 4.2(a), closer to \( E_{\text{norm}} = 0 \) in H-1NF. This “point” is related to the resonance between the \( \mathbf{E} \times \mathbf{B} \) and \( \mathbf{V} \times \mathbf{B} \) drifts, and is closer to \( E_{\text{norm}} = 0 \) in H-1NF because, at \( r_n = 0.75 \), \( \partial \varepsilon_h / \partial r \) is small so that \( \omega_{VB} \) is small. In contrast, at \( r_n = 0.25 \), (figure 4.2(b)) where \( \partial \varepsilon_h / \partial r \) is large in H-1NF and small in the torsatron, the torsatron curve has the same shape as before, but the “point” in the H-1NF curve is pulled so far to the left that it disappears, and the \( (E_{\text{norm}}, T_{\text{norm}}) \) relationship becomes one-to-one. This means that in H-1NF, \( E_r \) can vary smoothly from the ion to the electron root as \( T_{\text{norm}} \) is increased, because of the high values of \( \omega_{VB} \). This feature may make it easier to produce positive electric fields in magnetic geometries with high magnetic drift velocities, because it may be possible to induce the
interior positive radial electric field to diffuse outward to the plasma edge.

If this scenario proves to be true, then the feasibility of high-\(\omega_B\) magnetic geometries (which are expected to have poor confinement properties) will improve because of easier access to the electron root. In contrast, in a torsatron geometry, which is expected to have good confinement because of the relatively low magnetic drift velocity, the electron root will be harder to achieve. (This is related to the L-H transition model proposed by Itoh and Itoh [115].)

### 4.3.3 Density and temperature gradients

We can shed further insight on the results to come by isolating the effects of the \(n\), \(T_i\), and \(T_e\) gradients on the ambipolarity solutions in the \((E_{\text{norm}}, T_{\text{norm}})\) space. In figure 4.3(a) we show the \((E_{\text{norm}}, T_{\text{norm}})\) curves which are generated with flat temperature profiles and with \((a_p/n)(\partial n/\partial r) = -2, -1, 0, 1, 2\). Note that \((a_p/n)(\partial n/\partial r) = -1\) is the gradient expected at \(r = a_p/2\) when the density profile is parabolic. Figure 4.3(b) shows the ambipolar fields generated when \(\partial n/\partial r = 0\) and \(\partial T_e/\partial r = 0\) and \((a_p/T_i)(\partial T_i/\partial r) = -2, -1, 0, 1, 2\). Figure 4.3(c) shows the ambipolar fields generated when \(\partial n/\partial r = 0\) and \(\partial T_i/\partial r = 0\) and \((a_p/T_i)(\partial T_e/\partial r) = -2, -1, 0, 1, 2\). In each of these plots, the same conditions in H-1NF were assumed as in figure 4.2(b).

A negative density gradient will make the radial electric field more negative if \(T_{\text{norm}} < 1\), but will have the opposite effect when \(T_{\text{norm}} > 1\). A negative ion temperature gradient will have the same effect, but this will be greatly diminished when \(T_{\text{norm}} > 1\). \(T_{\text{norm}} = 1\) is significant because it represents the collisionality at which the ions change from the \(1/\nu\) regime to the \(\nu^{1/2}\) regime — i.e. it is the superbanana plateau. A negative electron temperature gradient will tend to have the reverse effect on the field. The effect changes sign not at \(T_{\text{norm}} = 1\), but at \(T_{\text{norm}} \approx 4.7\), where \(\partial D/\partial \nu\) changes sign for the electrons.
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Figure 4.3: Effect of density and temperature gradients on the ambipolar field.

(a) \( (a_p/n)(\partial n/\partial r) = -2, -1, 0, 1, 2 \) and \( T_i = T_e = \text{const.} \).

(b) \( (a_p/T_i)(\partial T_i/\partial r) = -2, -1, 0, 1, 2 \) and \( n = \text{const.}, T_e = \text{const.} \).

(c) \( (a_p/T_e)(\partial T_e/\partial r) = -2, -1, 0, 1, 2 \) and \( n = \text{const.}, T_i = \text{const.} \).

The thicker lines are the solutions for the negative gradients, the solid lines are where the normalised gradient magnitudes equal 2, and the dashed lines are where the normalised gradient magnitudes equal 1. (The dotted lines are where all gradients are zero.)
4.4 Monte Carlo Solution of Ambipolarity

In this section we solve the ambipolarity equation, using a model for the radial fluxes based on the Monte Carlo transport code described in chapter 3.

4.4.1 Assumptions

The following assumptions are made:

1. Guiding centre orbits are used, so there are no finite Larmor radius effects.

2. Boozer coordinates are used, so nested flux surfaces are assumed.

3. The electric field is purely radial, and no electrostatic fluctuations are included.

4. The density and temperature profiles are not self-consistent. That is, the test particle distribution is not used to update the background $n$, $T$ fields. In practice we have found that when the electric field is close to the ambipolar solution, the confinement is such that the background $n$ and $T$ profiles are not significantly modified from their initial conditions within the period of the simulation (see figure 4.4(a) and (b).)

5. Particle sources are modelled by assuming the plasma is in a steady state. The electric field is considered to be an equilibrium one, and therefore particle source terms are included in the code to ensure that the particle loss rate is equal to the particle replenishment rate. The radial profiles of the source terms are based on neutral penetration profiles.

6. Both RF heating and inelastic collision processes are not explicitly modelled. In practice, the inclusion of charge-exchange (CX) processes
in the absence of a heating model has a drastic effect on the tempera-
ture profile of the test particle population. Figure 4.4(d) shows an
example where, at the plasma edge, all hot test particles may have
been replaced by CX several times in the period of each simulation.
Since in experiment, temperatures are maintained in steady state (for
up to $30ms \approx 300\tau_{90} \approx 3000\tau_{CX}$) we assume that the plasma heating
must compensate for the energy loss due to charge exchange. There-
fore we model both RF heating and inelastic collision processes by
assuming that their associated heat fluxes exactly cancel. This is a
reasonable model for the calculation of ambipolar radial electric fields,
because charge exchange does not have a large associated particle flux;
it mainly affects the momentum and heat fluxes.

In the code, the radial particle fluxes are measured at the radial grid points,
r_j, and the electric field is determined at these grid points using the iteration
procedure in section 4.4.2 below. The electric field between the grid points
is specified using a cubic spline. This makes it possible to specify boundary
conditions at the ends of the $(0, a_p)$ interval. We have used $E_r(0) = 0$ in all
of our simulations so that the electric potential profile is flat at the magnetic
axis. In some of the simulations we have also employed an edge boundary
condition, $E_r(a_p) = 0$ to simulate the effect of the stochastic region immedi-
ately beyond the last closed flux surface; in the rest of the simulations, the
dge electric field was unconstrained.

The other issues involved in the calculation are in the inclusion of particle
sources and in the method of calculation of the test particle fluxes themselves.
These issues are addressed in sections 4.4.4 and 4.4.3 below.
4.4. Monte Carlo Solution of Ambipolarity

Figure 4.4: Evolution of density and ion temperature within the duration of one simulation (i.e. within one iteration cycle,) for a converged ambipolar radial electric field in "L-mode." The cell number shown indicates the interval in the radial coordinate in which \( n \) and \( T_i \) are calculated. The cell number increases with radius. The cases shown are (a) and (b), density and temperature evolution in the absence of inelastic collisions, and (c) and (d), density and temperature evolution including the effect of charge exchange. In (d) the edge ion temperature levels out at 10eV because this is the temperature of the neutral population in this simulation.
4.4.2 Iteration procedure

In the Monte Carlo code, test particles are free to sample an arbitrary region in the radial coordinate, and so the relationship between the fluxes and the electric field is non-local in the sense described in the review of section 4.2 above. Because of this, it was necessary to develop a new iterative procedure for the solution, which exploits the known tendencies of the system to arrive at an ambipolar result. [Both the bisection and false-position methods proved to be inadequate even with the use of dynamic brackets on the solution region. In trials of these methods the true ambipolar solution was often found to be outside the converged bracketed region which should include the result.]

There are three phases to the method:

Firstly, an initial guess to the solution is calculated, by measuring the ion and electron test particle fluxes, at the grid points $r_j$, in the absence of an electric field. From these fluxes, an initial guess at the field is calculated from $E_r^0(r_j) = k(\Gamma_i(r_j) - \Gamma_e(r_j))$. Here $k$, a relaxation parameter, is chosen so that the first guess will be an electric field of “thermal” magnitude, which will be of negative sign when $\Gamma_i(r_m) - \Gamma_e(r_m) > 0$. The subscript $m$ indicates the grid point at which $|\Gamma_i(r_j) - \Gamma_e(r_j)|$ is the largest, and the superscript indicates the iteration cycle number.

Secondly, if the ambipolar root has not occurred between $E_r^0$ and $E_r^1$ at the grid point $m$, then the $E_r(r_j)$ are increased with each iteration by the addition of $k(\Gamma_i(r_j) - \Gamma_e(r_j))$, until the ambipolar root has been crossed at the grid point $m$.

Thirdly, when the root has been crossed at $m$, the field is iterated on using $E_r^{n+1}(r_j) = E_r^n(r_j) + k_2(\Gamma_i^n(r_j) - \Gamma_e^n(r_j))$, where $k_2$ is another relaxation parameter, which is about an order of magnitude larger than $k$. This third phase converges to the root most of the time, even when the modification of the field in the neighbouring regions changes the value of the field at which the local ambipolar root occurs.
4.4. Monte Carlo Solution of Ambipolarity

4.4.3 Calculation of the fluxes

Each cycle of the iterative procedure involves the propagation of the electrons and the ions along their drift orbits, with an arbitrarily fixed background $E_r$. After a time $t_{1a} > \max(\tau_{90a}, 2\pi/\Omega_{Ea})$ ($a = i, e$, and $\Omega_{Ea}$ is the electric field drift frequency of species $a$), the particles are stopped and $\Delta \Gamma(r_k)$ is measured.

The numerical techniques used to measure test particle fluxes differ for ions and electrons because of the very large difference in radial orbit widths between the two species in the Improved Confinement Mode. The $\sim 10\text{eV}$ electrons are collisional and have a very small gyroradius, and therefore are in the ideal conditions for the Monte Carlo calculation of the diffusion coefficient and the thermal diffusivity. The ions on the other hand can have much larger radial orbit widths, so that it is not possible to calculate a series of local diffusion coefficients across the plasma radius.

Therefore, for the electrons we calculate the radial flux profile by calculating the Monte Carlo diffusion coefficient $D(r_j)$ and thermal diffusivity $\chi(r_j)$ at each of the grid points. The flux is then determined at each grid point by analogy with equation 4.2:

$$\Gamma_e = -D_e \frac{\partial n}{\partial r} + D_e n_e \frac{e}{T_e} \frac{\partial V}{\partial r} - \left( \chi_e - \frac{3}{2} D_e \right) \frac{n_e}{T_e} \frac{\partial T_e}{\partial r}. \quad (4.19)$$

The radial ion fluxes are calculated directly from the radial ion test particle fluxes at the grid points $r_j$. The test particle statistics are favourable for this technique when calculating fluxes of ions in a lossy plasma such as an Argon plasma in H-1NF, but they are less favourable when the confinement is very good, such as in the case of electrons in H-1NF, or of ions in a reactor.

The $\Gamma_i(r_j)$ are computed from the radial integral of the time averaged rate of change of the test particle number density. The time average is performed over the whole simulation period $t_{1i}$, and the test particle number densities are calculated using "flat," finite width, particles, so a linear smoothing pro-
cess is implied. The particle widths are chosen to be equal to the radial grid spacings, which are all of equal width in the flux surface label, $\psi \sim r^2$. Usually only 8 radial grid points are used, but having the grid points equally distributed in $\psi$ provides good resolution at the plasma edge, where it is needed the most. Simulations performed using 16 radial grid points have produced similar results, as is shown in figure 4.5. It would be difficult to justify the use of a finer radial grid than this in the ICM conditions, because of the size of the ion gyroradii.

An additional technique is used to improve the numerical resolution at the plasma edge. It is motivated by the necessity of modelling arbitrary ra-
4.4. Monte Carlo Solution of Ambipolarity

dial density distributions, and their effect on the electric field. In particular, if the initial test particle distribution is chosen to reflect realistic plasma density distributions, then the Monte Carlo statistics at the plasma edge will be poor (MC accuracy $\sim \sqrt{N}$.) To get around this problem, we assign statistical weights, $w_p \sim n(\psi_p)$, to each of the test particles $p$, and initially distribute the test particles uniformly in $\psi$. Then the initial statistical distribution has the same shape as the initial density distribution of the plasma, but the test particle distribution is actually linear in $r$ (because $\psi \sim r^2$.) This greatly enhances the accuracy at the plasma edge, although it is at the expense of the statistics at the center. Because the grid points are distributed uniformly in $r^2$ (so that they are farther apart in $r$ at the center,) and because we are more interested in what occurs at the plasma edge, the statistics at the plasma interior are still good enough for our purposes. This flux measurement method has been benchmarked in a tokamak, where it reproduced the expected transport scalings.

4.4.4 Particle Source terms

A particle source term of arbitrary shape is included in the calculation, using the assumption that the plasma is in steady state, so that the rate of plasma lost is exactly balanced by the source rate. Each time a particle is lost from the simulation it is replaced, and the position of replacement is determined by a probability distribution which is the same as the neutral particle density profile.

Two source terms, $S_1$ and $S_4$, were compared with the results obtained with a zero source term, $S_0$. The source term $S_1$ was edge peaked, and for $S_4$, all lost particles were reinjected at $r_n = 0.5$:

\begin{align}
S_1(r_n) &= 0.1 + 0.9r_n^3 \\
S_4(r_n) &= \delta(r_n - 0.5)
\end{align}
Figure 4.6(a) shows the electric fields obtained using $S_0$, $S_1$ and $S_4$, for an L-mode discharge with the $P_2$ background profiles. The edge peaked source profile reduces the electric field magnitude everywhere in the plasma. The $S_4$ source profile makes the field more negative outward of the source, and more positive inward of the source. The effect of the source terms is thus analogous to that of the density — a negative gradient makes the local field more negative, and a positive gradient makes the local field more positive.

To demonstrate the effect of including charge exchange without a heating model to compensate for the resulting heat loss, we have included figures 4.6(b) and (c). In each case, the field associated with charge exchange is markedly lower than without, because of the drop in ion temperature toward the edge.

4.5 ICM simulation conditions

In the first part of this section, we review the experimental results [49, 50] which have been observed near the transition to an Improved Confinement Mode in H-1NF. Then in section 4.5.2 we give some density and temperature profiles which are intended to model the conditions before and after the ICM transition. The ambipolar electric field profiles corresponding to these model profiles, calculated with the analytic and Monte Carlo flux models, are then presented in sections 4.6 and 4.7.

4.5.1 Experimental ICM results

The bifurcation to Improved Confinement Mode in H-1NF shares many of the characteristics of the L-H mode transition in tokamaks. The transition is quite sudden, lasting approximately 5ms in a discharge which may last several hundred milliseconds in the equilibrium states which precede and supersede the transition period. During the transition, the magnitude of the
4.5. *ICM simulation conditions*

Figure 4.6: (a) Effect of sources $S_0$ (zero source — solid line), $S_1$ (edge peaked source — dotted line), and $S_4$ (central source — dashed line) on the electric field profile. Also the effect of charge exchange (dotted lines) on the electric field profiles obtained using (b) $S_0$ and (c) $S_4$. 
Figure 4.7: Experimental result taken from Shats et al. [49]. The larger magnitude, bold curve represents the experimentally measured radial electric field 5ms after the transition to ICM, and the other curve represents $E_r$ 5ms before. The dotted vertical line represents the position of the plasma radius. Here $B = 0.0615T$.

electric field increases by 50–100%, but it remains negative at the plasma edge. An experimental result, taken from reference [49], shows the typical effect on the radial electric field. The bold curve in figure 4.7 is the ICM electric field, and the thin curve represents the electric field 5ms before the transition.

The ICM transition is triggered by the crossing of a critical $B$ value or a critical $\varepsilon$ value. When the critical value is crossed, there is an increase in the plasma density by 50–100%, and an increase in the ion temperature by 50–100%. The electron temperature, which is edge peaked before and after
the transition, similarly undergoes an increase, at the plasma edge, but a decrease at the interior, leading to an increase in $T_e(a_p) - T_e(0)$ of 50–100%. The plasma-potential well deepens by the same margin.

The transition to ICM has also been associated with the suppression of fluctuations in the density and electrostatic potential [49], which implies that the confinement improvement may be due to this mechanism. As a first approximation, we neglect fluctuations in the results that follow, and simulate quiescent, equilibrium plasmas, both before and after the ICM transition. Even with this simplification, we find good qualitative agreement with experimental results.

4.5.2 Model ICM background fields

At present it is not possible to make precise comparisons between experiment and the results of the models, because the ambipolar fields are quite sensitive to the density and temperature profiles, which are not measured to better than 10% in the experiments. Indeed, in the latest experimental results, depicted in figure 4.15, the ion temperature is only measured to within ±10eV. Therefore we choose to model the background density and temperature profiles in such a way that we get an overview of the possible effects of the density and temperature gradients.

To survey a range of possible conditions which may occur close to the Improved Confinement Mode threshold in H-1NF, electric fields were calculated using eight different radial profiles of background density and temperature. Results were taken using these profiles before the experimental results in figure 4.15 became available, but they remain relevant because the transition has been observed over a wide range of conditions.

The profiles, which we shall call $P_1$ to $P_8$, were described by:

$$T_{i1}(r) = T_{i0}(1 - 0.95r_n^2)$$ (4.22)
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\[ T_{i2}(r) = T_{i0} \quad (4.23) \]
\[ T_{i3}(r) = T_{i0} \quad (4.24) \]
\[ T_{i4}(r) = T_{i0} \quad (4.25) \]
\[ T_{i5}(r) = T_{i0}(1 + 0.5\exp(-2(r^2_0 - 1)^2)) \quad (4.26) \]
\[ T_{i6}(r) = T_{i0}(1 - 0.5\exp(-2(r^2_0 - 1)^2)) \quad (4.27) \]
\[ T_{i7}(r) = T_{i0} \quad (4.28) \]
\[ T_{i8}(r) = T_{i0} \quad (4.29) \]

and

\[ T_{e1}(r) = T_{e0}(1 - 0.95r^2_n) \quad (4.30) \]
\[ T_{e2}(r) = T_{e0} \quad (4.31) \]
\[ T_{e3}(r) = T_{e0}(1 + 1.5\exp(-25(r^2_n - 0.81)^2)) \quad (4.32) \]
\[ T_{e4}(r) = T_{e0}(1 + 1.5\exp(-25(r^2_n - 1)^2)) \quad (4.33) \]
\[ T_{e5}(r) = T_{e0}(1 + 1.5\exp(-25(r^2_n - 1)^2)) \quad (4.34) \]
\[ T_{e6}(r) = T_{e0}(1 + 1.5\exp(-25(r^2_n - 1)^2)) \quad (4.35) \]
\[ T_{e7}(r) = T_{e0}(1 + 1.5\exp(-25(r^2_n - 1)^2)) \quad (4.36) \]
\[ T_{e8}(r) = T_{e0}(1 + 1.5\exp(-25(r^2_n - 1)^2)) \quad (4.37) \]

and

\[ n_1(r) = n_0(1 - 0.95r^2_n) \quad (4.38) \]
\[ n_2(r) = n_0(1 - 0.95r^2_n) \quad (4.39) \]
\[ n_3(r) = n_0(1 - 0.95r^2_n) \quad (4.40) \]
\[ n_4(r) = n_0(1 - 0.95r^2_n) \quad (4.41) \]
\[ n_5(r) = n_0(1 - 0.95r^2_n) \quad (4.42) \]
\[ n_6(r) = n_0(1 - 0.95r^2_n) \quad (4.43) \]
\[ n_7(r) = 5n_0((1 - r^4_n)(0.2 + r^4_n) + 0.01) \quad (4.44) \]
\[ n_8(r) = 0.5n_0(1.1 + \cos(0.98\pi r_n)), \quad (4.45) \]
where $r_n$ is the normalised plasma radius $r/a_p$, and $n_0, T_{i0},$ and $T_{e0}$ are the central density, ion temperature, and electron temperature, respectively.

In Improved Confinement Mode, $n_0 = 0.02 \times 10^{20}$ m$^{-3}$, $T_{i0} = 60$eV and $T_{e0} = 10$eV, while in the conditions which have been observed before the bifurcation to ICM, $n_0 = 0.01 \times 10^{20}$ m$^{-3}$, $T_{i0} = 40$eV and $T_{e0} = 10$eV. The background profiles are summarised in table 4.1.

### Table 4.1: Summary of density and temperature profiles used in electric field calculations

<table>
<thead>
<tr>
<th>profile</th>
<th>ion temperature</th>
<th>electron temperature</th>
<th>density</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_1$</td>
<td>parabolic</td>
<td>parabolic</td>
<td>parabolic</td>
</tr>
<tr>
<td>$P_2$</td>
<td>flat</td>
<td>flat</td>
<td>parabolic</td>
</tr>
<tr>
<td>$P_3$</td>
<td>flat</td>
<td>peaked near edge</td>
<td>parabolic</td>
</tr>
<tr>
<td>$P_4$</td>
<td>flat</td>
<td>peaked at edge</td>
<td>parabolic</td>
</tr>
<tr>
<td>$P_5$</td>
<td>peaked at edge</td>
<td>peaked at edge</td>
<td>parabolic</td>
</tr>
<tr>
<td>$P_6$</td>
<td>minimum at edge</td>
<td>peaked at edge</td>
<td>parabolic</td>
</tr>
<tr>
<td>$P_7$</td>
<td>flat</td>
<td>peaked at edge</td>
<td>hollow</td>
</tr>
<tr>
<td>$P_8$</td>
<td>flat</td>
<td>peaked at edge</td>
<td>low edge gradient</td>
</tr>
</tbody>
</table>

4.6 Analytic ICM calculations

4.6.1 Results

Now let us look at the ambipolar radial electric field profiles for the cases $P_1$ to $P_8$, in figures 4.8–4.10. Each of the plots was calculated using an average plasma radius of $a_p = 0.124$m, but the electric fields have been renormalised so that they represent the fields that would be expected if they were measured, as they are in the actual H-1NF, along an axis where the
local minor radius is 0.0824m.

Comments on each of the resulting graphs are made below; the results of section 4.3.3 (and figure 4.3) are used to help interpret the electric fields.

**P_1** This case, where the density and both of the temperatures are parabolic, is intended as a reference case. The resulting electric field is approximately linear, so the potential will be approximately parabolic, in conformance with the model potential profiles used in chapters 2 and 3.

**P_2** Here the effect on $E_r$ of the density gradient is in direct competition with that of the collisionality (which is determined by the density since the temperatures are flat). Therefore the field magnitude increases with the radius as the density gradient increases, but, as the edge is approached, the normalised temperature increases and the solution shifts closer to $E_r = 0$. The marked decrease in $\partial\varepsilon_h/\partial r$ close to the edge also reduces the magnitude of the field required for ambipolarity.

**P_3** As in $P_2$, but at the edge the behaviour is dominated by the high $T_e$ gradient — the positive gradient increases the $E_r$ magnitude over the $P_2$ case and the negative gradient decreases the $E_r$ magnitude.

**P_4** As in $P_3$, but here there is no region where $\partial T_e/\partial r < 0$.

**P_5** As in $P_4$, but here the positive ion temperature gradient tends to reduce $|E_r|$.

**P_6** The effect of the negative temperature gradient, which would tend to increase $|E_r|$ is compensated for by the decrease in $T_i$ — and $|E_r|$ scales with $T_i$ so the field magnitude is smaller than in the $P_4$ case, close to the edge.

**P_7** A positive electric field is found in the interior because of the positive density gradient. The positive electron temperature gradient and strong
4.6. Analytic ICM calculations

Figure 4.8: (left column) Density and temperature profiles corresponding to $P_1$, $P_2$, and $P_3$, and (right column) resulting electric fields, in ICM (thicker line, larger magnitudes) and before ICM.
Figure 4.9: (left column) Density and temperature profiles corresponding to $P_4$, $P_5$, and $P_6$, and (right column) resulting electric fields, in ICM (thicker line, larger magnitudes) and before ICM.
4.6. Analytic ICM calculations

Figure 4.10: (left column) Density and temperature profiles corresponding to $P_7$ and $P_8$, and (right column) resulting electric fields, in ICM (thicker line, larger magnitudes) and before ICM.
negative density gradient reverse the sign at the edge.

\[ P_8 \] Within \( r_n < 0.8 \), the situation is very similar to the \( P_2 \) result, but outside this region the positive electron temperature gradient strongly influences the field.

### 4.6.2 Discussion

The experimental measurements extend beyond the last closed flux surface, which is beyond the scope of the present model. The inflection of the field about \((r, E_r) = (a_p, 0)\) is probably due to the stochastic region just outside the last closed flux surface, where the potential profile is expected to flatten out because of the ability of the electrons to rapidly respond to radial electric fields by moving along the field lines. In the analytic model, there is no such mechanism, and there is also no facility to impose a boundary condition on \( E_r \) because the model is entirely local (this is not the case with the Monte Carlo solutions in the next section). However, for many of the profiles studied, a similarly low value of \(|E_r|\) is observed at the edge because of the increase of \( T_{\text{norm}} \) toward the edge.

The main features of the experimental result within the last closed flux surface are the zero field at the edge, the strong peak to \(-5 \text{kVm}^{-1}\) just within the edge, and the drop in magnitude by a factor of 5 or more within \( r < a_p/2 \).

Some of the analytic calculations compare favourably with these results. Profiles \( P_4-P_8 \) reproduce the zero edge field, profiles \( P_4, P_5 \) and \( P_6 \) most closely reproduce the shape of the near-edge peak and also have a large drop in magnitude within \( r < a_p/2 \). Only \( P_3 \) and \( P_8 \) approach the same magnitude of field at the peak as in the experimental result. Only \( P_7 \) produces positive fields at the plasma interior. Also, in each case the "L mode" result is \( 1/2 \) to \( 3/5 \)ths of the size of the ICM result, as in the experiment. From what is
4.6. Analytic ICM calculations

known of the ICM conditions, the normalised temperature, $T_{\text{norm}} \approx 0.3$, so the discussion of section 4.3.2, and in particular the results in figure 4.3(a) and (b), indicate that the ambipolar electric field will be quite sensitive to the ion temperature and density gradients.

Because of the uncertainties in the experimental conditions, the analytic model cannot be dismissed: in conditions close to those observed in experiment, it produces ambipolar radial electric fields which are close to those which have been measured. Under these conditions the ion gyroradius is approximately $5\text{cm}$, so the plasma violates the condition, $\rho_i << a_p$, which is normally used to justify the use of the drift approximation in neoclassical transport. However, the method is still useful because it has allowed us to vary the density and temperature profiles of the plasma species, and observe the resulting effects upon the radial electric field that are expected from neoclassical theory. Furthermore, the ambipolar fields in the ICM situation are strong, so the radially local nature of the model formulation is valid because the drift surfaces are mostly closed and almost concentric. If finite orbit widths were taken into account in the model, one would expect the edge peaks in the electric field to become broader, and to become less sensitive to the narrow region of large $T_e$ gradient which occurs in profiles $P_3$ to $P_8$. This might make the resulting electric field profiles resemble the experimental results more closely.

Finally it should be emphasised that as well as finite Larmor radius (FLR) and finite drift radius effects, there are certain features which are entirely missing from this model. These include direct losses along unclosed drift surfaces, the influence of particle sources and inelastic collision processes such as charge-exchange, and the effect of the detailed 3-dimensional nature of the magnetic field. We address some of these issues in the next section.
4.7 Monte Carlo ICM simulations

In the Improved Confinement Mode conditions the electrons are in the collisional regime, so we applied a simplification to the calculation of the electron fluxes in the following calculations. We found that it was sufficient to only calculate $D_e$ and $\chi_e$ in the first cycle of the iteration procedure, because, in the collisional regime, the diffusion and thermal diffusivity coefficients are mainly independent of the electric field. The electron fluxes were calculated in subsequent iteration cycles by using these values of $D_e$ and $\chi_e$ and equation 4.19. The results were compared with a full simulation, and no appreciable difference was found, except that the computer time was reduced by a factor of approximately 50%.

4.7.1 Results

In figures 4.11–4.13 we present neoclassical ambipolar radial electric field profiles which have been computed using the Monte Carlo method of section 4.4. For comparison with the analytic results of section 4.6 we use $P_1 - P_8$ again as the background density and temperature profiles.

There are two columns of plots in figures 4.11–4.13: the left column of plots represents the model "L-mode" (before transition) ambipolar fields (where $T_{i0} = 40\text{eV}$ and $n_{i0} = 0.01 \times 10^{20} \text{m}^{-3}$,) and the right column represents the "H-mode" ambipolar fields (where $T_{i0} = 60\text{eV}$ and $n_{i0} = 0.02 \times 10^{20} \text{m}^{-3}$.) In each plot there are three curves. The dashed curves are the analytic fields of figures 4.8–4.10, repeated here to aid comparison with the MC results. The two solid curves in each plot are the MC results, calculated with a free boundary condition at the edge (thick solid curves, triangles) and with an $E_r(a_p) = 0$ boundary condition (thin curves, diamonds.) These solid curves are the cubic spline interpolants to the radial electric fields which are specified at the grid points (marked by triangles and diamonds) in the MC
4.7. Monte Carlo ICM simulations

code. The fields were calculated at the grid points using the iterative method of section 4.4.2 above, and the splines shown here were used to represent the electric fields in the MC code.

Effect of the boundary condition

Except for cases $P_1$ and $P_2$ (in figure 4.8) there is good agreement between the Monte Carlo results taken with and without a boundary condition. This is because, for cases $P_3$–$P_8$, the combination of edge gradients conspires to make the free-boundary edge electric field close to zero anyway. In the $P_1$ and $P_2$ cases, the MC results with the fixed boundary have a stronger field than the free-BC MC results, at $r = 0.075\text{m}$, to compensate for the low field magnitude at the edge.

Analytic/Monte Carlo comparison

When the MC results are compared with the analytic results the same general tendencies are observed throughout. We summarise the results below.

$P_1$ The analytic and MC results are in good agreement, except the MC results consistently display an inflection at $r \approx 0.06\text{m}$.

$P_2$ This result has the worst agreement between the analytic and MC codes because, in this case, the fluxes in the analytic model are determined entirely by diffusion in the presence of a density gradient, while the MC code includes convective effects due to the finite orbit widths.

$P_3$ In this case the number of grid points was doubled, to 16, because the negative field peak occurred between two grid points when there were only 8. There is good agreement between the analytic and Monte Carlo results, except for in the last centimetre.
Figure 4.11: Electric fields calculated with the Monte Carlo code, for profiles $P_1$, $P_2$, and $P_3$ in L-mode (left column) and H-mode (right column.) The thick solid curves have no edge boundary condition and the thin solid curves have an $E_r(a_p) = 0$ boundary condition. Triangles and diamonds represent the grid points. The dashed lines are the analytic results from figure 4.8.
4.7. Monte Carlo ICM simulations

Figure 4.12: Electric fields calculated with the Monte Carlo code, for profiles $P_4$, $P_5$, and $P_6$ in L-mode (left column) and H-mode (right column.)
Chapter 4. Neoclassical ambipolar radial electric fields in H-1NF

Figure 4.13: Electric fields calculated with the Monte Carlo code, for profiles $P_7$ and $P_8$ in L-mode (left column) and H-mode (right column.)
4.7. Monte Carlo ICM simulations

$P_4$–$P_6$ Ion temperature gradient:
These three cases display good agreement between the tendencies of the MC and analytic results, in both L and H modes, though the magnitudes differ by up to 25%. In $P_4$, the edge peak has the same width for both MC and analytic results, while for $P_5$ and $P_6$, the MC results have broader edge peaks than the analytic results. This is due to a non-zero ion temperature gradient in these plots, which has a less local effect in the MC code.

$P_7$–$P_8$ Density gradient:
In $P_7$, the MC results barely display a positive $E_r$ at all, in contrast to the analytic results, and they also have a smaller peak at the edge. The MC results are obviously less sensitive to the density gradient. The profiles in $P_8$ support this interpretation.

4.7.2 Discussion
Firstly, it is interesting to note that the dependence of the electric field on the edge density gradient, illustrated by cases $P_4$, $P_7$, and $P_8$, is reversed in the MC and analytic codes. A straightforward comparison of the analytic results for $P_4$, $P_7$, and $P_8$ shows that an increase in the magnitude of the edge density gradient leads to an increase in the magnitude of the electric field. Since an increased $|E_r|$ is associated with improved confinement, this could lead to a positive feedback effect between the density and potential gradients, which may even be strong enough to trigger the bifurcation to Improved Confinement Mode. The Monte Carlo results, in these conditions, display the converse relationship between the density gradient and the radial electric field at the edge. In the present Monte Carlo model, there can be no such positive feedback.

In general, the finite orbit widths in the MC code tended to “spread out”
the features of the radial electric field profiles. Another effect of the finite orbit widths (i.e. the "non-locality") is illustrated by a comparison between the analytic $P_2$ results and the free boundary condition MC results. In the analytic case (figure 4.8, middle row) the field magnitude decreases in the outermost eighth of the plasma because of the change in local collisionality. However in the MC case, test particles sample a finite region in the radius even in the presence of strong radial electric fields (partially due to chaotic scattering of trapped particles,) so there is no well-defined local collisionality. The local collisionality therefore does not out-compete the effect of the density gradient in the determination of the electric field, and so the field magnitude continues to increase toward the plasma edge. The finite orbit width may also obscure the effect of the small edge gradient of $\varepsilon_h$.

As well as the finite drift-orbit widths, it is worth considering the possible effect of a finite Larmor radius on the results, since in the ICM conditions, the ion Larmor radius is approximately 5cm. Recently, comparisons of guiding centre orbits with the full gyrating orbits, in ICM conditions, have demonstrated [116] that the drift orbits have an acceptable level of agreement with the exact orbits. Since the mean free path is not large ($L_{mfp} \approx 5L_c$) in ICM conditions, these small differences between the exact orbits and the drift orbits will not have time to take effect between collisions. There should still be a difference in the results though, because a strong positive radial electric field exists immediately outside the last closed flux surface, so FLR orbits may be lost if their gyration carries them beyond this surface. As a result, the ion loss rate in the outer 5cm of the plasma can be expected to be higher, when FLR effects are included, than the ion loss rate predicted using gyroaveraged orbits. This would tend to make the electric field more negative at the plasma edge, in the FLR case.

We make three other general observations. Firstly, the analytic results were more sensitive to the electron temperature gradient than the Monte
4.8. Ion–electron root simulations

Carlo results were. Because the region of finite electron temperature gradient was quite narrow in r, this difference can again be attributed to the finite orbit widths in the MC code. Secondly, the MC results were more sensitive to the ion temperature gradient than the analytic results were. This is because the \( \nabla T_i \) flux contribution is convective in nature, and it seems that the MC code finds this convective motion to be more significant, due to the realistic modelling of the drift surface geometry, and the finite orbit width. Furthermore, the region of finite \( T_i \) gradient was broad in comparison to the region of finite \( T_e \) gradient, and so it was not "ignored" by the test particles. Thirdly, in many of the results, the edge peaks in the Monte Carlo electric fields were broader than those in the analytic fields. This is again due to finite orbit width effects and realistic drift surface modelling.

4.8 Ion–electron root simulations

After the first stage of the National Facility upgrade, it may be possible to observe a transition to the electron root in H-1NF. We are interested in modelling the region of the transition with the MC code because, as in experiment, multiple roots and discontinuous electric field profiles cannot occur in the MC model, so it will not display the same bifurcation behaviour as is found in the results of local analytic models.

4.8.1 Results

We have calculated ambipolar radial electric fields, with the MC and analytic models, for the 200eV Hydrogen plasma which was studied (in a 1 tesla background field) in chapter 3. In figure 4.14, the results are plotted in a similar manner to those of figure 4.2, but this time the electric fields are not normalised, and also the central density rather than the normalised temperature is used as the (horizontal) collisionality coordinate. The figure shows
the ambipolar electric fields calculated using the MC model (connected diamonds) and the analytic model (smooth curves,) at 5 radii: \( r_n = 0.2, 0.4, 0.6, 0.8, \) and 1.0.

### 4.8.2 Discussion

In the ion root (where \( E_r < 0 \)) there is fair agreement between the two models over the range of collisionalities, except at the plasma edge. In the electron root the field magnitudes do not agree so well, and are substantially larger at \( n = 0.003, \) except at the plasma edge.

The collision frequency at which the bifurcation to the electron root occurs, at \( n_0 \approx 0.01, \) seems to be determined by the lowest collision frequency at which the ion root will exist in the plasma core (i.e. where \( r_n \leq 0.6. \)) The bifurcation to the electron root within \( r_n \leq 0.6 \) "drags up" the electric field at the plasma edge ((d) and (e)) even though an ion root still exists there, in the analytic results, for densities much less than 0.01. This supports the remarks in section 4.3.2, where we speculated that the lack of a resonant "point" between the \( \mathbf{E} \times \mathbf{B} \) and \( \nabla \times \mathbf{B} \) drifts near the magnetic axis (cf figures 4.2(b) and 4.14(a)), due to H-1NF's relatively strong helical ripple there, may make the electron root relatively easy to achieve in H-1NF.

There are two caveats that should be mentioned in relation to figure 4.14. The first is that the MC root finder of section 4.4.2 will have some bias in favour of the ion root, when both roots exist, because at zero \( E_r \) (i.e. in the first iteration step) the ion flux will slightly dominate, so the routine will begin stepping in the direction of an ion root. This could possibly be countered by initializing with a positive \( E_r. \) The second caveat is that the results in (e) may be due to a difficulty in calculating local values of \( D_e \) and \( \chi_e \) near the plasma edge.
Figure 4.14: Comparison of ambipolar radial electric fields calculated using the Monte Carlo and fitted analytic models, for a 200eV Hydrogen plasma in a 1 tesla background field in H-1NF. Results are shown at 5 radial positions, (a) $r_n = 0.2$, (b) $r_n = 0.4$, (c) $r_n = 0.6$, (d) $r_n = 0.8$, and (3) $r_n = 1.0$. 
4.9 Conclusions

A Monte Carlo code has been developed to solve the ambipolarity equation, for the radial electric field, by an iterative method. Over a wide range of conditions in H-1, the method obtains similar results to the ambipolar fields calculated using a geometrically-fitted version of Shaing's flux model.

The MC model has the advantages over the analytic model that it includes realistic magnetic field geometry, and finite drift-orbit-width effects. It appears to be more sensitive to the ion temperature gradient, and less sensitive to the electron temperature gradient than the analytic model. The MC model includes pitch-angle and energy scattering processes, but, like the analytic model, it neglects inelastic collision processes. Particle and energy sources are modelled using steady-state assumptions. Finite Larmor radius effects appear in neither of the two models.

The results of the two methods compare favourably with the Improved Confinement Mode fields which have been experimentally observed in H-1. It is not possible to make precise comparisons at present, because the model results are quite sensitive to variations, within the range of the experimental error bars, in the density and temperature. However, the same general trends are evident; in agreement with experiment, the models predict a 50–100% increase in the radial electric field after the transition to ICM, and they predict the same basic features in the electric field — negative electric fields, peaked at the edge, with a typical drop in magnitude by a factor of 5, within \( r < a_p/2 \). The agreement is surprisingly good, considering that we have neglected both finite Larmor radius effects, and the effect of fluctuations in the density and the potential.

The analytic and Monte Carlo models have also been used to find the predicted ion–electron root transition in H-1NF, in operating conditions which should be achievable after the National Facility upgrade. Positive electric
4.10. Addendum: Comparison with recent ICM experimental results

fields were observed, with multiple ambipolar roots in the analytic case, but only a single ambipolar root in the MC case. The critical density of the transition in the MC results appears to be determined by the disappearance of the ion root at the plasma interior, due to the significant helical ripple there. The transition at the interior appears to "drag" the field in the rest of the plasma into the electron root, where ion roots still exist in the local (analytic) model.

4.10 Addendum: Comparison with recent ICM experimental results

After this chapter was written, experimental results became available [50], which describe the ICM density and temperature profiles, before and after the crossing of a critical $B$, in more detail. In this addendum, we use these results to illustrate the effects of experimental uncertainty in the density and temperature profiles, on the ambipolar field estimates made using the analytic model and, by extension, by a full Monte Carlo simulation.

The experimental results, depicting the effect of the ICM transition on the density, the plasma potential, and the ion and electron temperatures, are shown in figure 4.15. The diamonds represent the profiles before the transition to ICM, and the triangles represent the profiles afterward. The error bars are not shown here, but the density, electron temperature, and plasma potential measurements are accurate to within ~10%, while the ion temperature measurements are accurate to within $\pm 10\text{eV} \ (i.e. \ to \ within \ 10\text{–}35\%)$.

As mentioned in section 4.6.2 above, the outputs of our models, the ambipolar radial electric fields, are sensitive to the input $n$ and $T_i$ profiles, because of the size of the normalised temperature ($T_{\text{norm}} \approx 0.3$). To illustrate this, we have fit two alternative curves to each of the density and ion
Figure 4.15: Experimental result taken from Shats et. al. [50]. The diamonds represent the experimental profiles before the transition to ICM \((B_0 = 0.061\, \text{T})\), and the triangles represent the experimental profiles after the transition \((B_0 = 0.072\, \text{T})\). The solid curves are analytic fits to the data, used to calculate radial electric fields in figure 4.16.
4.10. Addendum: Comparison with recent ICM experimental results

temperature profiles, in the L and H modes, in figure 4.15. Each of the fits is chosen such that it could represent the true profile, within the experimental uncertainty. The orange and red curves in figure 4.15(a) are fits to the density in L-mode, and the green and blue curves are fits to $n$ in H-mode. The dotted and solid curves are fits to $T_\text{i}$ in L-mode, and the dashed and dot-dashed curves are fits to the ion temperature in H-mode. There is only one fit to each of the electron temperatures, because $T_{\text{norm}}$ is small, so figure 4.3 in section 4.3.3 implies that variations in the electron temperature gradient will have minimal effect.

Using these alternative models of the background profiles, we have used the analytic flux model to calculate the ambipolar radial electric fields, and the resulting potential profiles. They are plotted in the left column of figure 4.16, where the colour of each curve indicates the density model that was used, and the linestyle (dotted, dashed, etc.) indicates the ion temperature model that was used. There is quite a large variation, especially in the H-mode results. For clarity, the ranges in L and H-mode results are plotted in the right column of the figure, with the H-mode range shaded in red, and the L-mode range shaded in green.

These results demonstrate that precise comparisons of theoretical, equilibrium ambipolar fields with experiment are not possible in the ICM regime, without quite accurate experimental density and temperature profiles. In these conditions, it is more valuable to compare the resulting potential profiles, which are less sensitive because they are the integrals of the electric field (compare the width of the red-shaded regions in the two plots in the right-hand column of figure 4.16). A comparison of the L-mode and H-mode electric potentials in figures 4.16 and 4.15 indicates that the analytic model can agree with the experimental results if the appropriate models for the density and temperature are chosen.
Figure 4.16: Analytic flux model results. Top row: the radial electric fields, and bottom row: the resulting potential profiles. In the left column, colours correspond to the four density fits in figure 4.15. Linestyles (solid, dashed, dash-dotted, dotted) correspond to the four ion temperature fits in figure 4.15. In the right column are the ranges in $E_r$ and $V$ spanned by the H-mode (red) and L-mode (green) fits to $n$ and $T_i$. 
Chapter 5

Conclusion

In this thesis, we have studied trapped particle drift-orbits in H-1NF, in the presence of electric fields, and have developed a neoclassical Monte Carlo transport code, MCMuPPeT, which has been optimised for use on both parallel and vector computer architectures. Monte Carlo transport calculations were examined in some detail, and the Monte Carlo code was further extended to calculate ambipolar radial electric fields in H-1NF.

In the magnetic ripple of H-1NF, we have described a hierarchy of trapped orbit types, ranging from the deeply trapped to the barely trapped. At the latter end of the spectrum are the toroidally trapped orbits, which can be "almost-closed" bananas, and at the former end are the helically trapped orbits, which are not almost-closed. In H-1NF, closed drift surfaces for trapped particles are not an intrinsic feature of the magnetic geometry, so that, for example, high levels of direct losses can be expected in the first few milliseconds of an H-1NF discharge, when the radial electric field is effectively zero. When electric fields of thermal magnitude are present, the topology of the trapped-particle drift surfaces is greatly improved for thermal particles. High energy particles are less effected by radial electric fields, with the result that H-1NF is expected to suffer from electron pump-out along unclosed drift surfaces, when ECH heating is used. Our orbit studies show that it may be
possible to ameliorate this problem, by positioning the ECH resonance layer so that the high energy, high $v_\perp$ electrons have their confinement improved by collisionless detrapping, from the helically trapped to the toroidally trapped state.

We have found that the total trapped particle fraction varies from 40 to 45% in H-1NF, in the three configurations studied, with approximately 5% deeply trapped, 15% helically trapped, and 20% of the particles toroidally trapped. If we define the trapped particle state using the number of maxima in the parallel kinetic energy between bounce points, $N_{\kappa}$, then we find that the radial electric field has a significant effect on the way the trapped particles are distributed between the trapping states. The work here could be extended using the $N_{\kappa}$ method, to numerically calculate, by a Monte Carlo technique, the probabilities of collisionless transition between the trapped particle states. This calculation would provide insight into the effective orbit width in the collisionless detrapping regime.

The Monte Carlo collisional transport code that we developed has been successfully benchmarked in both tokamak and H-1NF magnetic fields, and has been used to compare some of the Monte Carlo transport diagnostics from the literature. Of the confinement time methods we studied, we prefer the one due to Lotz, which simultaneously generates an equilibrium loss rate and an asymptotic test particle distribution function. A Multiple-Processor, Multiple-Data parallel algorithm was developed to efficiently implement this calculation on distributed computing architectures. A diffusion coefficient estimator due to Painter has also been described in some detail, and was used to verify in H-1NF a result which was obtained by Solano et al. using the DKES code: at collision frequencies much higher than the tokamak plateau collision frequency, the diffusion coefficient is a function of the radial electric field. An implication of this result is that the fitting of Shaing's flux model to H-1NF, performed by Painter and Gardner, might need to be improved in
the short mean-free-path regime.

We used the fitted version of Shaing's flux model to help understand the results of a Monte Carlo code for the self-consistent calculation of ambipolar radial electric fields. There was fair agreement between the ambipolar radial electric fields produced by the analytic model and the Monte Carlo code, over a broad range of conditions. With a reevaluation of the geometric parameters of the analytic model, it may be possible to obtain even closer agreement. In conditions surrounding the transition to the Improved Confinement Mode in H-1NF, both of the models produced ambipolar electric fields which are in qualitative agreement with the experimental results — in particular, the radial electric field predicted by the two neoclassical models displays similar profiles, and similar differences in magnitude between the low and high modes of confinement. The agreement with experiment is surprisingly good, considering that both finite Larmor radius effects, and density and electrostatic potential fluctuations, are neglected in our neoclassical predictions.

The Monte Carlo and analytic models were also used to investigate the transition from the ion to the electron root (from negative to positive ambipolar radial electric field) in H-1NF, in conditions which should be achievable after the National Facility upgrade. Both models predict positive ambipolar radial electric fields in the long mean free path regime, but close to the bifurcation point their results differed. In the Monte Carlo results, the transition to the electron root close to the magnetic axis appears to "drag" the field in the rest of the plasma along with it; a result which is consistent with the existence of an electric-field-diffusion coefficient. The results of both models suggest that the electron root may be easier to achieve in H-1NF than in a torsatron, where the helical ripple would be approximately parabolic in the minor radius.
Appendix A

The MCMuPPeT Code

In this chapter we describe the MCMuPPeT (Monte Carlo, Multi Processing Plasma Transport) code which has been written within the Multiple Processors, Multiple Data (MPMD) model of computer parallelism, using Fortran 90 and the Message Passing Interface (MPI) international standard [117, 118]. The code has been designed to be highly portable, and it requires relatively inexpensive computing resources. It was used to produce many of the results in chapter 3.

McMuPPeT can be ported to any distributed system for which an MPI implementation and a FORTRAN 90 compiler exist. It has been successfully run on a shared memory, superscalar SGI PowerChallenge XL, a shared memory, vector parallel Fujitsu VPP 300, a distributed memory, vector parallel Connection machine CM-5, and on a heterogenous network of DEC Alpha workstations. The code is suitable for each of these platforms, though for the current application it is difficult to find a large enough problem to justify the use of multiple processing on the VPP300.

Near-perfect parallelism is obtained on both scalar and vector parallel computers under normal operating conditions, and approximately 97% vectorisation was achieved in normal operating conditions on the VPP300.
Appendix A. The MCMuPPeT Code

A.1 Introduction

In Monte Carlo (MC) codes, collisions are modelled as interactions with a background plasma, using a Lorentz collision operator, so that individual test particles do not interact. As a result, MC codes are intrinsically parallelisable because the test particles can be distributed across a number of Processing Elements (PE's) and then integrated along their orbits independently of each other, without frequent interprocessor communication. Functionals of the test particle distribution which are required to calculate transport coefficients can be calculated from stored information after the simulation is over.

One way to parallelise a MC code is to use a Single Instruction Multiple Data (SIMD) model of parallelism. In this way, the test particles are distributed across the PE's, and all PE's perform the same instructions, and integrate their subset of the test particles in synchrony. However, different test particles require different-sized timesteps to obtain the same relative accuracy, so a SIMD implementation which allowed each test particle to find its own optimal timestep would tend to develop "race conditions" (where some processors finish their allocated work before others do,) while on the other hand, an implementation which gave all particles the same time step would tend to waste time on integrating some orbits with unnecessarily high accuracy. Painter [59] overcame this by implementing a stochastic integrator in a SIMD code, and giving each test particle the same timestep. The integrator was a weak, 2nd order, stochastic predictor-corrector method due to Platen [95], which guaranteed that the test particle distribution was integrated with a required degree of accuracy, irrespective of the accuracy of individual orbits. The distribution of test particles was allowed to find its own optimal timestep.

In this chapter, we describe parallel MC algorithms which effectively distribute the computational burden across the processors, regardless of the
particular choice of integrator. The methods enable us to relax the requirement of uniform timestep. This is especially desirable for the simulation of a Maxwellian distribution of test particles, where, for example, one might otherwise be simulating a high-energy passing particle and a low-energy deeply-trapped particle, with the same timestep. The relaxation of the uniform timestep also allows us to carry out detailed and accurate orbital analyses such as those presented in chapter 2.

We also "relax" the form of parallelism to fit the Multiple Processes, Multiple Data (MPMD) paradigm, which is applicable over a wider range of computers (including relatively affordable platforms such as workstation clusters.) Dynamic load balancing is an implicit feature of the algorithms, so the code is suitable even for heterogeneous networks.

A priority of the project was to make the code as portable as possible, so that it can be run on almost any parallel computer. This has been achieved by using the Message Passing Interface (MPI) international standard to perform all interprocessor communications. MPI is becoming ubiquitous in parallel computing; a list of machines that one free MPI implementation will support is given in table A.1. In contrast, it is not possible to write a portable SIMD code because SIMD implementations are generally machine-specific or vendor-specific.

Two Message Passing (MP) algorithms were developed for the data transactions which are required to get the Monte Carlo code to work. Each algorithm is based on a "master-slave" model, where the master processor\textsuperscript{\dag}, PE 0, distributes jobs, coordinates the activities of the other processors, and processes all of the output data. The slave processors integrate test particle orbits, and record the information which is required to calculate the transport coefficients. Since the "master" role is not very demanding, PE 0 also

\textsuperscript{\dag}Here and in what follows we mean virtual processor or virtual PE, since several processes (e.g. a master and several slaves) will often reside on a single physical PE when the machine is heavily loaded.
Appendix A. The MCMuPPeT Code

Convex Exemplar
Cray multiprocessor, Cray t3d
Intel Paragon, Intel i860, Intel Delta
IBM SP2
Meiko CS-2
DEC Alpha
IBM RS6000
SGI multiprocessors (e.g. PowerChallenge, Origin 2000)
Sun SunOS, Sun Solaris
PC networks using FreeBSD or LINUX or Microsoft Windows
Nexus device
HP HPUX
Fujitsu VPP, M780, AP1000
NEC SX-4

Table A.1: Architectures supported by the MPICH implementation of MPI [119]. There are several other free implementations of MPI available, and many computer vendors have their own implementations.

integrates test particle orbits. A schematic diagram of this setup is given in figure A.1.

The ratio of MP time to CPU time used in these algorithms depends mainly on how lossy the plasma is, since (other than in the distribution and collection phases) message passing only occurs when a test particle is lost from the plasma. In lossy conditions, or on a network with very slow interprocessor communication, the communication times can become a significant factor. In both of the algorithms below, we use two devices to get around this:

1. *non-blocking* sends (ISEND's) are used so that the sending PE need not wait for the matching RECV operation

2. Each PE propagates a vector of test particles so that, if MP is required regarding a subset of the test particles on a PE, then the PE can
A.2. The MPMD Algorithms

Figure A.1: The master-slave methods have three phases; the distribution of data by the master, the integration of orbits by the slaves, and the collection of output data by the master. All three phases operate concurrently.

continue to propagate the rest of the particles while waiting for the MP to complete

These two devices ensure that the wall time is determined by the required CPU time. The use of non-blocking sends also prevents deadlocks.

A.2 The MPMD Algorithms

The choice of these parallel algorithms which we apply to a problem is determined by the transport coefficient which will be measured, since this dictates both the particle source terms, and the functionals of the test particle distribution that will be calculated. For these reasons we have found it necessary to develop two separate master-slave algorithms, for two separate classes of problem.

The first method is designed to handle Monte Carlo calculations where the particle source terms are independent of the test particle distribution. As pointed out by Meglicki [120], this situation is suitable for implementation
of a bank-queue algorithm, which is described in section A.2.1 below. In this algorithm, no more than 2 PE's are ever required to participate in a message passing transaction. The method is very general, and is suitable for the parallelisation of standard ray-tracing calculations, such as those required for the calculation of drift wave growth rates.

The second MPMD algorithm is more complicated than the first, because it has been designed to cater for simulations which have a particle source term, $S$, that is a function of the test particle distribution, i.e. $S(r, t) = S(f(r, t), r, t)$. One such calculation is the asymptotic decay rate method, introduced in scalar form by Lotz and coworkers [44, 40]. For these types of simulations, message passing transactions involving up to 3 PE's are required, so we have developed a new algorithm to parallelise this calculation within the master-slave model. PE 0 is involved in every transaction, but the other participants may be completely arbitrary. Because the "queue" of new test particles is distributed across all of the PE's in this case (since the "queue" is the confined test particle population) we call this method the Dynamic Queue algorithm. We use Lotz's asymptotic decay rate calculation to illustrate the Dynamic Queue algorithm in section A.2.2 below.

A.2.1 Method 1: The Bank-queue algorithm

The name "bank-queue" refers to an analogy between processor load distribution and queues for teller service in a bank. In a large bank with many tellers, there is usually only one queue for customers which serves all tellers, so the occasion never arises where a teller sits idle while there are still jobs queued.

When this philosophy is applied to a parallel network of processing elements (PE's) one of the processors has to be responsible for administering the queue of jobs, and for sending new jobs to PE's when they finish with a "customer." Since this usually requires very little work, this processor (the
A.2. The MPMD Algorithms

“master”) also gives jobs to itself.

The algorithm begins with PE 0 reading input files, calculating data for the specification of the background fields, and establishing a queue of test particles. PE 0 then broadcasts the information required to calculate the background fields to each slave. A subset (numbering $N_s$ test particles) of the $N_q$ test particles in the queue is then given to each of the $M$ slave PE's. Usually we use $N_s \times M \ll N_q$, since this provides optimal load balancing.

Each slave then integrates the $N_s$ test particles along their orbits, recording the positions of each particle at $N_{\text{traj}}$ times. Each trajectory of recorded positions, $T_{j,1:N_{\text{traj}}}$, is used in the calculation of transport coefficients when the simulation is complete. The CPU time required to integrate the orbits dominates the wall time.

When a test particle is lost from the simulation, or when its simulation time is complete, a bank-queue transaction occurs where the test particle’s host PE (PE $a$) sends its trajectory of recorded positions, $T_{j,1:N_{\text{traj}}}$, to PE 0. PE 0 stores the trajectory, and then sends back to PE $a$ the next test particle, $p_{n_{\text{queue}}}$, in the queue. This transaction is summarised in figure A.2. Since the first send operation is a non-blocking one (a call to the MPI_SEND routine,) PE $a$ does not wait for a response — it continues computing the orbits of its remaining test particles, until the response from PE 0 is registered. Likewise, PE 0 does not wait for PE $a$ to receive the new test particle; it immediately recommences propagating its own set of orbits. If a particle is lost from PE 0, then a new particle is provided by PE 0 in the same way.

This process continues until the queue is exhausted, and all of the orbits have finished. The slave processes then return, and the transport coefficients are calculated by PE 0 from the stored trajectories $T_{j,1:N_{\text{traj}}}$, using the techniques described in chapter 3.

The slave algorithm, SLAVE1, is shown in table A.2. The algorithm, WHIP1, used by the master process to communicate with the slave, is given
in table A.3. There are several extra message passing transactions in the code which are not shown here; they ensure that the slave PE's enter and exit the integration routines correctly.

A.2.2 Method 2: The Dynamic Queue algorithm

As discussed in chapter 3, an asymptotic loss rate can be calculated from the slowest rate of decay of a test particle distribution. For the calculation of Lotz et al [84], each time a particle is lost from the simulation region (by crossing the last closed flux surface) it is replaced by duplicating one of the other test particles. The index of the particle which is duplicated is chosen using a cyclic procedure which ensures that the indices are uniformly sampled. The result is equivalent to the presence of a source term which has the same shape as the test particle distribution function. An "asymptotic" state is reached when the MC replenishment rate becomes constant in time, at which point the asymptotic decay rate is equal to the MC replenishment
A.2. The MPMD Algorithms

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subroutine SLAVE1:

initialize background fields
initialize test particles \( p_j \) with coordinate vector \( y_j \), length \( N/M \)
initialize coordinate vector \( \text{lost}_j \), length \( N/M \)
set \( m_{\text{local}} \) to actual PE number
set the number of stored trajectory points, \( i_j \), for \( p_j \) to 0
determine simulation time \( \tau_{\text{sim}} \)
do
1. advance each test particle \( p_j \) by its timestep \( dt_j \)
2. record trajectories:
do
j = 1, \( N_{\text{vec}} \)
   if \( t_j > \tau_{\text{sim}} \times i_j/N_{\text{traj}} \) then
      \( i_j = i_j + 1 \)
      record trajectory, \( T_{j,i_j} = y_j(t_j) \)
   endif
endo
3. where \( t_j > \tau_{\text{sim}} \) or \( p_j \) is lost, \( fin_j = \text{true} \)
3. if any(\( fin_j \)) then
   ISEND_1 trajectory \( T_{j,1:N_{\text{traj}}} \) to WHIP1 on PE 0
endif
4. do
   IPROBE – probe for pending messages
   if message for WHIP1 then call WHIP1 routine
      (this only occurs on PE 0)
   if other message then
      \( \text{RECV}_2 \) new \( p_j \) from bank queue
      \( y_j = y_{\text{new}} \)
or \( \text{RECV}_3 \) termination order
      exit outer do loop
   if no message then exit inner do loop
endo
return

Table A.2: The algorithm followed by each slave PE when the bank-queue algorithm is used (see section A.2.1.) Numbered subscripts on the SEND/RECV operations indicate the number of the matching RECV/SEND operations in the WHIP1 routine (table A.3.)
subroutine WHIP1:

1. **RECV**$_1$ trajectory $T_{j,1:N_{queue}}$ from PE $a$
   store $T_{j,1:N_{queue}}$
   if $n_{queue} < N_{queue}$ and PE $a$ not stopped then
   $n_{queue} = n_{queue} + 1$
   get replacement particle $p_{n_{queue}}$ for PE $a$ from queue
   ISEND$_2$ new particle $p_{n_{queue}}$ to PE $a$
   endif

2. if any(slaves not stopped) and $n_{queue} >= N_{queue}$ then
   ISEND$_3$ a termination order to PE 0
   SEND$_3$ termination orders to all other PE’s
   endif

return

Table A.3: The algorithm followed by PE 0 when a call to WHIP1 is made, when the bank-queue algorithm is used (see section A.2.1.) Numbered subscripts on the SEND/RECV operations indicate the number of the matching RECV/SEND operations in the SLAVE1 routine (table A.2.)
As before, the algorithm begins with the master processor (PE 0) reading data files and generating the initial test particle distribution. The master process then distributes all of the $N_q$ test particles uniformly across the $M$ processors, by making each processor solely responsible for the propagation of $N_q/M$ test particles along their orbits. Each slave then integrates the $N_q/M$ test particles along their orbits. When a test particle on, for example, PE $a$ is lost from the simulation (or when its simulation time is complete) one of the transactions in figure A.3 is performed: first, PE $a$ sends the time at which the test particle was lost to PE 0, which then calculates the index $n_i$ of the test particle which will be duplicated to replace it, from the cyclic relationship $n_i = (n_i + k_{cyc}) \mod N_q$. If this new test particle, $p_{n_i}$, already resides on PE $a$, then the transaction in the top half of figure A.3 occurs: PE 0 sends the index $n_i$ of the test particle to PE $a$, and then PE $a$ duplicates the test particle itself. If $p_{n_i}$ resides on a different PE, then the transaction in the bottom half of figure A.3 occurs: PE 0 sends an instruction to PE $b$ (where $p_{n_i}$ resides,) telling it to send the full details of test particle $p_{n_i}$ to PE $a$. All the PE's involved in the transaction then continue integrating orbits. As in the bank-queue algorithm, PE's do not wait for a message that they send to be received — they fill the time by integrating orbits.

This process continues until $n_{\text{limit}} \geq N_q$ test particles have been lost and replaced in this fashion. The slave processes then return, and the loss rate is calculated as in section A.2.2, from the loss times $t(\text{lost})$ which were stored by the master process.

The slave algorithm, SLAVE2, is presented in table A.4. The algorithm, WHIP2, used by the master process to communicate with the slaves, is given in table A.5. As in the bank-queue algorithm, there are several other message passing transactions which are not shown here.
Figure A.3: Source term transactions for Dynamic queue algorithm, used when a test particle is lost from PE $a$. Top: the transaction which occurs if the new test particle $p_{ni}$ is on PE $a$ (in this case either $a = 0$ or $a \neq 0$.) Bottom: the transaction for the case where $p_{ni}$ is on PE $b$ (here $a = 0 \neq b$ or $a \neq 0 = b$ or $a \neq 0 \neq b$.)
A.2. The MPMD Algorithms

subroutine SLAVE2:
  initialize background fields
  initialize test particle coordinate vector \( y \), length \( N_q/M \)
  initialize coordinate vector \( \text{lost} \), length \( N_q/M \)
  set \( m_{\text{local}} \) to actual PE number
  do
    1. advance particles by \( dt \)
    2. where a particle is lost, \( \text{lost} \) = true
    3. if any(\( y(\text{lost}) \)) then
      ISEND\(_i\) \( t(\text{lost}) \) to WHIP2 on PE 0
    endif
    4. do
      IPROBE – probe for pending messages
      if message for WHIP2 then call WHIP2 routine
        (this only occurs if \( m_{\text{local}} = 0 \))
      if other message then
        RECV\(_2\) index \( n_r \) of replacement particle
        \( y(\text{lost}) = y(n_r) \)
        or RECV\(_3\) new particle coordinates, \( y_{\text{new}} \)
        insert \( y_{\text{new}} \) into test particle vector
        or RECV\(_4\) order to send coordinates of test particle \( n \) to PE \( m \)
        ISEND\(_3\) coordinates of \( n \) to PE \( m \)
        or RECV\(_5\) termination order
        exit outer do loop
      if no message then exit inner do loop
      enddo
    enddo
  ISEND\(_6\) final coordinate vector to WHIP2
return

Table A.4: The algorithm followed by each slave PE when the dynamic queue algorithm is used (see section A.2.2.) Numbered subscripts on the SEND/RECV operations indicate the number of the matching RECV/SEND operations in the WHIP routine (table A.5.) The exception is ISEND\(_3\)/RECV\(_3\), which is a message between SLAVE2 routines on processors \( a \) and \( b \).
subroutine WHIP2:

1. either: \text{RECV}_1 \ t(\text{lost}) \text{ from PE } a
   \[ n_{\text{lost}} = n_{\text{lost}} + 1 \]
   \text{if } n_{\text{lost}} \leq n_{\text{limit}} \text{ and PE } a \text{ not stopped then}
   \text{store } y(\text{lost})
   \text{get index of replacement particle for PE } a,
   \[ n_i = (n_{i-1} + k_{cyc}) \text{ mod } N_q \]
   \text{if } n_i \text{ is on PE } a \text{ then}
   \text{ISEND}_2 n_i \text{ to PE } a
   \text{elseif } n_i \text{ is on PE } b \text{ then}
   \text{ISEND}_4 \text{ order to PE } b: \text{ "send } y(n_i) \text{ from PE } b \text{ to PE } a" \]
   \text{endif}
   \text{endif}

or:
 \text{RECV}_6 \text{ final coordinate vector from SLAVE2}

2. if \text{any(slaves not stopped)} \text{ and } n_{\text{lost}} > n_{\text{limit}} \text{ then}
   \text{ISEND}_5 \text{ a termination order to PE } 0
   \text{SEND}_5 \text{ termination orders to all other PE's}

\text{return}

Table A.5: The algorithm followed by PE 0 when a call to WHIP2 is made by the dynamic queue algorithm (see section A.2.2.) Numbered subscripts on the SEND/RECV operations indicate the number of the matching RECV/SEND operations in the SLAVE2 routine (table A.4.)
A.3 Discussion

The parallelism of each of these methods is high because they are naturally load-balanced across the processors, even on a heterogenous distributed machine. “Slave” processes which are running fastest submit more requests to the “master” process, and end up performing more of the computation.

An ideally parallel algorithm will have a linear speedup in computing time as the number of processing elements (PE’s) is increased. In figure A.4 we have plotted this relationship for the MPMD code when run on an SGI PC and a Fujitsu VPP. It is clear that the code attains excellent parallelism on both the SGI PC and the VPP 300. Since the ratio of CPU time per PE is approximately constant for the SGI PC up until 18 PE’s are used (the largest number of PE’s available at the time of this test) it is also clear that the code displays excellent scalability. On the VPP300, overall vectorisation varies from 90% to 98%.

As a further test of the method, we saturated the MP network, to see what effect it would have on the parallel performance. The saturation condition used was the requirement that each process had more than one (we used 10) requests pending with the master process at any time. (A process “requests” a new particle when one is lost from the simulation region.) This saturated-state message burden is several orders of magnitude greater than that which occurs in normal operation. Using this condition, there was no discernible impact on parallel performance of the code, on either the VPP300 or the SGI PC.

A more stringent saturation condition was also tested on the VPP, in which every process submitted a request to the master once in each timestep. The algorithm remained stable under this condition, though the vectorisation was poor, and, when a slave reached its exit condition in $N$ timesteps, it required approximately $N$ more time steps to finish receiving its requests.
Figure A.4: Run times on the SGI PC XL and the Fujitsu VPP 300. A zero gradient corresponds to perfect parallelism.
Because of this it was difficult to draw meaningful runtime comparisons between this case and the other cases.

A.4 Summary

A scalable MPMD Monte Carlo code has been developed which exhibits excellent vectorization, and a linear speedup with PE number. The code is portable, and can be compiled on any system supporting FORTRAN 90 and a Message Passing Interface library. The bank-queue and dynamic queue algorithms which we have developed allocate work so that the code is always optimally load balanced. The disparate computing requirements of different test particles are catered for by allowing each test particle to have a self adaptive timestep. The code has been successfully benchmarked, and was used to produce many of the results in chapter 3.
Appendix A. The MCMuPPeT Code
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