Electrostatic Energy Exchange in Shock Acceleration

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ABSTRACT

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Plasma shocks are very common occurrences, and diffusive shock acceleration is a simple and efficient mechanism for generating cosmic rays. A shock’s main effect is turbulent dissipation, which rapidly thermalizes the downstream plasma. Diffusive shock acceleration produces a nonthermal component to the particle distributions (quasi-power-law tails) which translates to nonthermal photon spectra, as seen in supernova remnants, jets in active galactic nuclei, and gamma-ray bursts. In supernova remnants, X-ray observations show that inferred proton temperatures are considerably cooler than standard shock heating predicts. A cross-shock electrostatic potential, akin to a double layer, is reasoned to exist in certain conditions due to the different inertial gyration scales of the plasma species. It provides a mechanism for energy exchange between species, and should result in a respective heating/cooling of the electrons/ions. It modifies the electron/ion distributions, which couple through radiative processes to the observed X-ray emission. In this thesis, the effects of cross-shock electrostatics are explored using a Monte Carlo simulation, where test particles gyrate and stochastically diffuse in a background fluid pre-defined by MHD jump conditions. A cross-shock electric field is derived from the steady-state spatial distribution of particles via a modified Poisson’s equation that includes Debye screening, and the simulation is rerun with this field superimposed on the background magnetic
and drift electric fields. This feedback loop continues until a self-consistent solution is obtained. Results show a significant departure of the particle distributions from the usual thermal+power-law form, and clearly demonstrates substantial energy exchange between the electron and ion populations.
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CHAPTER 1
Introduction

The process of shock acceleration is a convenient mechanism for generating high energy particles. Shocks are ubiquitous in the cosmos due to an abundance of supersonic flows, and it takes only a few simple assumptions to produce acceleration in a shock environ. Shock acceleration provides a convincing explanation on the origin of cosmic rays as well as nonthermal photon spectra seen in supernova remnants, jets in active galactic nuclei, and gamma-ray bursts. Starting from simple ideas in the late 1940’s the field has progressed towards complicated numerical models.

1.1 History of Diffusive Acceleration

In the early 20th century, several experiments investigating ionization found that observed ionization rates increase with altitude. A daring balloon flight by Victor Hess (1912) to a height of 5.3 km during a solar eclipse helped to establish this. With terrestrial and solar origins ruled out, the best explanation for such a result is strongly penetrating radiation of some cosmic origin. Further observations showed a latitudinal dependance, suggesting that most cosmic rays were charged particles. Rossi (1930) predicted the magnetic deflection of cosmic rays, and by 1945 it was evident that cosmic rays are mostly protons. Fig. 1.1 depicts the all particle spectrum of cosmic rays. A straight line seen on a log-log plot is the signature of a power law dependence; the slope gives the corresponding power (called a spectral index). The energy spectrum of cosmic rays follows a power law \( \frac{dN}{dE} \propto E^\alpha \) with spectral index
Figure 1.1: The all particle spectrum of cosmic rays as seen by a variety of experiments. The flux for the lowest energies ($< 10^{10}$ eV) are mainly attributed to solar cosmic rays, intermediate energies ($10^{10}-10^{15}$ eV) to galactic cosmic rays, and highest energies ($> 10^{15}$ eV) to extragalactic cosmic rays. Credit: W. F. Hanlon; a polished update of the original plot by Swordy (2001). http://www.physics.utah.edu/~whanlon/spectrum.html
\( \alpha \) near -3 in a wide energy range. The “knee” refers to the change of the power law index from -2.7 to -3.1 at energy \( 10^{15} \) eV; this probably reflects the transition from galactic to extragalactic cosmic rays. Why does cosmic ray flux obey an inverse power law in energy, and why \( \alpha \approx -3 \) ?

1.1.1 Second-order Fermi Acceleration

The first serious attempt to explain the origin of cosmic rays was proposed by Fermi (1949). He imagined test particles traversing a region with numerous magnetized clouds of gas. If a particle encounters a cloud, it is scattered by a magnetic mirror effect. This can be modeled as elastic scattering with a perfectly rigid moving target.

If the scatterers are at rest, then scatterings can only change the direction of the particle’s momentum as it traverses the region. If the scatterers are allowed nonzero motion, i.e. an isotropic velocity distribution, then particles can gain (lose) energy in head-on (trailing) collisions. However, the odds of a particle encountering a cloud head-on are greater than the odds of a trailing collision. If this is not intuitive, consider the analogy of driving down a busy two-way road: obviously, more cars on average pass traveling the opposite way than pass traveling the same way.

Give the scatterers an isotropic velocity distribution, where the average speed \( V \ll c \) is nonrelativistic. Particles then enjoy a mean energy gain per collision that is second order in cloud velocity: \( \Delta E/E = (V/c)^2 \). The particles gain energy at a rate proportional to their energy, \( dE/dt = E/\tau_{acc} \), where the acceleration time scale \( \tau_{acc} \) varies with the mean collision time and average cloud velocity. Consider a steady injection of particles into the region of moving clouds while allowing their escape from the region with a probability per unit time \( \tau_{esc}^{-1} \). The steady-state energy distribution
is an inverse power law in energy with spectral index $\alpha$:

$$
\frac{dN}{dE} = \frac{\alpha - 1}{mc^2} \left( \frac{mc^2}{E} \right)^\alpha ; \quad \alpha = 1 + \frac{\tau_{acc}}{\tau_{esc}}. \quad (1.1)
$$

Note that power laws are scale-invariant; seen another way, this means that cosmic ray flux obeys a power law in energy because the process that creates it has no characteristic energy scale. Here this implies that $\tau_{esc}$ and $\tau_{acc}$ must have the same dependence on momentum/energy, so that their ratio is independent of such.

A Fokker-Planck formalism can also be used to approach the problem. A simple model is momentum space diffusion, isotropic scatterers/scattering, and a “leaky box” term:

$$
\frac{\partial f}{\partial t} + (\vec{v} \cdot \nabla) f = \frac{\partial}{\partial \vec{p}} \cdot \frac{c \rho^2}{3v\tau_{acc}} \frac{\partial f}{\partial \vec{p}} - \frac{f}{\tau_{esc}}. \quad (1.2)
$$

Here the LHS is a convective derivative, the first term on the RHS describes momentum space diffusion, and the second term represents the “leaky box” escape rate; see Blandford & Eichler (1987) for more details. This equation has a steady-state power law solution of index

$$
\alpha = -\frac{1}{2} + \frac{3}{2} \sqrt{1 + \frac{4}{3} \frac{\tau_{acc}}{\tau_{esc}}}. \quad (1.3)
$$

This solution is different from (1.1) because it includes momentum diffusion; the solutions match in the limit $\tau_{acc}/\tau_{esc} \ll 1$.

Fermi’s stochastic acceleration process is of limited use. It is relatively inefficient due to being second order in cloud velocity. Comparison with the galactic cosmic ray spectrum tells us $\tau_{acc}/\tau_{esc} \approx 1.7$, but there is no good reason why this should be. It is more reasonable to expect that $\tau_{acc}/\tau_{esc}$ varies from place to place as well as with energy/momentum. Also, when ionization losses are considered, only particles
above a threshold energy of about 100 MeV can gain net energy in the process; see Morrison et al. (1954) for discussion. How do enough above-threshold particles enter the process? This is called the injection problem.

1.1.2 First-order Fermi Acceleration

Darwin (1949) was the first to predict the importance of shocks as an origin for cosmic rays. It was then shown by Bell (1978), Krymskii (1977), Axford et al. (1977), and Blandford & Ostriker (1978) that particles can accelerate to high energies in astrophysical shock fronts. Energetic plasma particles gyrate along the local field lines near a shock, and in doing so they naturally excite helical plasma wave modes, i.e. Alfvén waves. This results in a turbulent magnetic field structure near the shock, and this turbulence acts to deflect particles from their original trajectories. Particles departing downstream are sometimes deflected back towards the shock, recrossing it. It is helpful to recognize that the shock can be seen as two converging flows; crossing the shock in either direction guarantees a head-on collision with the opposing flow.

Particles that recross scatter off turbulence in the opposing flow, sampling the change in flow speed. This leads to an average energy gain upon crossing that is first order in the flow speed difference. Also, the probability of recrossing increases with particle speed, with fast particles simply random walking off the turbulence. Once a particle is sufficiently energetic it is virtually guaranteed to continue recrossing the shock; this results in a highly efficient acceleration mechanism.

This is called first-order Fermi acceleration, diffusive shock acceleration (DSA), or the Fermi-I mechanism. Diffusive shock acceleration is far more efficient than the second-order stochastic acceleration, although both mechanisms can be present. As before, the process has no energy scale and thus produces a power law spectrum. The
spectral index is no longer arbitrary but is determined by the shock kinematics.

The flow velocities, magnetic fields, pressures and densities describing the shock structure are prescribed with a fluid model, using magnetohydrodynamic equations to describe the steady-state far-upstream and far-downstream states. This gives bulk properties to each side of the shock; the convention is to use a subscript 1 (2) to label the upstream (downstream) quantities (see Appendix). Turbulence certainly needs to be considered though, as diffusive shock acceleration relies on a scattering mechanism to enable recrossing and to allow energy gains from sampling the different flow speeds. It is worth highlighting that Coulomb collisions are usually negligible in most astrophysical systems; the mean free path for Coulomb collisions is often much larger than the physical structure of a system. Shocks with this large Coulomb collisional scale are called collisionless shocks, and are common in astrophysics.

An exact description of shock turbulence generation is possible with full plasma codes, but this is outside the scope of this work. Luckily, diffusive shock acceleration is insensitive to the details of the scattering process, and we can model turbulence parametrically as stochastic diffusion in the local fluid frame. By approximating turbulence in this way we gain a resemblance to second order Fermi acceleration on each side of the shock; the connection is described in Fig. 1.2. In this work, scattering events are approximated as elastic scatterings with perfectly rigid targets that are tied to the flow. The frequency and strength of an individual scattering is decided stochastically and is parameterized by defining a mean free path (see Appendix).

In the beginning diffusive shock acceleration was modeled with simple 1-D momentum space diffusion; see Krymskii (1977), Axford et al. (1977), and Blandford & Ostriker (1978). This is similar to (1.2), but with a spatially-dependent scatterer velocity profile that represents the shock discontinuity. Bell (1978) instead used a
Figure 1.2: A cartoon of Fermi acceleration. A test particle is pictured entering a region of rigid scatterers (blue dots) interacting with them, then departing. The trajectory is in red and red arrows show the initial and final velocities. Green arrows show the motion of the scatterers. In (a) the scatterers are at rest. There is no acceleration; elastic scattering serves only to rotate the velocity. In (b) the scatterers have some isotropic motion. Particles gain energy on average; this represents 2nd order acceleration. In (c) the scatterers divide into two converging regions of flow as indicated by the grey line. The particles always gain energy in the first scatter after crossing the boundary; this represents 1st order acceleration (DSA). If the scatterers are allowed some isotropic motion in their co-moving frame, we have both 1st and 2nd order acceleration; this is shown in (d).
kinetic theory viewpoint to model diffusive shock acceleration, considering particle fluxes and recrossing probabilities to obtain a downstream spectrum. Either case describes the evolution of a test particle population, recognized to be separate from the shock representation which is often pre-defined.

The power-law spectrum that resulted was found to be independent of the injection spectrum (provided the latter was initially steeper), independent of the details of the scattering process (assuming to first order an isotropic accelerated particle distribution), and independent of the shock geometry (if the diffusion scale is larger than the shock thickness and smaller than the shock curvature). The resulting spectral index depends only on one parameter called the density compression ratio $r$:

$$dN \propto p^{-\sigma} dp, \quad \sigma = \frac{r + 2}{r - 1}, \quad r = \frac{\vec{u}_2 \cdot \hat{n}}{\vec{u}_1 \cdot \hat{n}}$$  \hspace{1cm} (1.4)

Note that a power law in energy $dN \propto E^{-\alpha} dE$ is equivalent to a power law in momentum $dN \propto p^{-\sigma} dp$, where $\sigma$ is related to $\alpha$ by $\sigma = 2\alpha - 1$ for non-relativistic particles; for relativistic particles, $\alpha = \sigma$. For strong shocks, the compression ratio is constrained to be near $r = 4$, which gives $\sigma \simeq 2$. This property was a huge success for diffusive shock acceleration because, when source-to-Earth propagation effects are taken into account, $\sigma \simeq 2$ approximately matches the inferred particle spectrum for galactic cosmic rays as well as a wide variety of other astrophysical sources. The current paradigm for the origin of galactic cosmic rays is diffusive shock acceleration in supernova remnant shocks; see Reynolds (2008). The detection of pion-decay signatures in supernova remnants (SNRs) by the Fermi-LAT gamma-ray telescope by Ackermann et al. (2013) provides direct evidence of accelerated protons that can explain the origin of galactic cosmic rays. The particle spectrum produced near a
shock by diffusive shock acceleration also couples to radiation through processes such as synchrotron, bremsstrahlung, and inverse-Compton scattering. When astronomers see a nonthermal power-law photon spectrum, they are likely to be looking at energetic particles participating in diffusive shock acceleration. This is exactly what is observed in supernova remnants such as Cassiopeia A (Fig. 1.3), in jets in active galactic nuclei such as the jet in M87 (Fig. 1.4), in gamma-ray bursts, and in many other sources. It has become the theorist’s job to model these observations with increasing accuracy using increasingly sophisticated shock models, including numerical simulations.

1.1.3 Other Mechanisms

There exists some other forms of acceleration that should be mentioned since they are relevant to various astrophysical environments. In shock drift acceleration (SDA) work is done by drift electric fields which occur in the shock rest frame when the upstream flow and upstream magnetic field are not parallel. While a drift electric field does no work when phase-averaged, the shock discontinuity provides the non-uniformity needed for work to be extracted. Repeated reflections and upstream excursions are a hallmark of shock drift acceleration; see Decker & Vlahos (1986). Jones & Ellison (1991) point out that there has been confusion in the past as to the nature of this mechanism. Because we can eliminate drift electric fields by choice of frame, shock drift acceleration can be thought of as a purely relativistic effect; a sub-set of diffusive shock acceleration that is already present in the formalism. Shock drift acceleration dominates in low turbulence near-perpendicular shocks where injection into diffusive shock acceleration from the thermal spectrum is inefficient. It makes for more efficient trapping upstream and so enhances the acceleration once it is started; see Summerlin & Baring (2012).
Figure 1.3: Multi-wavelength images of Cassiopeia A, a 320 year old supernova remnant. Going clockwise from the top left: radio, infrared, optical, and x-ray images. The x-ray image captures the expanded shock-heated gas, while the radio shows high energy electron synchrotron emission. Infrared shows dust grains swept up and heated by the expanded gas, and optical shows wisps of matter thought to be clumps of stellar ejecta. Credits: Radio: NRAO/AUI/NSF; Infrared: ESA/ISO, CAM, P. Lagage et al.; Optical: MDM/R. Fessen; X-ray: NASA/CXC/SAO. http://chandra.harvard.edu/photo/1999/0237/
Figure 1.4: Multi-wavelength images of the jet flowing from the nucleus of M87, a giant elliptical galaxy 50 million light years away in the constellation Virgo. The jet is thought to be produced when gas and magnetic fields from matter accreting onto the central supermassive black hole becomes pulled away along its axis of rotation by strong electromagnetic forces. Inside the jet, shock waves produce high-energy electrons that emit synchrotron radiation, creating the observed radio, optical and X-ray knots. Credits: X-ray: NASA/CXC/MIT/H.Marshall et al. Radio: F. Zhou, F.Owen (NRAO), J.Biretta (STScI) Optical: NASA/STScI/UMBC/E.Perlman et al. http://chandra.harvard.edu/photo/2001/0134/
Shock surfing acceleration (SSA) was originally proposed by Sagdeev (1966) and bears similarities to shock drift acceleration as pointed out by Lever et al. (2001). Shock surfing acceleration recognizes that a cross-shock electrostatic potential should exist in the shock layer. A particle may be repeatedly reflected by this potential, "surfing" it and extracting energy from the drift electric field until sufficient energy is reached to breach the potential barrier; see Lee et al. (1996). This is very similar to shock drift acceleration, although in shock drift acceleration any reflection is from the magnetic gradient at the shock or backscattering. The form of the cross-shock potential is specified \textit{a priori} in models of shock surfing acceleration; some simple form is often assumed. Shock surfing acceleration is very phase-sensitive and can be easily disrupted by diffusive turbulence in an astrophysical shock. It is useful to invoke as a pre-acceleration mechanism for bootstrapping the injection process.

Magnetic reconnection can also accelerate particles efficiently; see de Gouveia dal Pino & Lazarian (2005). The motion of magnetic fluxes during reconnection allows for acceleration analogous to diffusive shock acceleration to take place. While not germane to shock acceleration, it does contribute to the overall cosmic ray abundance. Reconnections occur on fast time scales of minutes to hours, while shocks can persist and propagate for thousands of years. In this way shocks and reconnections are differentiable; so while we know reconnection occurs in places such as solar flares, shocks provide a much steadier source of cosmic rays.

Malkov & O’C Drury (2001) describe how overly efficient acceleration in diffusive shock acceleration leads to nonlinear effects that break down the test particle approximation. Diffusive shock acceleration alters the injection spectrum, moving particles from a thermal injection into the high-energy cosmic ray tail. When the cosmic ray contribution is a significant fraction of the total energy flux, the magnetohydrodynamics...
namic structure of the shock becomes altered. Energetic plasma particles near a shock drive Alfvén waves, producing turbulence in the magnetic fields. However, the super-Alfvénic particles produced by diffusive shock acceleration cause the majority of the magnetic turbulence in the first place. Also present is the aforementioned injection problem. Diffusive shock acceleration may start slowly as only minor turbulence is present and few particles are injected. These low-wavenumber excitations can interact to create a new wave with a higher wavenumber, which can excite waves of even higher wavenumber, leading to a cascade of energy from low to high wavenumbers. This avalanche increases the acceleration efficiency until the point where the cosmic ray contribution is significant, altering the MHD structure and reducing efficiency until an equilibrium is reached. To account for these effects, models of nonlinear diffusive shock acceleration were developed, e.g. Ellison & Eichler (1984). These models aim to treat these issues in a self-consistent way. Caprioli et al. (2010) provides a comparative review of different popular methods.

1.1.4 Numerical Methods

The advent of numerical simulation reinvigorated shock acceleration theory. Now the field is dominated by simulation models that can solve analytically non-tractable problems. Diffusive shock acceleration simulations fall into two major camps: Monte Carlo (MC) and particle-in-cell (PIC). Monte Carlo models diffusion in prescribed turbulence or parametrically, and particle-in-cell is a full plasma code.

Particle-in-cell simulations solve the differential equations of particle/fluid and field dynamics numerically. Particles (or fluid elements) alternate between two roles: being moved by the fields, and being the source terms used to calculate the fields. In this way, particle-in-cell codes incorporate all the complex microphysics within
the framework of electrodynamics, such as magnetic turbulence and nonlinear effects. However, particle-in-cell has some shortcomings. One or more dimensions are sometimes ignored to simplify the simulation and speed up runtime, but this unphysically prevents particles from crossing magnetic field lines. Diffusive shock acceleration spans large spatial, temporal, and momentum scales in order to accelerate particles into the TeV range. A particle-in-cell code must use a relatively small time step to reach an incredibly large (TeV-scale) acceleration time; this makes the computational requirements far too much for even modern computers. Vladimirov et al. (2008) present these arguments in more detail; see Kang et al. (2009) for an example of a nonlinear particle-in-cell code that uses a diffusion-convection model.

Monte Carlo simulations such as that by Ellison et al. (1990) use the test particle approach of Bell (1978). Particles are inserted upstream of a pre-defined shock, the trajectories are followed as they convect and scatter, and ‘detection data’ is obtained in the time-asymptotic steady-state. Nonlinear effects can be addressed by an iterative feedback mechanism that allows the final test particle steady-state properties to modify the initial background properties. For example, with a discontinuous subshock this will smooth a step function flow profile into a softer sigmoid function. Monte Carlo simulations have a significant runtime advantage over particle-in-cell codes, and have additional redeeming features such as easily obtainable time-asymptotic states and the ability to isolate various elements of the physics involved. Moreover, they can model acceleration up to the highest energies inferred in astrophysical systems such as SNRs, extragalactic jets in blazars, and gamma-ray bursts. Monte Carlo simulations remain useful in the current state of the field, although sometime in the future computing power will allow for full 3-D particle-in-cell simulations that model 4-5 orders of magnitude in momenta and diffusive mean free path.
1.2 Motivation

What is the degree of energy exchange and equilibration between thermal ions and electrons in hydrogenic shocks? This is a key question for shock acceleration studies. Chandra X-ray observations have significantly enhanced the understanding of supernova remnant structure. However, the observed degree of energy exchange is not correctly predicted.

Inferred proton temperatures in SNR shocks can be made using proper motion studies or spectroscopic methods, as Ghavamian et al. (2003) did. Electron temperatures are determined using ion line diagnostics (assuming $T_p = T_e$). Combining these, Hughes et al. (2000) noticed that proton temperatures are significantly lower than what is predicted from standard magnetohydrodynamic (MHD) shock heating, where the inertia from the bulk flow is converted to heat. Combining these measurements and others, the inferred temperature ratio for various SNR shocks have been calculated by Hwang et al. (2002), shown in Fig. 1.5. This property is expected in nonlinear shock acceleration, since moving a significant fraction of energy into the tail will lower the effective temperature of the thermal population. Could we be missing an extra ingredient that allows for electrons and protons to exchange energy at a shock?

SNR shocks are almost always collisionless, and therefore lack the usual avenue of Coulomb collisions to thermalize the plasma species. However, charge separation in the shock layer and thus a cross-shock potential is argued to occur because the plasma species react to the shocked magnetic field on different inertial scales. Baring & Summerlin (2007) describe how the magnetic field discontinuity at the shock leads to coherent gyrations that create a charge buildup downstream of the shock, as seen in Fig. 1.6. Note that strong turbulence that will act to destroy the coherence, so that it only occurs in weaker turbulence. The combined effect of electrons and protons
Figure 1.5: Ratios of electron and proton temperatures inferred for supernova remnant shocks at various wavelengths, from Fig. 9 of Hwang et al. (2002). In order of increasing shock velocity, the plot shows the temperature ratios for the Cygnus Loop, RCW 86, Tycho’s SNR in optical, SN 1006, SN 1987A, Tycho’s SNR in X-ray, and SNR E0102-72.
Figure 1.6: Plot showing charge buildup in a shock layer. The shock is at rest at \( x = 0 \), and particles enter from the upstream (left). The upstream magnetic field is tipped 30° towards +z of the shock normal, and a drift electric field ensures particles move normal to the shock. The downstream magnetic field is significantly enhanced, while the drift electric field remains unchanged. This causes the trajectories to bend towards the magnetic field and gyrate more coherently, yielding an obvious density enhancement. Credit: Baring & Summerlin (2007).
leads to a cross-shock potential akin to a capacitance. Note that pair plasmas should not produce this since there is only one inertial scale, and the buildups will cancel.

Intuition indicates that this capacitance should quickly be shorted out by the plasma due to efficient Debye screening. However, it has been known since the discovery by Bernstein et al. (1957) that there is an unlimited class of solutions the Vlasov equation that contains layered potential structures. Such a structure need not be associated with a shock and is known as a double layer; for it to exist there simply must be a way to maintain trapped electron and ion populations. In this case electric fields can be maintained on scales many times larger than the screening depth.

Net energy gain (loss) for the electrons (ions) is expected in such charge separation potentials, raising effective electron temperatures and thus increasing their contribution to radiative emission. This provides an intimate connection to the thermalization questions raised by Chandra and other X-ray spectroscopy for SNRs. The shapes of the full particle energy distributions will also be altered by such cross-shock potentials, renormalizing the power law portions of the cosmic ray electron and proton distributions. This influences predictions of neutrino flux, calculations of the ratio of electron/proton cosmic ray abundance, as well as determinations of the emission mechanism in SNRs, gamma-ray bursts, and blazars. Direct measurements of cross-shock potentials in the bow shock and attempts to parameterize the cross-shock potential have been made, see Mandt & Kan (1991), Baring & Summerlin (2007), Dimmock et al. (2012). In this paper, we use a Monte Carlo simulation of diffusive shock acceleration to analyze the cross-shock potential. We will model charge transport near a shock using the test particle approach in order to obtain charge densities. These densities will be fed to a version of Poisson’s equation that accounts for Debye screening. The resulting electric field can then be fed back to the simulation.
Chapter 2
Monte Carlo Simulation

The MC simulation used in this thesis is a C++ program coded from scratch.* It uses a test-particle approach that follows the theoretical approach of Bell (1978). In this picture, test particles gyrate about bulk magnetic fields in convecting plasma flows, their trajectories perturbed by stochastic deflections that are presumed to be precipitated by charges’ interactions with MHD turbulence. Using a test particle approach means we assume the particle’s presence does not alter the system, and the particle motion (between scatterings) is described by the Lorentz force. This approach is a simulational proxy for solving the Boltzmann equation with a collision operator, and has been successfully applied in a variety of environments such as the Earth’s bow shock, interplanetary shocks, and blazar jets; see Ellison & Eichler (1984), Ostrowski (1991), Baring et al. (1993), Jones et al. (1993), Baring et al. (1997), et cetera. The major difference of this code is an inclusion of arbitrary electric fields.

The simulation can be roughly divided into four main algorithmic elements. A fluid description of the shock structure is needed to provide a background for the test particles. A trajectory calculator for the test particles is needed to follow their evolution. A stochastic scattering scheme is needed to model the effects of turbulence. Finally, a calculation of the cross-shock electric field in background plasma based on

*Some C++ template libraries were used. The trajectory calculator utilizes an arcsinh function defined in math headers of the Boost C++ Library (http://www.boost.org). The electric field calculation uses some matrix manipulation functions that come from Eigen (http://eigen.tuxfamily.org), a template library for linear algebra. Some 3D plotting functionality, though unrelated to the simulational function, uses openGL. Other than that, the code (including vector manipulation) is custom made from scratch.
the test particle density in the neighborhood of the discontinuity is needed to obtain the cross-shock electric field. The strategy is to reinsert the output (cross-shock electric field) as input into a new simulation with the aim of iteratively producing a self-consistent field profile and test particle spectrum.

2.1 Shock Structure

A shock, sometimes called a shock wave or shock front, is a propagating disturbance characterized by a near-discontinuous change in the characteristics of the medium it occurs in. When an object or disturbance moves faster than the speed at which ‘information about its existence’ can propagate into the surroundings, then the media near the disturbance cannot react or ‘get out of the way’ before the disturbance arrives; this leads to the formation of a shock. The shock is itself the medium’s surprised reaction to the disturbance; the medium is shocked.

In a gas, the bulk properties are temperature, pressure, and density. Information about changes in these properties propagate at the speed of sound: sound waves are the carriers of this information. The sonic Mach number gives the relative speed with respect to the gas, in units of the gas sound speed:

\[
M_S = \frac{u}{v_s}
\]  

(2.1)

For an ideal gas, \( v_s = \sqrt{\gamma P/\rho} = \sqrt{\gamma kT/m} \), where \( \gamma \) is the adiabatic index. When \( M_S > 1 \), the sound speed is exceeded and a gas shock is formed. Density, pressure, and temperature all increase sharply upon the shock’s passing (\( P \propto \rho^\gamma \) is the equation of state).

Once formed, a shock wave propagates in a characteristic way, independent of its
detailed history. Shocks are exceedingly thin, hence the near-discontinuous change they induce. As such, a shock front can be thought of as a plane of zero width that divides space into an upstream and downstream side. In the shock’s rest frame, the upstream side convects towards the front at supersonic speed, and the downstream side is compressed, heated, and subsonic. The flow direction can change as well.

A plasma differs from a gas mainly in that it is conducting; this creates an assortment of effects. Free charges can both generate electric fields and quench them, i.e. short them out. Background magnetic field lines (i.e. those averaged over larger spatial volumes) will move with the plasma: the field lines essentially become ‘frozen’ in. A whole zoo of new wave types will exist as well. Alfvén waves traveling along field lines are a good example; they are analogous to tension waves on a guitar string, with magnetic tension and ion inertia replacing the string tension and inertia. As such, the background magnetic field will be considered a bulk property of the plasma, and it is noted that Alfvén waves are the propagators of magnetic field information in the plasma. We therefore define the Alfvénic Mach number:

$$M_A = \frac{u}{v_A}$$  \hspace{1cm} (2.2)

where $v_A = B/\sqrt{4\pi\rho}$ is the Alfvén speed and $\rho$ here is the ion mass density. When $M_A > 1$, the direction and magnitude of the magnetic field (among other things) will change upon the shock’s passing. In this thesis, we restrict ourselves to only supersonic, super-Alfvénic hydrogenic ‘fast-mode’ collisionless shocks. This means respectively that $M_s > 1$, $M_A > 1$, the plasma is composed of only electrons and protons, the shock mode is such that the downstream magnetic field is enhanced and points further from the shock normal than the upstream (depicted in Fig. A.1), and
the mean free path for Coulomb collisions is much larger than the shock thickness. Such ‘collisionless’ shocks are usually what are encountered in tenuous astrophysical supersonic environments.

We can relate the bulk properties of a gas on either side of (but far from) a gas shock wave using the Rankine-Hugoniot jump conditions. They enforce the continuity of equations describing the conservation of mass, momentum, and energy upon crossing the shock. Magnetic jump conditions also exist; they relate the properties of a MHD plasma with background magnetic field on either side of a plasma shock. They include the magnetic contributions to energy and momentum, and enforce Maxwell’s equations in addition to the conservation laws. The solution to the nonrelativistic magnetic jump conditions is given in the Appendix. Relativistic jump conditions are more complicated and are solved numerically; see Summerlin & Baring (2012) and Double et al. (2004) cited therein. Note that in deriving the jump conditions it is assumed that effective Debye screening is present, so that there is zero electric field in the fluid rest frame. While drift electric fields can still exist in certain frames, there are no electric fields in the local fluid frame at this point.

To better quantify the bulk properties of the shock, we take as a general convention the +x direction as the shock normal and place all vectors in the x-z plane. We prefer to propagate charges and perform statistical accounting of their distributions in the normal-incidence frame (NIF) of the shock, where the shock front is at rest and the upstream flow is normal to the plane of the shock (see Fig. A.1). The shock is placed at \( x = 0 \) and is assumed to be of negligible thickness. In reality it is of small, finite thickness that scales with the inertial scale \( (u/\omega_p) \) of the charges, where \( \omega_p \) is the electron plasma frequency; it is intimately connected to screening and plasma dissipation in the shock layer. The flow is directed in the +x direction, therefore
$x < 0$ is upstream and $x > 0$ is downstream. In the Monte Carlo simulation, a sizable region of the $x$-axis is selected and divided equally into a large number of ‘grid zones’ or ‘$x$-bins’. Each $x$-bin is associated with an electric field, magnetic field, flow velocity, and ‘detected’ electron and proton densities. ‘Detection’ is simply a raw count that has been properly normalized to match the far upstream background fluid density. The shock is mathematically treated as an infinite plane, so there is no variation of any quantities along the $y$-$z$ directions. This is generally appropriate since all inertial and gyrational scales are normally far inferior to the spatial scale of astrophysical shock curvature.

### 2.2 Test Particle Evolution

The test particles must move through the fields as represented by the grid zones while participating in scattering events that simulate turbulence. Symmetry along $y$ and $z$ means we only need to track the $x$ position (and 3-D momentum) of the particles. To code this we will need a trajectory solver and a scattering algorithm. For the former, we make use of an exact analytic solution to the full relativistic Newton-Lorentz equation derived for this purpose from scratch, including arbitrary electric field (see Appendix). This calculator needs to accommodate the full range of field orientations in order to allow for the presence of a cross-shock component to the electric field. This is different than the common strategy such as Ellison et al. (1995): transform to a special frame where the drift electric field disappears, then calculate the pure magnetic trajectory in that frame. de Hoffmann & Teller (1950) noted the existence of a shock rest frame with no drift electric fields under certain conditions, namely that the upstream flow speed is not too close to $c$ for a given magnetic field obliquity to the shock normal. The de Hoffmann-Teller frame is commonly used as
a calculation frame for test particle trajectories due to its computational economy. Since we know that cross-shock electric fields will usually be present in the simulation, we must use a trajectory calculator that accommodates the full range of orientations. The full-range trajectory calculator is more computationally expensive; with it there is nothing to gain from transforming to a de-Hoffman-Teller frame. Note that Double et al. (2004) and Summerlin & Baring (2012) have also dispensed with boosts to the de Hoffman-Teller frame in their simulations. Including electric fields in the trajectory is a necessary step towards the analysis.

As stated, we use stochastic scattering to model the effect of MHD turbulence; this scattering is parameterized by a mean free path proportional to a particle’s gyroradius:

\[ \lambda = \eta r_g, \quad r_g = \frac{p_\perp c}{qB}. \]  

(2.3)

This simple form is reasonably justified.\(^\dagger\) To simulate a scattering event, the momentum vector is tipped by some amount in the local fluid frame. This is equivalent to elastic scattering with rigid comoving scatterers. Super-Alfvénic particles will see the turbulence as magnetostatic, and magnetostatic forces do no work. Therefore, as long as the Alfvénic Mach number is not very low, fluid frame elasticity is a valid assumption. The direction and the amount of deflection is determined stochastically; it is a solid angle mapping about the pre-scattering momentum vector. This means phase angles are sampled randomly, uniformly from \( 0 \leq \phi \leq 2\pi \), and deflection angle cosines are sampled randomly, from \( \cos \delta \theta_{\text{max}} \leq \cos \theta \leq 1 \). If the half angle of the

\(^\dagger\)For example, Baring et al. (1997) begin with a more general form \( \lambda \propto (r_g)^\alpha \). They point out the values of \( \alpha \) that are compatible with evidence drawn from observations of planetary bow shocks, interplanetary shocks, plasma simulations, etc.; this varies with the environ, and in general \( 1/2 < \alpha < 3/2 \) (the union of the ranges). Therefore \( \alpha = 1 \) is reasonably justified and is an attractive choice due to its simplicity. \( \eta \) is simply the constant of proportionality.
scattering solid angle cone is small ($\delta \theta_{\text{max}} < 15^\circ$), we have small-angle scattering, and multiple scatterings will be necessary to realize a full mean free path. The alternative is large-angle scattering, where a single event is enough to isotropize a particle (i.e. $\delta \theta_{\text{max}} \sim \pi/2$). We stay in the small-angle scattering regime in the simulation, and following the work of Ellison et al. (1990), we use their derived relation between small-angle scattering coefficient and mean free path:

$$\delta \theta_{\text{max}} = \sqrt{\frac{6 \delta t}{t_c}},$$  \hspace{1cm} (2.4)

where $t_c = \lambda/u = \eta pc/\eta quB$ is the mean collision time, $\lambda \equiv \eta r_g$ is the mean free path, defined to be proportional to gyroradius $r_g$, $\eta$ is the constant of proportionality, called the gyrofactor, and $\delta t$ is the time increment between scatterings measured in the fluid frame. Note that if we set the charge’s velocity to be equal to the flow speed $u$, then $t_c = \eta \gamma u mc/q B$ is independent of speed for nonrelativistic $u$ (since $\gamma u \approx 1$).

We hand pick $\delta t$, such that $\delta \theta_{\text{max}} < 15^\circ$ to ensure a small-angle scattering regime in the simulation. This also means the scattering is continuous, and contrasts with a stochastically sampled $\delta t$. Here the stochastic nature of the scattering is due to random sampling of the scattering angle. Over a collision time $t_c$, the cumulative effect of numerous small-angle scattering events on a charge isotropizes its fluid frame momentum vector and all memory of the initial direction is lost.

The initial conditions of a test particle should sample the fluid properties given to the background MHD plasma by the jump conditions. In other words, they should represent the temperature and flow speed of the upstream plasma. We sample a thermal Maxwellian distribution $f(p) \propto e^{-p^2/2mkT}$ to generate the momentum magnitude in the fluid frame. This is a nonrelativistic distribution; this can be generalized to
the relativistic Maxwell-Jüttner distribution (see Jüttner (1911)) in due course. The momentum orientation is sampled isotropically in the fluid frame. We then move to the NIF, Lorentz boosting by the upstream flow speed \( u_1 \hat{x} \). The initial \( x \)-position is somewhat arbitrary; we simply require that particles start upstream, and there be no phase bias induced. This is safely done by uniformly sampling an upstream region that is at least as wide as the average proton gyroradius. This region can be as close to the shock as we like in theory, since the momentum is already isotropic in the fluid frame. In practice, we keep some distance between the initial \( x \)-position injection distribution and the shock front.

A particle is removed from the simulation only if it is determined to continue downstream indefinitely. This determination is done via a probability-of-return calculation (see Appendix). We pick a distance downstream and call it the free escape boundary. It needs to be far enough downstream that we can assume particles are isotropic in the local fluid frame. This means it needs to be at least a scattering mean free path downstream. At the free escape boundary, the assumption of isotropy can be used to obtain the probability of escape and the momentum distribution for particles deemed to return. We can then sample these to determine whether a specific particle returns or not, and what its vector momentum will be upon returning (see Appendix). This lets us ignore all motion past the free escape boundary, instead assessing the outcome probabilistically; this significantly speeds up runtime. If desired, we can also set up a flux detection plane, so that we can record the momentum flux distribution of each species; this is expected to be roughly a thermal+power-law form.

To summarize, the evolution of a single particle goes as follows. The particle’s initial momentum samples a thermal Maxwellian beamed with the flow, its \( x \)-position sampled uniformly from an upstream ‘\( x \)-injection region’. The simulation determines
which \( x \)-bin the particle is in, records a ‘detection’ there (i.e. collects its velocity/momentum component information), then advances the trajectory by the small time-step \( \delta t \) before performing a small-angle scattering. This last step is repeated many times until the particle reaches the free escape boundary; the particle either returns and the evolution continues, or it escapes and the evolution ends.

This evolution is done for \( N \) protons and \( N \) electrons in each iterative run; a run with excellent statistics \((N = 10^6)\) takes roughly 4 hours on a modern desktop computer for typical simulation parameters. It should be noted here that \( N \) is not a physical parameter. However, the ‘detected’ number density is easily normalized to the true density, independent of computational parameters like \( N \) and \( \delta t \). We know that far upstream, each of the \( N \) particles will be detected on average \( N_{\text{avg}} = u_1 \delta t/\Delta x \) times in each \( x \)-bin it passes, where \( \Delta x \) is the \( x \)-bin width (which is unchanging for a given run). So, if we call \( N_{\text{det}} \) the detected number count, then the true density in each bin is approximated by \( n_{\text{true}} = n_1 N_{\text{det}}/(N_{\text{avg}} N) \). In this way the true density can be simulated without needing to use the true number of particles that would be present. This is a common technique in Monte Carlo simulations.

It should also be noted how steady-state densities are obtained with this method. In a physical shock where there is a steady number flux entering the shock, the resulting (instantaneous) density is steady-state because it is dynamically maintained by this flux. This could be modeled in the simulation by a steady injection; then at far later times an instantaneous density (or flux) could be detected, and would correspond to the physical case. However, in the simulation a single injection of particles occurs over a spatially-distributed range upstream, and the detected density is summed over the full simulation time (and properly normalized). This method is valid thanks to a trick: the time-instantaneous density due to a passage of a constant flux is equivalent
to the time-integrated density due to the passage of an impulse of flux. Both avenues were explored; the statistics and runtime involved the steady injection method make it an inefficient approach by orders of magnitude when compared to the single injection method.

### 2.3 Cross-shock Electric Field Calculation

Once the particle evolution is completed, we have values for the proton and electron number densities in each \( x \)-bin based on the ‘detections’ made there. It is trivial to obtain a charge density for each \( x \)-bin based on these number densities: \( \rho = e(n_p - n_e) \).

The task will then be to calculate the cross-shock electric field for each bin based on this. This is done electrostatically since the densities obtained are steady-state. If the background is considered to be vacuum, Poisson’s equation will describe the solutions:

\[
\nabla^2 \Phi = -4\pi \rho, \quad \vec{E} = -\nabla \Phi \tag{2.5}
\]

However, taking a vacuum background with our iterative scheme will lead to a complete omission of the influences of electric field (Debye) screening. Debye screening occurs in any system with mobile charges and an electrostatic field: the nearby charges are quickly rearranged by the field, creating a large cancellation and thus reduction in field strength. As argued in the next section, the most computationally efficient strategy is to take the MHD background plasma described by the jump conditions as the background for the field calculation. This leads to a screened version of Poisson’s equation, derived in the Appendix:

\[
\left( \nabla^2 - \frac{1}{\lambda^2} \right) \Phi = -4\pi \rho \tag{2.6}
\]
where $\lambda$ is the screening length; if the plasma is assumed to be quasi-neutral ($n_e \approx n_p \approx n_0$) and ion contribution is neglected, it is equal to the Debye length:

$$\lambda = \lambda_D = \sqrt{\frac{kT}{4\pi n_0 e^2}} \quad (2.7)$$

Here, $T$ is electron temperature; Note that temperature and density (and thus $\lambda$) differs between the upstream and downstream regions.

Solving either of these equations is easily handled in the discrete case (for individual bins) using the method of finite differences. This method converts the differential equation into a set of linear equations that can be solved with linear algebra. A sizable region of the $x$-axis (from $x_a$ to $x_b$) is selected and divided into a large number ($N_{bins}$) of $x$-bins. So, the $i^{th}$ grid zone begins at $x_i = x_a + i \Delta x$ and ends at $x_{i+1}$, where $\Delta x = (x_b - x_a)/N_{bins}$, and $i$ goes from 0 to $N_{bins} - 1$. The $i^{th}$ bin also has a charge density $\rho_i$ and screening length $\lambda_i$ associated with it. To apply the method of finite differences, we need to convert $\nabla^2$ into a finite difference. Due to the $y$-$z$ symmetry, $\Phi$ can only vary with $x$, and $\vec{E} = E_x \hat{x}$. So, we can take $\nabla^2 \rightarrow d^2/dx^2$ and use the central finite difference to lowest order:

$$\left( \frac{d^2 \Phi}{dx^2} \right)_i \approx \frac{\Phi_{i-1} - 2\Phi_i + \Phi_{i+1}}{\Delta x^2} \quad (2.8)$$

The screened Poisson’s equation now reads:

$$\frac{\Phi_{i-1} - 2\Phi_i + \Phi_{i+1}}{\Delta x^2} - \frac{\Phi_i}{\lambda_i^2} = -4\pi \rho_i. \quad (2.9)$$

This can be recast as a $N_{bins}$-dimensional matrix equation $Ax = b$, where we set $\Phi_{-1} = \Phi_{N_{bins}} = 0$ (which is equivalent to choosing the boundary condition $\Phi = 0$).
This can be visualized in matrix notation:

\[
\begin{bmatrix}
\left( \frac{-2}{\Delta x^2} - \frac{1}{\lambda_0^2} \right) & \frac{1}{\Delta x^2} & 0 & \cdots & 0 \\
\frac{1}{\Delta x^2} & \ddots & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \frac{1}{\Delta x^2} & \left( \frac{-2}{\Delta x^2} - \frac{1}{\lambda_{N_{\text{bins}}-1}^2} \right) & \ddots & \vdots \\
0 & \frac{1}{\Delta x^2} & \ddots & \ddots & \vdots \\
\end{bmatrix}
\begin{bmatrix}
\Phi_0 \\
\vdots \\
\vdots \\
\Phi_{N_{\text{bins}}-1} \\
\end{bmatrix}
= 
\begin{bmatrix}
-4\pi\rho_0 \\
\vdots \\
\vdots \\
-4\pi\rho_{N_{\text{bins}}-1} \\
\end{bmatrix}
\]

Obtaining \( \Phi_i \) then amounts to calculating \( x = A^{-1}b \), a task easily handled with a numerical solver.\(^\dagger\) The electric field in each bin \((E_x)_i\) can then be calculated straightforwardly from \( \Phi_i \) using a central finite difference to lowest order:

\[
(E_x)_i \approx \frac{d\Phi}{dx}_i \approx \frac{\Phi_{i+1} - \Phi_{i-1}}{2\Delta x} \quad (2.10)
\]

### 2.4 Iterative Scheme

So far we have described how the Monte Carlo simulation sets up the shock, propagates and scatters the particles, and calculates the electric field. We will call this a run. In order to analyze the effect that the cross-shock electric field has, we take the electric field output from the end of a run and insert it as input in a new run. The new run will have exactly the same parameters as the previous run; the only difference is the vector addition of the previous run’s cross-shock field into the background field.

\(^\dagger\)This is done in the code with the help of Eigen (http://eigen.tuxfamily.org), a template library for linear algebra. The code simply needs to pass the matrix coefficients of \( A \) and \( b \) to one of Eigen’s many linear system solvers in order to obtain the solution \( x = A^{-1}b \). The specific solver used (SimplicialLDLT) provides a Cholesky decomposition without square root \( A = LDL^T \) of the sparse matrix \( A \) into lower unitriangular matrix \( L \) and diagonal matrix \( D \) in order to efficiently obtain \( A^{-1} \). This is stable and faster than alternative solvers (twice as fast as a LU decomposition), but can only be used when \( A \) is self-adjoint and positive definite. This happens to be the case for our \( A \), and leads to a quick solution (< 1s) even for large values of \( N_{\text{bins}} (> 10^4) \).
We call the primary run the zeroth iteration run, and expect that after a number of iterations the electric field will be self-consistent, i.e. it will converge on a form that reproduces itself. Of course, the opposite is also possible: this method could lead to a divergent feedback. The determining factor is how strongly the particles react to the field, which is decided by the field strength itself.

There are various ways to implement Debye screening computationally, and they vary in physical precision and ease of implementation. If the unscreened field calculation is used, then the iterative process itself accounts for screening in a sense: the charges are rearranged by the field in each iteration. This is the simplest case, but how well does it model Debye screening? After all, the simulation injects particles far upstream some distance from the cross-shock electric field, and they eventually leave the simulation through the free escape boundary. This contrasts with the physical picture of screening, where charges are already present locally and rearrange in a short time ($\sim \omega_p^{-1}$, where $\omega_p = \sqrt{4\pi ne^2/m}$ is the plasma frequency).

There is also a particle-in-cell-style approach: recalculate the field very frequently, perhaps on the order $\sim \omega_p^{-1}$. This would likely be quite self-consistent and model screening to the precision permitted by the number of particles employed, but like a particle-in-cell code it is CPU-intensive. Also, it doesn’t lend well to the single-injection approach, since charges would need to be present locally in order to screen on short timescales. Both of these methods can suffer from statistical fluctuations; the Monte Carlo density is not the true density by orders of magnitude.

The screened Poisson’s equation provides an intermediate approach. It’s far less sensitive to statistical fluctuations, since the screening is provided by the uniform MHD background density. It’s also compatible with the single-injection approach, and is not CPU-intensive. This provides a strong computational motivation for this
approach. This is expected to be a good approximation that will capture the character on $u_1/\omega_p$ spatial scales, particularly once iterative convergence is achieved.

Momentum distributions obtained after the first run will reflect the effect of the cross-shock electric field inserted from last run. In this way we obtain the cross-shock electric field as well as the test particle reaction to it. The application of this scheme in the code is straightforward: to obtain the electric field for the next run we add the cross-shock electric field from the last run to the background’s drift electric field. The addition is vectorial and within each $x$-bin.
CHAPTER 3

Results for a SNR-like shock

This chapter explores the character of the cross shock potential feedback on the shock acceleration process by examining some specific examples taken from the Monte Carlo simulation. The simulation parameters are chosen to be in the regime belonging to supernova remnant shocks: upstream flow speed \( u_1 = 0.03c \), magnetic field \( B_1 = 10^{-3} \text{ G} \), and number density \( n_1 = 10 \text{ g cm}^{-3} \). This sets the Alfvénic Mach number to \( M_A \approx 13 \). The sonic Mach number here is chosen to be \( M_S = 10 \), which effectively sets an upstream proton temperature \( T_{p,1} \approx 2.5 \text{ keV} \). The incoming flow is assumed to be in velocity equipartition; this sets the electron temperature as being cooler by the mass ratio \( T_{e,1}/T_{p,1} = m_e/m_p \). With this choice of parameters, the density compression ratio \( r = n_2/n_1 = 3.85 \). The largest spatial scale is set by the maximum upstream proton gyroradius, \( r_{g,p,1} = \gamma_1 m_p u_1 c/q B_1 \), where \( \gamma_1 \) is the Lorentz factor for the upstream flow speed \( u_1 \). For these parameters, \( r_{g,p,1} = 939 \text{ km} \). The downstream properties will depend on the choice of magnetic field obliquity \( \theta_{B_1} \).

Results are presented for \( \theta_{B_1} = 30^\circ \), in which case \( u_2 = 0.468 u_1, \theta_{u_2} = 1.63^\circ, B_2 = 2.14 B_1, \theta_{B_2} = 66.1^\circ, \) and \( n_2 = 3.858 n_1 \). These values are derived from the jump conditions discussed in Appendix A and serve to set up our background fields and flows. The small amount of deflection seen in \( u_2 \) is currently neglected in the simulation for simplicity. The electron mass is artificially set to be \( 1/20^{\text{th}} \) the proton mass instead of \( 1/1836^{\text{th}} \); this is to speed up the initial analysis and is commonly done in plasma simulations, since they must capture the electron gyrational and inertial
scales as well as for the protons. We anticipate that this expedient step will not incur significant loss of physics content.

We must also choose the gyrofactor $\eta$, which sets the scattering strength. The code allows for the gyrofactor to differ between location (upstream/downstream) and species (e/p); however for this run we choose $\eta = 5$ everywhere. This corresponds physically to fairly strong turbulence everywhere, the situation expected for efficient acceleration in SNR shocks. Zeroth iteration results are first presented. Next, the details of the cross-shock electrostatics and its proper application is analyzed. Finally, the multiple-iteration results are presented and discussed.

### 3.1 Zeroth Iteration

As previously stated, the zeroth iteration run is the initial run required to obtain the charge densities used to compute the initial cross-shock electric field. The test particle spatial densities can be seen in Fig. 3.1, and for an individual species the shape is determined by three factors: the shock compression, the gyrational contribution, and the precursor contribution.

The shock compression is the main effect of a shock and the easiest to understand: material crossing the shock is slowed down, heated, and compressed. We could also call it the thermal diffusive contribution. In the simulation, this occurs because of particle scattering and isotropization in the local fluid frame. The far-upstream density is normalized to $n_1$, and the downstream densities converge towards $n_2 = r n_1$: once the test particles have isotropized their momentum in the downstream fluid frame, the average velocity is reduced to $u_2$ which necessarily causes a density enhancement. The location downstream where the charges are fully isotropized will depend on the strength of scattering (the choice of gyrofactor). It can be seen in Fig.
Figure 3.1: Test particle spatial densities for the zeroth iteration run with the above parameters. The proton density is blue, the electron density is in green, and the charge density is traced in red, all in units of the far upstream density $n_1 = 10 \text{ g cm}^{-3}$. Note that on all plots showing spatial structure, the shock normal distance ($x$) is in units of the typical upstream proton gyroradius, $r_{g,p,1} = \gamma_1 m_p u_1 c/qB_1$. 
3.1 that this compression is reached rather quickly for this set of parameters.

The gyrational contribution is due to the cusp-like enhancement discussed at length in Chapter 2; it is caused by a coherent gyration of particles as they first sample the kinked and enhanced downstream magnetic field. This effect is sensitive to the field obliquity and the scattering strength. If the magnetic field is parallel (or near-parallel) to the shock normal, then there will be zero (or negligible) field kinking, and the gyrational enhancement will not be produced. For this run, the thermal smearing of momenta and the diffusive scattering smear out the cusp-like profiles into smoother forms as in Fig. 3.1.

If the scattering strength is extremely strong, coherent gyration is never realized; the charges are isotropized too quickly. Bohm diffusion sets a realistic upper limit on the scattering strength ($\eta \approx 1$, $\lambda \approx r_g$). If the scattering strength is extremely weak, coherent gyration can continue for quite some distance before being ‘damped out’. The situation is somewhat analogous to a damped oscillator, with scattering strength playing the role of damping strength. Note that for our choice of parameters there happens to be only one easily visible cusp in the gyrational enhancement.

The precursor enhancement refers to the effect of diffusive shock acceleration on the spatial density: upstream of the shock in the precursor, information (i.e. density and flow speed) is partially transmitted to the upstream side by the accelerated population. It could also be thought of as the nonthermal diffusive contribution. The upstream excursions by accelerated charges occur within a diffusive mean free path scale, which can be quite large for the highest energy particles. Precursor enhancements were also seen by Baring & Summerlin (2007); their presence hints at the need for a nonlinear treatment. We acknowledge the need for a nonlinear treatment, but remind the reader that much can be learned from an initial analysis before including
the complication of nonlinear effects.

Diffusive shock acceleration can be effectively ‘turned off’ in the simulation by eliminating charges that are found to recross the shock; when this is done, it results in the elimination of the precursor enhancement (as well as the elimination of the power-law tail in the downstream spectrum). With diffusive shock acceleration ‘off’, the upstream density is exactly $n_1$, as opposed to what is seen in Fig. 3.1: the difference is the precursor enhancement. This enhancement is larger for protons since their larger mean free path means longer upstream excursions. The overall result is a net positive charge density upstream. In the far-upstream limit, the charge density does indeed go to zero.

The downstream charge density structure is dominated by a set of two extrema corresponding to the electron and proton gyralional cusps. This charge separation somewhat resembles a capacitance; this will be discussed shortly. Note that the sharpest change in charge density is due to the different diffusion scales for each species. Electrons isotropize a short distance downstream while protons take much longer, leading to a large electron excess extending to about $x = 0.25r_{g,p,1}$ downstream. This sharp change near $x = 0$ due to this electron excess will play an important role in the electrostatics.

The test particle momentum-space density distributions are shown in Fig. 3.2. For each species they show a thermal peak corresponding to shock compression heating, and a nonthermal power-law tail corresponding to the accelerated population. This is the signature of diffusive shock acceleration.
CHAPTER 3: RESULTS FOR A SNR-LIKE SHOCK

Figure 3.2: NIF test particle momentum-space densities for the zeroth iteration run with the above parameters. The proton density is blue and the electron density is in green. This density effectively samples the far-downstream value; it samples the NIF momentum magnitude at the moment the free escape boundary calculation determines that the charge is lost downstream. The structure seen in the distribution is easily explained. The tallest peak corresponds to the thermal distribution: particles detected in this peak have not been scattered back towards the shock at all. As discussed in Ch.2, these peaks sit apart because the species are not in thermal equilibrium. The peak next to it has particles that have returned upstream exactly once; they are bumped up in energy in the crossings, and this peak’s shape therefore mirrors the thermal peak. The rest of the tail structure is the superposition of peaks for larger numbers of crossings; energy is proportional to the number of shock crossings.
3.2 Electrostatics

The addition of electrostatics can be thought of as a potential barrier problem. A crucial threshold occurs when the cross-shock potential energy exceeds the average kinetic energy; charges of the right sign with energy lower than the barrier height $q\Phi$ will be reflected. If this barrier is due to a positive $E_x$, then electrons reflecting upstream will contrast protons that are driven downstream. In order to pass downstream, charges trapped by the barrier must participate in the shock surfing acceleration mechanism, extracting energy from the drift electric field and the upstream flow, eventually gaining enough to be able to pass downstream.

There is initially an equipartition of velocity between the two species, the electrons have far less kinetic energy (by the mass ratio) and therefore are much more likely to be reflected. The average kinetic energy of an incoming simulated electron can easily be estimated: $\langle K_e \rangle = (\gamma_1 - 1)(m_p/20)c^2 \approx 3.4 \times 10^{-8}$ erg. If the maximum potential barrier is greater than this, i.e. $q\Phi_{\text{max}} > \langle K_e \rangle$, then virtually all incoming electrons will be reflected. An accurate estimate of $\Phi_{\text{max}}$ is difficult to pin down; it depends on the assumptions under which the potential is calculated.

The electric field strength for the unscreened problem has been roughly estimated by Baring & Summerlin (2007) using Poisson’s equation: $E_x \sim 4\pi e n_1 r_{g,p,1}$ and $|E_x/B_1| \sim M_A^2(c/u_1) \gg 1$. The potential can also be estimated: $q\Phi \sim qE_x r_{g,p,1} \approx .255$ erg $\approx 10^6 \langle K_e \rangle$; it implies a very large reflection barrier. We can make a similar estimate for the screened Poisson’s equation: $E_x \sim 4\pi e n_1 r_{g,p,1} \exp(-r_{g,p,1}/\lambda)$, where we need to make some assumptions about screening to obtain $\lambda$. We use upstream electronic Debye screening, then $\lambda = \lambda_{e,1} = \sqrt{kT_{e,1}/4\pi n_1 e^2} = 26.5$m. This contrasts the enormous proton gyroradius, $r_{g,p,1} = 939$ km. This gives $e^{-r_{g,p,1}/\lambda_{e,1}} = 1.7 \times 10^{-15389} \sim 0$, which tells us proton-scale charge density structure is screened out.
quite well by electrons.

The screened Poisson’s equation with a single screening length for a 1-D symmetry leads to electric field solutions that are not directly sensitive to the charge density, but rather the rate of change of the charge density:

$$E_x(x) = -2\pi\lambda \int_{-\infty}^{+\infty} \frac{d\rho(s)}{ds} e^{-|x-s|/\lambda} ds$$

(3.1)

This means the areas of largest density gradient correspond to the strongest field rather than the areas of density enhancement; see the Appendix for more details.

For the geometry in our simulation, the screening length will change on either side of the shock. This makes the solutions more complicated, and the numerical method described in Chapter 2 is used. The screening length on either side depends on the local temperatures and densities; for this simulation run, $\lambda_1 = 36.5m$ and $\lambda_2 = 251m$. Although one would expect the density compression to reduce the downstream screening length, the temperature increase is much larger, leading to an increase instead. The change in screening length is not modeled as a step function discontinuity, but is softened slightly into a hard sigmoid function

$$\lambda(x) = \lambda_1 + \frac{1}{2}(\lambda_2 - \lambda_1) \left[ 1 + \tanh(x/\eta_{g,e,2}) \right]$$

(3.2)

This softening must be done to avoid the pathological effect that a discontinuity in screening length causes. The downstream electron diffusive scale $\eta_{g,e,2} = 28.5$ km is used to set the hardness; electrons are the main players in screening, and the density and temperature that feed into the screening length are adjusted on this scale.

In light of this discussion, we see that the screening becomes weaker going from upstream to downstream, and that the field will be strongest where the charge density
Figure 3.3: Cross-shock electric field profiles for the zeroth iteration run with the above parameters. The charge density is shown again in red in units of the far upstream density $n_1 = 10 \text{ g cm}^{-3}$. The screened electric potential energy is shown in pink in units of electron rest energy, scaled up by a factor of 20 for visibility. The screened cross-shock electric field is shown in brown in units of the upstream magnetic field $B_1 = 10^{-3}\text{G}$, scaled up by a factor of 10 to make it visible on the plot. The field calculated from the unscreened Poisson’s equation is shown in purple for comparison, and is scaled down by a factor of 200.

change is sharpest. So, the sharp change in density mentioned near $x = 0$ due to the electron excess should cause the dominant feature in the cross-shock electric field profile. Indeed, this is what is seen, as shown in Fig. 3.3. We can estimate from this that $|q\Phi_{max}| \approx 5.5 \times 10^{-8} \text{ ergs} \approx 1.3 \langle K_e \rangle$. This means we will see electrons reflected by this potential, although the barrier is not nearly large as is estimated for the unscreened case.
3.3 Multiple Iterations

For the first iteration run, the electric field profile (shown in orange in Fig. 3.3) is superimposed with the background drift electric field. Based on the estimate of $\Phi_{max}$, we would expect there to be a signature of reflection in this run. Indeed, this is what is seen, shown in Fig. 3.4: a large cusp in the electron density occurs due to trapped electrons. This correspondingly alters the shape and strength of the electric field.

The effect on the momentum distributions is shown in Fig. 3.5. The electron distribution is profoundly affected, while the proton distribution is barely changed.
Figure 3.5: First iteration spectral momentum distributions. The same colors are used as in Fig. 3.2, with the zeroth iteration run now in dashed lines. As before, this samples the NIF momentum magnitude at the moment the free escape boundary calculation determines that the charge is lost downstream.
CHAPTER 3: RESULTS FOR A SNR-LIKE SHOCK

Protons have opposite charge, and see an accelerating potential instead of a barrier. The effect is weak; the protons are more massive, and their net energy gain relative to their kinetic energy is much less than the corresponding ratio for electrons. Meanwhile, the entire electron population is trapped behind the electrostatic barrier and must gain energy through diffusive scatterings to overcome the barrier. This has led to a corresponding shift upwards in energy, producing a very nonthermal structure to the distribution. Once the barrier is overcome, the electrons are free again to proceed with diffusive shock acceleration, and indeed this is seen as a high-energy power-law tail. This tail in the electron spectrum is significantly more populated than it was for the zeroth iteration. This is because the barrier-induced energy shift has improved the ratio of particles exceeding the momentum threshold for injection into the diffusive shock acceleration process.

In going to further iterations, we would like to see the field profile converge on a self-consistent form. Since the density gradient plays an important role in screened electrostatics, \( E_x \propto -d\rho/dx \), we can look at the density profiles to get an idea of the electric field that they will produce. We only need to look at electron densities, since electrons are the only species whose density gets significantly altered.

We see in Fig. 3.6 the electron density profiles for the first four iterations. The rise in upstream density going from 0 to 1 is due to reflection; a cusp-like feature can be seen that signifies the mean reflection point. Going from 1 to 2, the density is increased further; this implies that an increase in the potential barrier has occurred, and this is exactly what is seen in the potential profile. The same thing occurs going from iteration 2 to iteration 3.

We observe a pattern: the presence of a potential barrier creates a density enhancement whose effect increases the height of the barrier with each iteration. The
Figure 3.6: Electron density for multiple iterations. The potential barrier is rising each iteration, causing the electrons to be trapped for longer periods.

The potential barrier is due to the gyrational enhancement of electrons: the concentration of electrons there repels other electrons. For each further iteration the barrier is due to the density peak caused by reflection. In this way, the potential barrier is self-reinforcing, and there is no sign of convergence in these early iterations. In going to further iterations (not shown), there is also no convergent solution.\(^*\)

The situation is unphysical and can be seen as a partial failure (at least) of the current iterative scheme. In reality, a buildup of (negative) charge density would mean a local excess of electrons, and would cause a spatial rearrangement of those very

\(^*\)In further iterations there is an oscillatory behavior in the solutions which can be interpreted as follows. The electron cusp feature moves upstream with each iteration. When the cusp reaches the stronger screening upstream, the potential is weakened. Once weakened, charge can build up further downstream, and the process resets. This prevents a runaway buildup of density from occurring, though the solutions oscillate significantly instead of converging.
Figure 3.7: Screened potential profiles for multiple iterations. When $-e\Phi/\langle K_e \rangle > 1$, electron reflection is predicted. In going to further iterations, we see the barrier height increase and the location of the reflection threshold move upstream. Note that the reflection cusps seen in Fig. 3.6 align with the location of the corresponding reflection threshold.
electrons. In our scheme, charges come from far upstream and leave far downstream, interacting with any charge buildup from the last iteration as they pass through. With screening included in the field calculation, we are effectively allowing the background MHD gas to rearrange, and this background always has constant density (though different between upstream and downstream); it never accounts for the effect that these density buildups have on the screening length itself. As a future plan for this research program, we would like to improve the model to address this.

Despite this shortcoming, we would expect that simulation charges in a weak electric field (without a potential barrier) will largely maintain their co-moving speed due to diffusion and would not cause any extreme modification to density, although their fluid-frame energy would still be altered. Thus, as an immediate task we would like to explore a regime where reflection is not occurring.

### 3.4 Discussion

So far we have shown results for an artificial mass ratio \( m_p/m_e = 20 \). An artificial mass ratio is a necessary sacrifice for a PIC code; the full ratio often makes runtime unmanageable. However, the diffusive shock acceleration process is scale-invariant, and the assumptions about scattering, shock structure, etc., makes the entire process independent of the mass ratio (to first order, neglecting shock structure). However, some back-of-the-envelope electrostatic scale estimates do have mass dependence, due to changes in gyroscale and screening properties.

To make this concrete: we estimate the electric field scale \( E_x \approx 4\pi e^2 n_1 x_\rho \exp(-x_\lambda/\lambda) \), and the potential scale \( \Phi \approx E_x x \nabla \), where the \( x \)'s are estimates. \( x_\rho \) is a den-

---

†The diffusive shock acceleration process is scale-invariant in space and momentum, provided that the particles are test particles. This is not the case for nonlinear diffusive shock acceleration.
sity/potential scale, $x_\lambda$ is a screening scale, and $x_\nabla$ is a density/potential gradient scale. We have previously set them all equal to the upstream proton gyroradius $x_{g,p,1} = \gamma_1 \beta_1 m_p c^2/eB_1$, but there is also the corresponding electron gyroscale $x_{g,e,1} = \gamma_1 \beta_1 m_e c^2/eB_1$ and the relevant electron Debye length $\lambda = \sqrt{kT_e/4\pi n e^2} \sim \sqrt{\beta_1^2 m_e c^2/4\pi n_1 e^2}$. We define the shorthand $\Phi(x) = 4\pi n_1 x^2 \exp[-x/\lambda]$ to describe the potential estimate. We combine this with $\langle K_e \rangle = (\gamma_1 - 1) m_e c^2$ to form a relative barrier height $|e\Phi|/\langle K_e \rangle$ that predicts reflection if greater than one (recall that $|e\Phi_{max}|/\langle K_e \rangle \approx 150$ from the simulation). Using the proton gyrational scale,

$$\frac{|e\Phi(r_{g,p,1})|}{\langle K_e \rangle} = (\gamma_1 + 1) \frac{m_p}{m_e} \left( \frac{c}{v_A} \right)^2 \exp \left[ -\gamma_1 \sqrt{\frac{m_p}{m_e}} \left( \frac{c}{v_A} \right) \right]$$

where $v_A = B_1/\sqrt{4\pi n_1 m_p} \approx c/435$. This case has been treated before; the barrier height is $\sim 0$ due to large negative numbers in the exponential. With the Debye scale,

$$\frac{|e\Phi(\lambda)|}{\langle K_e \rangle} = \frac{\gamma_1 + 1}{\gamma_1^2} \exp[-1]$$

Mass falls out of this estimate entirely, and for $\gamma_1 \sim 1$ this is less than unity. While this is informative, we are most interested in the electron gyrational scale:

$$\frac{|e\Phi(r_{g,e,1})|}{\langle K_e \rangle} = (\gamma_1 + 1) \frac{m_e}{m_p} \left( \frac{c}{v_A} \right)^2 \exp \left[ -\gamma_1 \sqrt{\frac{m_e}{m_p}} \left( \frac{c}{v_A} \right) \right]$$

This case is most relevant to our situation: the electron gyrational scale is the closest of these three estimates to the scale of sharp change in the density as seen in Fig. 3.6 that produces the dominant feature in the cross-shock electric field profile. This gives $\approx 0.01$ for the relative barrier height; it is also less than unity. So our estimate is perhaps too coarse, but it can still be used to give the approximate mass-ratio.
dependence of the problem; we can use it to see how the barrier height will change when going to the full mass-ratio, to see if it increases or decreases. The barrier height is scaled by $H$ in moving from the artificial to full mass, where

$$H \equiv \frac{|e\Phi(r_{g,e,1})/\langle K_e \rangle|_\mu}{|e\Phi(r_{g,e,1})/\langle K_e \rangle|_{\mu_a}} = \frac{\mu_a}{\mu} \exp \left[ -\frac{c}{v_A} \left( \mu^{-1/2} - \mu_a^{-1/2} \right) \right]$$  \hspace{1cm} (3.6)$$

where $\mu_a = 20$ is the artificial ratio and $\mu = 1836$ is the true ratio. This expression also depends on $v_A$; density and magnetic fields affect the estimate. For our case of interest, $v_A/c = 1/435$, and $H \sim 10^{35} \gg 1$, meaning reflection increases drastically going to the full ratio. So, according to our coarse estimate, moving to the full mass for this choice of parameters will only make the reflection more prolific. And, unlike a pure diffusive shock acceleration problem, the realistic mass ratio will be necessary for accurate modeling that includes cross-shock electrostatics.

The code can be upgraded to handle nonlinear diffusive shock acceleration, so that the test particle distributions themselves feed into the shock structure. This would follow the ideas of the nonlinear Monte Carlo simulation by Ellison et al. (1996), a method that agrees with other nonlinear simulations as noted by Caprioli et al. (2010). The largest modification comes from the highest energy particles, and they affect the shock structure on larger scales. The result is a weakened shock with a lower effective compression ratio in the cross-shock potential zone, which forms part of the so-called subshock. There is also some modification to the surrounding densities and pressures. This large scale modification is distinct from the region of weakened discontinuity (the subshock). The addition of nonlinear effects can translate to changes in the screened electric field, and is likely to weaken it.

The code is designed to allow the user to prescribe a density, temperature, flow
speed, magnetic field, etc., different for each bin. Therefore, if we can parameterize
the effects of nonlinear modification, they can be plugged into the model directly.
This would be a more expedient to implement than a full self-consistent nonlinear
code. However, the potential interplay between nonlinear density/temperature mod-
ifications and screening effects would be included only in a full code.

We would also like to resolve the shock structure on a finer scale, particularly the
reflection cusp seen in electron density. This can be done directly by defining a finer
binning, but this comes at a computational cost: smaller timesteps are necessarily
involved, and larger statistics are likely needed. This is inefficient, since we are only
interested in finer structure close to the shock, not everywhere. A more efficient tech-
nique would have finer resolution only in the shock layer. This can be used together
with a statistical technique called particle splitting‡ to allow for finer resolution with
good statistics; this is being planned for the next step of the investigation.

‡Particle splitting is a common technique for increasing statistics in test particle Monte Carlo
simulations. For example, in simulations of DSA, the very high energy part of the power-law tail
suffers from poor statistics, since only a few particles make it to that energy. Particle splitting
alleviates this: particles above a certain energy are ‘split’: the simulation now contains two or
more particles at that energy, each with the appropriate fractional statistical weight of the original.
Diffusion gives the split particles different evolution, and the statistics are improved at minimal
expense. In the context of this simulation, splitting could be used to improve resolution in the shock
layer.
Chapter 4

Conclusions

The evidence is clear that diffusive shock acceleration is an important astrophysical mechanism. While its presence is well established, data (such as Fig. 1.5) shows that the degree of proton and electron heating in SNR shocks doesn’t agree with predictions for simple hydrodynamical shock structures. Shock layer electric fields can influence these predictions, but cross-shock electrostatic energy exchange had not been isolated or treated in much detail in the literature so far.

We have built a robust tool to study and diagnose the electrostatic structure in a shock layer and the energy exchange that it produces in the context of shock acceleration. Using it, we have been able to determine the initial structure and iterative evolution of the cross-shock electric field in a plasma shock under the assumptions described. We have learned that the electron cross-shock density enhancement to be the dominant feature with screened electrostatics, at least in our study case. Electron reflection is prolific in our model; it has a large effect on the final electron energy spectrum, and therefore plays the dominant role in electrostatic energy exchange.

There are several improvements to the simulation that have been considered for the near future. We plan to parameterize the effects of nonlinear shock modification, which will give a more realistic (and weaker) shock with higher downstream flow speed. We will implement finer resolution in the simulation near the shock (using the particle splitting technique to maintain good statistics) in order to precisely define the reflection cusp structure and thereby refine the electrostatic feedback determination.
The artificial mass ratio has provided a useful test case, used mostly for its expedience (following precedence in plasma simulations); however, since the electrostatics have some dependence on this ratio, we plan in the near future to simulate the full mass in order to make physical predictions.
A.1 MHD Jump Conditions

The far-upstream plasma is characterized by a flow vector $\vec{u}_1$, mass density $\rho_1$, pressure $P_1$, and frozen-in background magnetic field $\vec{B}_1$. The (non-relativistic) MHD jump conditions relate these properties on either side of the shock:

\begin{align*}
0 &= (\rho \vec{u} \cdot \hat{n})^2, \quad \text{(A.1)} \\
0 &= \left[ \rho \vec{u} \vec{u} \cdot \hat{n} + \left( P + \frac{B^2}{8\pi} \right) \hat{n} - \frac{\vec{B} \cdot \hat{n} \vec{B}}{4\pi} \right]^2_1, \quad \text{(A.2)} \\
0 &= \left[ \vec{u} \cdot \hat{n} \left( \frac{\gamma P}{\gamma - 1} + \frac{\rho u^2}{2} + \frac{B^2}{4\pi} \right) - \frac{(\vec{B} \cdot \hat{n})(\vec{B} \cdot \vec{u})}{4\pi} \right]^2_1, \quad \text{(A.3)} \\
0 &= \left[ \hat{n} \times (\vec{u} \times \vec{B}) \right]^2_1, \quad \text{(A.4)} \\
0 &= \left[ \vec{B} \cdot \hat{n} \right]^2_1, \quad \text{(A.5)}
\end{align*}

where $\gamma$ is the adiabatic index*, $\hat{n}$ is a unit vector in the shock normal direction, and $[\cdots]^2_1$ refers to a difference, i.e. $[P]^2_1 = P_2 - P_1$. The subscript 1 (2) refers to the upstream (downstream) properties. Note that (A.4) and (A.5) codify the continuity of Maxwell’s equations, while (A.1), (A.2), and (A.3) respectively codify the conservation of mass, momentum, and energy fluxes at the shock boundary. We will be most concerned with fast shocks, where the shock speed $u_1$ exceeds the sound speed $v_s = \sqrt{\gamma P/\rho} = \sqrt{\gamma kT/m}$ as well as the Alfvén speed $v_A = B/\sqrt{4\pi\rho}$. This is

*The adiabatic index is the ratio of specific heats at constant pressure and constant volume, and for an ideal monatomic gas, lies between 4/3 (relativistic value) and 5/3 (non-relativistic value).
Figure A.1: The normal incidence frame (NIF). The shock layer is at rest, is located in the $(y, z)$-plane at $x = 0$, and is considered to be negligibly thin. The upstream flow incoming from $x = -\infty$ is normal to the shock (is in the $+x$ direction).

best expressed in terms of Mach numbers: the sonic Mach number $M_S = u_1/v_s$ and Alfvénic Mach number $M_A = u_1/v_A$ will both be greater than one in this case.

We prefer to express flux conservation in the normal incidence frame described in Fig. A.1: the shock is at rest and the incoming upstream flow is normal to the shock. The vectors are all coplanar; components perpendicular to the shock normal are placed along the $z$-axis by convention. We can decompose the vectors into magnitudes and angles as defined in the figure. The general solution in this geometry is
\[ \tan \theta_{B_2} = \tan \theta_{B_1} \left( \frac{r M_A^2 - \cos^2 \theta_{B_1}}{M_A^2 - r \cos^2 \theta_{B_1}} \right), \quad (A.6) \]

\[ \tan \theta_{u_2} = \tan \theta_{B_2} - r \tan \theta_{B_1}; \quad (A.7) \]

\[ B_2 = \frac{B_1 \cos \theta_{B_1}}{\cos \theta_{B_2}}, \quad (A.8) \]

\[ u_2 = \frac{u_1}{r \cos \theta_{u_2}}, \quad (A.9) \]

\[ R = 1 + \gamma M_S^2 \left( 1 - \frac{1}{r} + \frac{\sin^2 \theta_{B_1} - \cos^2 \theta_{B_1} \tan^2 \theta_{B_2}}{2 M_A^2} \right), \quad (A.10) \]

where \( r = \rho_2/\rho_1 \) is called the compression ratio, \( R = P_2/P_1 \) is the pressure ratio, and \( \theta_{B_1} = \theta_{B_1} \). The solution for \( r \) is given by the roots of the following polynomial:

\[ 0 = (r - 1) \left[ r^3 \cos^2 \theta_{B_1} \left( \gamma - 1 + \frac{2 \cos^2 \theta_{B_1}}{M_S^2} \right) - r^2 \left( M_A^2 (\gamma - 2) + \left( \gamma + 1 + M_A^2 \left( \frac{4}{M_S^2} + \gamma \right) \right) \cos^2 \theta_{B_1} \right) + r M_A^2 \left( \gamma + M_A^2 \left( \gamma - 1 + \frac{2}{M_S^2} \right) + (\gamma + 2) \cos^2 \theta_{B_1} \right) - M_A^4 (\gamma + 1) \right]. \quad (A.11) \]

This has the trivial solution \( r = 1 \), corresponding to no shock transition, as well as a single real solution to the cubic in the brackets, corresponding to the shock solution. For the special case \( M_A \to \infty \), this cubic reduces to a linear equation:

\[ r = \frac{\gamma + 1}{\gamma - 1 + 2/M_S^2}; \quad (A.12) \]

In the MC simulation, the values \( u_1, B_1, \theta_{B_1}, \rho_1, T_1 \) are passed as input parameters. This is equivalent to specifying \( u_1, B_1, \theta_{B_1}, M_S, M_A \). The cubic is solved numerically in the code, and the value obtained for \( r \) is used to calculate the remaining properties \( \theta_{B_2}, \tan \theta_{u_2}, B_2, u_2, R \). A relativistic version of the jump conditions has been solved.
for by Summerlin & Baring (2012); the resulting polynomial for $r$ is seventh-order.

**A.2 Test Particle Trajectory**

Consider uniform, static electric and magnetic fields (constant in space and time) in some arbitrary configuration $\vec{E}, \vec{B}$. As long as $\vec{E} \cdot \vec{B} \neq (E^2 - B^2) \neq 0$, we can perform a Lorentz boost from this frame to a new frame such that the fields are parallel; $\vec{E}_\parallel \times \vec{B}_\parallel = 0$ (subscript $\parallel$ for parallel field frame vectors). This is encoded in the following equation due to Landau & Lifshits (1939):

$$\frac{\vec{\beta}}{1 + \beta^2} = \frac{\vec{E} \times \vec{B}}{E^2 + B^2}. \quad (A.13)$$

Of course, if $\vec{E} \times \vec{B} = 0$ were true already then we have no need to transform frames ($\vec{\beta} = 0$). This equation has one root satisfying $0 \leq \beta^2 < 1$:

$$\vec{\beta} = \frac{2\vec{E} \times \vec{B}}{E^2 + B^2 + \sqrt{(E^2 - B^2)^2 + 4|\vec{E} \cdot \vec{B}|^2}}. \quad (A.14)$$

The radical has been rewritten in terms of field invariants.\(^1\) Once in the parallel field frame we can also rotate such that the fields lie in the x-direction. The test particle trajectory in such a frame can be obtained exactly and is

\(^1(E^2 - B^2)^2 + 4|\vec{E} \cdot \vec{B}|^2 = (E^2 + B^2)^2 - 4|\vec{E} \times \vec{B}|^2\)
\[ \vec{r}(t) - \vec{r}_0 = \frac{c}{\omega} \left[ \sqrt{(\omega t + \psi)^2 + 1} - \sqrt{\psi^2 + 1} \right] \hat{x} \]  
(A.15)

\[ + r_g [\sin (\Omega(t) - \xi) + \sin \xi] \hat{y} \]

\[ + r_g [\cos (\Omega(t) - \xi) - \cos \xi] \hat{z}; \]

\[ \epsilon(t) = Mc^2 \sqrt{(\omega t + \psi)^2 + 1}; \]

\[ \vec{p}(t) = Mc (\omega t + \psi) \hat{x} \]

\[ + p_\perp \cos (\Omega(t) - \xi) \hat{y} \]

\[ - p_\perp \sin (\Omega(t) - \xi) \hat{z}. \]

The definitions of these terms are as follows: \( p_\parallel \), \( p_\perp \), and \( \xi \) come from a cylindrical decomposition of the initial momentum in this parallel, rotated frame; \( \vec{p}_0 = p_\parallel \hat{x} + p_\perp (\hat{y} \cos \xi + \hat{z} \sin \xi) \). The perpendicular momentum \( p_\perp \) is conserved; work is done only in the parallel direction. Due to this, the particle mass \( m \) and \( p_\perp \) appear together often, and we define \( Mc = \sqrt{p_\perp^2 + m^2 c^2} \) as a shorthand. The gyroradius, \( r_g = \frac{p_\perp c}{qB_\parallel} \), is well known. Note that \( \omega = \frac{qE_\parallel}{Mc} \) is not the Larmor frequency, but is instead related to the acceleration rate, and often appears with \( \psi = \frac{p_\parallel}{Mc} \). As a check, note that \( p_x(t) = p_\parallel + qE_\parallel t \), as it should. The most interesting term is perhaps \( \Omega(t) \), which describes the combination of electric acceleration and magnetic gyration on the perpendicular directions:

\[ \Omega(t) = \frac{\vec{E}_\parallel \cdot \vec{B}_\parallel}{E_\parallel^2} \left[ \sinh^{-1}(\omega t + \psi) - \sinh^{-1} \psi \right]. \]  
(A.16)
This is an exact, analytic, relativistic solution\(^\ddagger\). Note that when \(E_\parallel = 0\) this is a pure gyrohelix solution, and when \(B_\parallel = 0\) it is a pure electric acceleration solution.

### A.3 Probability of Return Calculation

We present results presented previously by Bell (1978) and later in Summerlin & Baring (2012) related probability-of-return calculations. The basic idea is that tracking particles directly when they are far enough downstream to be considered isotropized is a tremendous waste of CPU power. It’s much faster to calculate a probability of return based on the statistical properties of an isotropic flow. Consider a particle with momentum \((p_f/mc = \gamma_f\beta_f, p_s/mc = \gamma_s\beta_s)\) and angle cosine with respect to the shock normal \((\mu_f, \mu_s)\) in the (fluid, NIF) frame. The probability of return is nonzero only if the particle speed in the fluid frame is greater than the flow speed; it is:

\[
P_r = \left(\frac{\beta_f - \beta_s}{\beta_f + \beta_s}\right)^2.
\]

(A.17)

This probability expresses the ratio of number fluxes heading downstream to that heading upstream at a given detection plane. In the simulation, the boundary will be located downstream of the shock, and thus \(\beta = \beta_2\). Those particles which do not return are eliminated from the simulation. Those that return will have momentum vectors which obey the following angular distribution:

\[
\frac{dF}{d\mu_s} = C|\mu_s| \frac{(S + \mu_s\chi)^3}{S(1 - \beta^2\mu_s^2)^3},
\]

(A.18)

\(^\ddagger\)In the simulation, due to machine precision, we must also code the limiting cases and perform the limiting explicitly. In practice this is done by defining an effective tolerance (\(\sim 10^{-7}\)), and when the ratio of fields \((B_\parallel/E_\parallel\) or \(E_\parallel/B_\parallel\)) is less than this, we use the appropriate limiting case. This introduces a maximum range for this field ratio that the simulation will permit the full solution to be used in. In particular, when \(E_\parallel/B_\parallel < 10^{-7}\), the pure gyrohelix case will be used; this means the simulation cannot ‘feel’ electric fields past this ratio.
where \( C = \frac{2\gamma f^2 \beta_f^2}{\Gamma^6/(\beta_f - \beta)^2} \), \( S = \frac{\Gamma f}{\gamma f} \sqrt{1 - \chi^2(1 - \mu_s^2)} \), and \( \chi = \frac{\Gamma \beta}{\gamma f \beta_f} \). There is also a useful relationship between the two momenta:

\[
\frac{p_s}{p_f} = \frac{\gamma f S + \chi \mu_s}{\Gamma^2 (1 - \beta^2 \mu_s^2)}.
\]

Equations A.18 and A.19 are due to Summerlin & Baring (2012) (A7 and A3 in their paper, respectively).

In the simulation, a location sufficiently far downstream is selected, called the free escape boundary; it is here that the calculation takes place. A returning particle will have its \( \mu_s \) distributed according to (A.18), momentum \( p_s \) which obeys (A.19), and a phase around the shock normal distributed evenly on \([0, 2\pi]\). The \( x \) position is the location of the free escape boundary. The \((y,z)\) position is chosen to be the same as it was pre-crossing; the choice of \( y \) and \( z \) is irrelevant and does not introduce bias in the simulation.

### A.4 Screened Electrostatics

Poisson’s equation describes the electrostatic potential in terms of its source, charge density:

\[
\nabla^2 \Phi = -4\pi \rho.
\]

Consider a plasma where each species obeys Maxwell Boltzmann statistics:

\[
n_s = n_{0,s} \exp(-q_s \Phi/kT_s).
\]

We allow for the species to have different temperatures and densities (i.e., \( T_s = T_e \) or \( T_p \), and for a shock these differ upstream and downstream). For a plasma of electrons...
and protons, we have

\[ n_p = n_{0,p} \exp(-e\Phi/kT_p), \quad n_e = n_{0,e} \exp(e\Phi/kT_e), \quad \rho = e(n_p - n_e). \] (A.22)

This gives for Poisson’s equation:

\[ \nabla^2 \Phi = -4\pi e \left[ n_{0,p} \exp(-e\Phi/kT_p) - n_{0,e} \exp(e\Phi/kT_e) \right]. \] (A.23)

If we want the electric field to be zero everywhere, then \( \nabla \Phi = 0 \). We can set \( \Phi = 0 \) with electrostatic gauge freedom, and we see this forces \( n_{0,e} = n_{0,p} \) in the above equation. We would like to be as general as possible, so this assumption will not be made (yet). We look at the perturbation \( \Phi \rightarrow \Phi + \delta \Phi \) and \( \rho \rightarrow \rho + \delta \rho \). This gives

\[ \nabla^2 \Phi + \nabla^2 \delta \Phi = -4\pi \rho - 4\pi \delta \rho; \] (A.24)

\[ \nabla^2 \delta \Phi = -4\pi \delta \rho. \] (A.25)

The total perturbed charge density is written

\[ \delta \rho = \delta \rho_{ext} + e(\delta n_p - \delta n_e), \] (A.26)

where \( \rho_{ext} \) is an external charge density, provided by something besides the background plasma, and the other term gives the perturbation to the background plasma:

\[ n_s + \delta n_s = n_{0,s} \exp(-q_s(\Phi + \delta \Phi)/kT_s). \] (A.27)
This yields

\[ \delta n_s = n_{0,s} \left[ \exp(-q_s(\Phi + \delta\Phi)/kTs) - \exp(-q_s\Phi/kTs) \right] \]  \hspace{1cm} (A.28)

\[ = \frac{-q_s n_{0,s}}{kTs} \exp(-q_s\Phi/kTs) \delta\Phi + \cdots \]  \hspace{1cm} (A.29)

We assume the perturbation is small, i.e. \( \delta\Phi \ll kTs/q_s \), and keep only first order terms. This gives a quasi-linear approximation

\[ \nabla^2 \delta\Phi = -4\pi \left( \delta\rho_{ext} - e^2 \delta\Phi \left[ \frac{n_{0,p}}{kT_p} \exp(-e\Phi/kT_p) + \frac{n_{0,e}}{kT_e} \exp(e\Phi/kT_e) \right] \right). \]  \hspace{1cm} (A.30)

We can rewrite this as

\[ (\nabla^2 - \lambda^{-2})\delta\Phi = -4\pi \delta\rho_{ext}, \]  \hspace{1cm} (A.31)

where

\[ \lambda^{-2} = 4\pi e^2 \left[ \frac{n_{0,p}}{kT_p} \exp(-e\Phi/kT_p) + \frac{n_{0,e}}{kT_e} \exp(e\Phi/kT_e) \right]. \]  \hspace{1cm} (A.32)

Note we have imposed no restrictions on densities, temperatures, or the initial fields. In the usual calculation of Debye screening, we assume the plasma species are thermalized, so \( T_e = T_p = T \), and we assume the plasma is neutral and uniform, so \( n_{0,e} = n_{0,p} = n_0 = const. \) and \( \Phi = const. \) (set \( \Phi = 0 \) with gauge freedom). This gives

\[ \lambda^{-2} = 4\pi e^2 \left[ 2 \frac{n_0}{kT} \right] = \frac{2}{(\lambda_D)^2}, \quad \lambda = \frac{1}{\sqrt{2}} \sqrt{\frac{kT}{4\pi e^2}} = \frac{\lambda_D}{\sqrt{2}}, \]  \hspace{1cm} (A.33)

where we obtain an extra factor of \( 1/\sqrt{2} \) over the traditional Debye screening length \( \lambda_D = \sqrt{kT/4\pi e^2} \) because we allow the protons to participate in screening as well; calculations that lack this factor model the ion population as effectively immobile.
Let’s drop the δ-notation and the ext-subscript. So we have:

\[
\left( \nabla^2 - \frac{1}{\lambda^2} \right) \Phi(\vec{r}) = -4\pi \rho(\vec{r}).
\]  
(A.34)

Assume that density and potential depend only on x (planar symmetry), then

\[
\left( \frac{\partial^2}{\partial x^2} - \frac{1}{\lambda^2} \right) \Phi(x) = -4\pi \rho(x).
\]  
(A.35)

This captures the symmetry of our shock geometry. If we allow \( \lambda \) to be a function of \( x \) as well, the equation becomes more complicated. In the simulation, we need to use the solution for \( \lambda \to \lambda(x) \). This lends well to a numerical solution, and in the simulation we use the method described in Section 2.3 to obtain \( \Phi \).

In the rest of this section, we look at some analytic solutions to (A.35) in order to get a feel for the character of the solutions for the simpler, constant \( \lambda \) case. The usual intuition about electrostatics in the unscreened case is distorted in an interesting way.

We solve Eq. A.35 using the method of Green’s functions:

\[
\Phi(x) = 2\pi \lambda \int_{-\infty}^{+\infty} \rho(s) e^{-|x-s|/\lambda} ds.
\]  
(A.36)

Note we are more concerned with knowing \( \vec{E}(x) = E_x(x)\hat{x} = -(\partial \Phi/\partial x)\hat{x}; \)

\[
E_x(x) = -\frac{\partial \Phi(x)}{\partial x} = -2\pi \lambda \int_{-\infty}^{+\infty} \rho(s) \frac{\partial}{\partial x} \left( e^{-|x-s|/\lambda} \right) ds
\]
\[
= 2\pi \int_{-\infty}^{+\infty} \rho(s) \frac{x-s}{|x-s|} e^{-|x-s|/\lambda} ds.
\]  
(A.37)
In the limit of $\lambda \to \infty$ we obtain the original solution to the Poisson equation:

$$E_x(x) = 2\pi \int \rho(s) \frac{x - s}{|x - s|} ds. \quad (A.38)$$

We can use integration by parts to get another formula for the screened electric field. Note that $\partial / \partial x = d / dx$; it is the only variable. Also note $\partial \left( e^{-|x-s|/\lambda} \right) / \partial x = -\partial \left( e^{-|x-s|/\lambda} \right) / \partial s$. So, if we take $\partial / \partial s$ into a full derivative,

$$E_x(x) = 2\pi \lambda \int_{-\infty}^{+\infty} \rho(s) \frac{d}{ds} \left( e^{-|x-s|/\lambda} \right) ds$$

$$= 2\pi \lambda \left[ \rho(s) e^{-|x-s|/\lambda} \right]_{-\infty}^{+\infty} - 2\pi \lambda \int_{-\infty}^{+\infty} \frac{d\rho(s)}{ds} e^{-|x-s|/\lambda} ds \quad (A.39)$$

$$= -2\pi \lambda \int_{-\infty}^{+\infty} \frac{d\rho(s)}{ds} e^{-|x-s|/\lambda} ds.$$

This shows that, with screening, only gradients in charge density are important.

We now look at some specific examples of $\rho$. Consider a constant $\rho(x) = \rho_1$. In this case we have $E_x(x) = 0$. This makes sense when you imagine how only charge within roughly a Debye length is influencing any one value of $x$; a uniform charge density within that region would then produce fields that cancel. Now take a step function $\rho(x) = \rho_1 + (\rho_2 - \rho_1) \Theta(x)$. Here we have $E_x(x) = 2\pi \lambda (\rho_1 - \rho_2) e^{-|x|/\lambda}$. So only differences in density appear in screened fields. Next try a linear function $\rho(x) = \rho_1 + ax$. In this case, $E_x(x) = -4\pi \lambda^2 a$. So it takes a linear change in density to maintain a constant field.
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