Proton Acceleration in Colliding-Wind Binaries

Dissertation

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Preamble

This thesis was part of the PhD programme in physics of the University of Innsbruck. The work was supervised by Assoc. Prof. Dipl.-Phys. Dr. Anita Reimer, and Assoc. Prof. Dr. Ralf Kissmann.
List of papers being part of the thesis


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Abstract

The acceleration of a fraction of the thermal protons (ions) and electrons of the wind plasmas in colliding-wind binary (CWB) systems – binary systems of hot, massive stars with supersonic stellar winds – is expected to produce relativistic non-thermal populations of particles. At the position where the stellar winds collide, two collisionless shocks form, which are suitable sites for diffusive shock acceleration. The accelerated, non-thermal particles can then produce $\gamma$-rays, mainly via inverse Compton scattering from relativistic electrons in the stellar radiation field, or the decay of neutral pions produced in hadronic interactions (protons and ions). Despite decades of efforts, only two of such systems have been detected as sources of non-thermal $\gamma$-rays: $\eta$ Carinae and $\gamma^2$ Velorum. The non-detection of other colliding-wind binaries, despite the predictions of models for several systems, reveal that the processes of particle acceleration and the production of non-thermal radiation in those environments is not fully understood.

This thesis studies particle acceleration in colliding-wind binaries. For this purpose, a method has been developed, combining 3D magnetohydrodynamic numerical models of such systems, and Monte Carlo simulations of proton acceleration at collisionless shocks. The local nonlinear modification of the shocks delimiting the wind-collision region, caused by the backreaction of the accelerated protons, is modelled, also including magnetic field amplification due to resonant-streaming instability. The investigation presented in this thesis supports the hypothesis that the differences between the shock conditions at the two sides of the wind-collision region can result in differences between the spectra of the accelerated particles. Moreover, it suggests that previous models, which were not considering the backreaction of the non-thermal protons in the process of shock acceleration, may be overestimating the acceleration efficiencies in CWBs. The presented results also allow to formulate the hypothesis that magnetic field amplification may cause severe synchrotron energy losses of non-thermal electrons, preventing the efficient production of $\gamma$-rays via inverse Compton scattering. This effect may be one of the reasons for the elusiveness of CWB systems in the $\gamma$-ray band.
List of Abbreviations

CR Cosmic ray
CWB Colliding-wind binary
DSA Diffusive shock acceleration
HD Hydrodynamic
IC Inverse Compton
MFA Magnetic field amplification
MHD Magnetohydrodynamic
PIC Particle in cell
RSI Resonant-streaming instability
SC Superimposed cell
SNR Supernova remnant
WCR Wind-collision region
WR Wolf-Rayet
Chapter 1

Introduction

This thesis investigates colliding-wind binary (CWB) systems. More precisely, we are interested in modelling the acceleration of particles which form a non-thermal energy distribution in CWB systems. To this end, we have developed a code that combines three different numerical methods to catch different aspects of the system and of the acceleration process.

In this introduction, we will not give any details of the code or the simulations. Instead, we will describe CWBs and their components, and provide an overview of observations and of other works modelling these systems. We will also briefly summarize the predictions made by models of the fluxes of $\gamma$-rays produced by the interaction of the accelerated particles with the local environment. This summary will provide a clear motivation for the work presented in this thesis. The actual mechanism of particle acceleration expected to take place at CWBs will be treated in Chapter 2. There we will review the literature on the subject, which constitutes the foundation of this work, as well as several methods for the study of particle acceleration at collisionless shocks. The model developed for this PhD project will be described in Chapter 3 and the results will be presented in Chapter 4. The latter also delineates the path followed in the project, providing the motivations for the single steps taken. Finally, Chapter 5 is devoted to the conclusions and an outlook concerning possible future research directions to be undertaken.

1.1 Colliding-wind binary systems

Colliding-wind binary systems consist of two hot, massive stars, gravitationally bound to one another, which generate supersonic stellar winds. The stellar winds are composed of a plasma of electrons and ions flowing outwards from the stellar surfaces. Depending on the type of the star, the ratio of ions of different elements in the wind can vary, as well as the physical mechanisms accelerating them up to the so-called terminal velocity (see, e.g., Lamers and Cassinelli (1999)). In a CWB, the winds of the two stars eventually reach each other, forming the so-called wind-collision region (WCR), which is a three-dimensional, bow-shaped region of denser and hotter plasma delimited by two shock fronts. This is schematically represented in Figure 1.1.

The location of the WCR can be estimated by computing the position where the ram pressures of the two winds are equal. Let us put the two stars on the $x$-axis, at a distance $d_{12}$ from each other, and let us find the distance $x_1$ of the WCR from star 1, and the distance $x_2$ from star
2 (see Figure 1.1). Assuming an isotropic outflow of the winds from the stars, the density at a distance $x_i$ from star $i$ is given by $\rho_i = \dot{M}_i/(4\pi x_i^2 v_i)$, where $\dot{M}_i$ is the mass-loss rate, and $v_i$ is the wind velocity. Assuming that the stellar wind has reached its terminal velocity, $v_{\infty,i}$, its ram pressure is given by $\rho_i v_{\infty,i}^2$. Solving the simple system of equations:

\[
\begin{cases}
\rho_1 v_{\infty,1}^2 = \rho_2 v_{\infty,2}^2 \\
d_{12} = x_1 + x_2
\end{cases}
\]

yields the solutions:

\[
x_1 = \frac{\sqrt{\eta_{12}} d_{12}}{1 + \sqrt{\eta_{12}}}, \quad x_2 = \frac{d_{12}}{1 + \sqrt{\eta_{12}}},
\]

with $\eta_{12} = \dot{M}_1 v_{\infty,1}/(\dot{M}_2 v_{\infty,2})$. Hydrodynamic (HD) and magnetohydrodynamic (MHD) simulations yield more detailed information concerning position, width, and actual shape of the WCR. However, the crude analytic model works as a fairly good approximation, and has been used in several studies (e.g. Reimer et al. (2006), Reimer and Reimer (2009), Eichler and Usov (1993), Benaglia and Romero (2003)).

Early observations of CWBs showed a thermal X-ray component, which can be associated with the hot, shocked plasma in the WCR (Moffat et al., 1982; Pollock, 1987; Usov, 1992). In addition, some of those systems showed a non-thermal radio component (Abbott et al., 1984, 1985; Williams et al., 1990). This led Eichler and Usov (1993) to develop a model in which a non-thermal distribution of accelerated electrons is produced at the shock fronts of the WCR.

![Figure 1.1: Schematic representation of a colliding-wind binary system. The stellar wind of Star 1 has not been depicted for display convenience.](image-url)
In fact, they noticed that such environments should provide suitable conditions for a fraction of the thermal particles to gain energy via first-order Fermi acceleration, also called diffusive shock acceleration (DSA).\footnote{The details of the process are reviewed in Chapter 2.} In their model, the electrons, accelerated to relativistic energies, emit the detected non-thermal synchrotron radiation by spiralling along the local magnetic field lines. In this picture, electrons, protons and ions are accelerated, forming a non-thermal tail towards high energies of the respective spectral energy distributions. More recent observations have confirmed the presence of non-thermal radio synchrotron radiation from many CWBs (e.g. Chapman et al. (1999); Dougherty et al. (2005); Williams et al. (1997)).

Observations of CWBs in the $\gamma$-ray band would provide strong supporting evidence for this hypothesis. The accelerated electrons and protons are expected to interact with the ambient photon field or matter, and produce $\gamma$-rays, via inverse Compton (IC) scattering, relativistic bremsstrahlung (for electrons), or the decay of neutral pions produced in hadronic interactions (e.g. proton-proton collisions). The great advantage of the detection of photons, as compared to the possible direct detection of the accelerated charged particles, lies in the fact that they are not deflected by the Galactic magnetic field. Therefore, they point directly towards the source of their emission, which is expected to coincide with, or be close to, the particle-acceleration site.

Unfortunately, and contrary to the expectations (see Section 1.3), the analysis of 24 months of Fermi LAT data by Werner et al. (2013) did not provide any evidence for $\gamma$-ray emission which could be related with WR 11, WR 70, WR 125, WR 137, WR 140, WR 146, or WR 147. A catalogue of “particle-accelerating colliding-wind binaries” was compiled by De Becker and Raucq (2013) (also including the above cited results of Werner et al. (2013)). The authors listed 43 confirmed or strongly suspected binary (or multiple) systems, which presented non-thermal radiation associated with particles accelerated in the systems. Amongst them, only $\eta$ Carinae was seen as a $\gamma$-ray emitter. However, it was (and still is) not detected as a non-thermal radio emitter, as opposed to all other systems identified as particle-accelerating. The fascinating system of $\eta$ Carinae is very peculiar and complex. It is embedded in an expanding bipolar shell, the Homunculus Nebula (see Figure 1.2). This beautiful structure results from the so-called “Great Eruption”, which took place in the mid of the 19th century. Both the Homunculus Nebula and the CWB have been popular objects for observations (e.g. Davidson et al. (2001); Smith (2006); Weigelt et al. (2016), and references therein). The lack of radio emission is likely attributable to synchrotron self-absorption in the environment surrounding the CWB and its WCR. It is interesting to note that the $\gamma$-ray flux from $\eta$ Carinae shows a clear orbital modulation, which allows unambiguous identification of the source. Hints of phase-locked flux changes were found by Reitberger et al. (2012) and were confirmed by Reitberger et al. (2015) by analysing the Fermi LAT data over a full orbit. In the latter work, the authors, citing an idea of Farnier et al. (2011), claim that the most plausible cause for the orbital flux modulation is the presence of two different $\gamma$-ray components, one at energies up to $\approx 10$ GeV and another between $\approx 10$ GeV and $\approx 300$ GeV, possibly produced by different mechanisms (leptonic and hadronic). The hypothesis is based on the fact that the conditions (such as the particle and photon densities) at the WCR of a CWB vary, depending on the orbital phase. Therefore, the production of $\gamma$-rays via $\pi^0$ decay might be enhanced at periastron, due to the increased particle density, and in turn...
more frequent nucleon-nucleon collisions, resulting in the additional high energy component in the measured spectra.

In a more recent analysis of almost 7 years of Fermi LAT data, Pshirkov (2016) found evidence for a $\gamma$-ray source in spatial coincidence with $\gamma^2$ Velorum (WR 11). For this system, the flux is much lower and the author could not find any orbital periodicity.

This section surveyed the evidence supporting the claim that charged particles are accelerated to relativistic energies in CWBs. In the next section, we introduce the indispensable environment in the scenario of DSA, namely collisionless shocks.

![Figure 1.2: View of $\eta$ Carinae taken by the Wide Field and Planetary Camera 2 instrument of the Hubble Space Telescope. Credit: NASA, ESA, and the Hubble SM4 ERO Team.](image)

### 1.2 Collisionless shocks

A central role for particle acceleration in CWBs is played by collisionless shocks. Indeed, collisionless shocks are a necessary ingredient for the above-mentioned process of DSA to take place.

Shocks form in a variety of contexts, for example explosions, supersonic flight, and “Goasl-schnöllen” on Earth, as well as in many astrophysical objects and events, such as the solar wind (and, in general, stellar winds), jets of active galactic nuclei, gamma-ray bursts, supernova explosions, and, of course, colliding-wind binaries. A shock is, ideally, a discontinuity where a supersonic fluid is compressed, heated and slowed down to subsonic speeds.\(^2\) In the simplest configuration of a hydrodynamical shock, the fluid, described by its density, velocity and temperature, moves in the $x$-direction, perpendicular to the shock surface. The region where the fluid flows towards the shock is the upstream region, while the hotter and denser fluid leaving the shock defines the downstream region. A qualitative illustration of how the parameters of the fluid change is given in Figure 1.3. The conditions downstream are fully determined by the well

\(^2\)Microphysically, the shock is not a sharp discontinuity, but rather a (thin) transition layer.
known Rankine-Hugoniot relations, which are derived from the equations for mass, momentum and energy flux conservation across the shock surface. More general solutions are obtained by also considering the electromagnetic fields, and for configurations where the fluid velocity and the magnetic field lines are not necessarily parallel to the shock normal (i.e. the normal to the shock surface). These are given in Chapter 2, and we will not discuss them further in this introduction. Instead, we want to focus on the definition of collisionless – as opposed to collisional – shocks, and on the key difference between them which allows particle acceleration.

In collisional shocks (the kind of shocks that form, for example, in the Earth’s atmosphere), the width of the shock transition is on the order of a few collision mean free paths. In collisionless shocks, the shock transition is much smaller than the particle collisional (Coulomb) mean free path. The charged particles in a collisionless shock are not scattered by collisions with each other, but rather by electromagnetic turbulences in the plasma. The detailed mechanism of shock formation is currently a research topic, but the MHD equations and jump conditions for describing collisionless shocks are commonly employed (see Bret (2015) for a review focussed on the collisional behaviour of collisionless plasmas at shocks). However, as a consequence of the fact that the collisions between the particles are not the dominant scattering mechanism, the thermalisation process is not as efficient as in collisional plasmas. In other words, if a fraction of the thermal particles is accelerated by some mechanism (e.g., by means of the Fermi process, described in Chapter 2), the collisions with the other plasma particles are not sufficient to efficiently recover a Maxwell-Boltzmann distribution. This provides a necessary condition for the development of a non-thermal tail in the particle spectra.

It is enlightening to verify that typical shocks in CWBs are indeed collisionless, and therefore, in the presence of efficient scattering in the plasma flows, can accelerate particles. The Coulomb mean free path is given by

$$\lambda_{\text{mfp}}^C = \frac{1}{n\sigma^*},$$

(1.3)

where $n$ is the target particle density, and the cross section for Coulomb collisions of a test particle in a plasma can be written as (e.g. Bellan (2008)):

$$\sigma^* = \frac{1}{2\pi} \left( \frac{q_t q_b}{\varepsilon_0 \mu v_0^2} \right)^2 \lambda,$$

(1.4)

where $q_t$ is the charge of the test particle, $q_b$ that of the background plasma particle, $\varepsilon_0$ is the vacuum permittivity, $\mu$ is the reduced mass of the two colliding particles, $v_0$ is the initial relative velocity between them, and $\lambda$ is the Coulomb logarithm. Considering collisions between protons upstream and downstream of a shock, with parameters typical for CWBs, i.e. with the bulk-flow velocity $v_0 = 10^6$ m s$^{-1}$, $\lambda \approx 20$, and $n = 10^{13}$ m$^{-3}$, the mean free path is $\lambda_{\text{mfp}}^C \approx 3 \times 10^9$ m. The commonly used mean free path for scattering off electromagnetic waves in the Bohm limit is (see also next chapter for more details):

$$\lambda_{\text{mfp}}^B = \frac{p_t}{q_t B},$$

(1.5)

where $p_t$ is the momentum of the test particle and $B$ is the magnetic field. At the shocks of CWBs the magnetic field is expected to be $\gtrsim 10^{-9}$ T, so that the mean free path is
λ_{\text{mfp}}^B \lesssim 10^7 \text{ m} \ll \lambda_{\text{mfp}}^C \text{, confirming that typical shocks in CWB systems are collisionless.}

For the sake of completeness, we note that the expected magnetic field in CWBs has been derived in the literature either by using the upper limit of 100 G for the surface magnetic fields of specific B and Wolf-Rayet (WR) stars (e.g. Barker (1986) and references therein), combined with numerical MHD models of CWB systems (e.g. Reitberger et al. (2017)), or by assuming equipartition between the magnetic field energy density and the energy density of the accelerated particles, at the WCR (e.g. Benaglia and Romero (2003)). We are not aware of any quantitative detection or measurement of magnetic fields in CWBs. However, Neiner et al. (2015) provided upper limits for the surface magnetic fields of the stars of nine CWB systems, ranging from \approx 180 \text{ G} \text{ to } \approx 4400 \text{ G}, which is consistent with the estimate for the lower limit of the magnetic field at the WCR used in this section.

Figure 1.3: Sketch of a shock and of the qualitative change in the hydrodynamical quantities. The shock is located at the centre, coincident with the dashed line. The height of the lines indicates the magnitude of the variable. \(T\) represents the temperature, \(\rho\) is the density, and \(u\) is the velocity of the fluid.

1.3 Models of colliding-wind binaries

In several works CWBs have been modelled and simulated. In some cases, the goal was to shed light on the 3D hydrodynamical structure of the WCR in CWBs (e.g. Lamberts et al. (2011, 2012)). In other works, the three-dimensional HD simulations where used to model the thermal (radio and/or X-ray) emission of the stellar winds and the shocked plasma in the WCR (Madura et al., 2013; Parkin et al., 2010; Pittard, 2009, 2010; Pittard and Parkin, 2010).

The non-thermal emissions from CWBs have also been investigated (Balbo and Walter, 2017; Benaglia and Romero, 2003; del Palacio et al., 2016; Eichler and Usov, 1993; Falceta-Gonçalves and Abraham, 2012; Pittard and Dougherty, 2006; Pittard et al., 2006; Reimer et al., 2006; Reitberger et al., 2014a,b, 2017). In the following, we will review some of these investigations, allowing the reader to get an idea of what approximations have been typically used in those studies. The approaches can be roughly divided into analytical, semi-analytical, and numerical.

Analytical and semi-analytical models rely necessarily on a plethora of approximations, concerning the geometry of the system, as well as the strength and topology of the magnetic field, and the particle-acceleration process itself. In their first study of particle acceleration in CWBs,
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Eichler and Usov (1993) first considered a generic system of a WR star and an OB star, showing that in such a system the necessary conditions for particle acceleration are typically fulfilled. The position of the WCR was estimated by means of Eq. (1.2), while for the magnetic field, the authors used the following approximation, which we specify here for later reference:

\[
B(r) \approx B_\ast \times \begin{cases} 
\left(\frac{R}{r}\right)^3 & \text{for } R \leq r < r_A \text{ (dipole)}, \\
\frac{R^4}{r_A^2 \mu_0^2} & \text{for } r_A \leq r < \frac{v_\gamma}{v_{\text{rot}}} \text{ (radial)}, \\
\left(\frac{R}{r}\right)^3 & \text{for } R \frac{v_\gamma}{v_{\text{rot}}} \leq r \text{ (toroidal)}. 
\end{cases}
\] (1.6)

Herein, \(R\) is the stellar radius, \(B_\ast\) its surface magnetic field, \(v_{\text{rot}}\) the stellar rotational velocity (assumed to be \(v_{\text{rot}} = 0.1 \, v_\infty\)), and the Alfvén radius \(r_A\) is given by the solution to\(^3\)

\[
1 - \frac{R}{r_A} = \frac{4\pi B_\ast^2 R^2}{\mu_0 M v_\infty^2} \left(\frac{R}{r_A}\right)^4,
\] (1.7)

where \(\mu_0\) is the permeability of free space and \(\dot{M}\) is the mass loss rate of the star. They then estimated the radio and \(\gamma\)-ray emission due to the accelerated electrons, predicting that the space telescope EGRET could not only detect \(\gamma\)-ray emission from WR 140, but also measure its orbital modulation, and be able to discriminate between the contributions from IC scattering and pion decay. Later observations of WR 140 close to periastron did not detect the system. Mücke and Pohl (2002) proposed that the non-detection could be interpreted as an effect of the anisotropy of the IC scattering, combined with the geometrical orientation of the system. They expected Fermi LAT to provide a possible confirmation to this hypothesis.

Benaglia and Romero (2003) considered the three binary systems WR 140, WR 146, and WR 147. Like in the above-cited studies, the distance of the WCR from the stars was estimated with the aid of Eq. (1.2). The magnetic field strength at the WCR was estimated from radio observations, assuming equipartition between the magnetic field energy density and the energy density of the accelerated particles (see Benaglia and Romero (2003) and references therein for further details). The obtained magnetic field value was then compared to the value calculated with Eq. (1.6), assuming the surface magnetic field of the stars to be within the range allowed by dedicated studies (e.g. Ignace et al. (1998); Maheswaran and Cassinelli (1994)).

For WR 140, which was expected to be detectable with Fermi LAT, they claimed a possible association with the EGRET source 3EG J2022+4317. For WR 146 and WR 147, on the other hand, they estimated fluxes below the detection threshold of EGRET, but possibly high enough to allow detection with INTEGRAL and Fermi LAT.

A more sophisticated model was developed by Reimer et al. (2006). The authors performed a first attempt to consider the geometry of the WCR when calculating the high-energy emission from CWBs. The shock acceleration and energy losses (synchrotron, IC, bremsstrahlung, and

\(^3\)This equation follows from requiring the Alfvén Mach number, defined in the next chapter, to be one, while assuming an isotropic wind and a wind velocity given by \(v(r) = v_\infty(1 - R/r)\), and using Eq. (1.6) for the magnetic field.
Coulomb losses) for both electrons and protons (ions) were considered using the transport equation for energetic particles (see Reimer et al. (2006) for further details concerning the transport equation and the individual terms used). The WCR was divided into a cylinder and a coaxial disk, with inner boundary coincident with the outer boundary of the cylinder, and with the axis coincident with the imaginary line connecting the two stars of the binary system (see Figure 1.4). The internal cylinder was the “acceleration zone”. There, the particles were accelerated and produced radiation. The particles were allowed to leave the acceleration zone by diffusion, entering the outer disk, which they named the “convection zone”. Here, they could not gain further energy, but they were assumed to still emit radiation (and lose energy), by means of IC scattering, relativistic bremsstrahlung, and neutral pion decay. From the convection zone, the particles were finally advected out of the extended emission site. The distance of the WCR from the stars was estimated by means of Eq. (1.2). Only the dominant magnetic field was considered at the WCR, assuming \( B = 100 \text{ G} \) for both stars and, again, using the approximation of Eq. (1.6). The authors applied the model to WR 140 and WR 147, using the observed parameters of these binary systems, and concluded that both would be detectable by Fermi LAT. Moreover, WR 147 was predicted to be possibly detectable by other instruments, such as MAGIC, VERITAS, and HESS, at least for a favourable range of orbital phases.

Pittard et al. (2006) and Pittard and Dougherty (2006) used 2D axisymmetric HD simulations for modelling the geometry of the WCR. They assumed a power-law dependence on the particle momentum \( p \) for the distribution of the relativistic particles at the shocks, i.e. \( n(p) \propto p^{-\sigma} \), and, including IC cooling, calculated the spectrum at each cell in the WCR.\(^4\) The magnetic field strength was assumed to be proportional to the thermal energy density of the plasma

\[
U_{\text{th}} = \frac{n k_B T}{\gamma - 1},
\]

where, \( n \) is the particle number density of the plasma, \( T \) is its temperature, \( \gamma = 5/3 \) is the

---

\(^4\)As shown in Section 2.1, the non-thermal distribution of particles accelerated via DSA, in the test-particle approach, has the form of a simple power-law.
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adiabatic index, and $k_B$ denotes the Boltzmann constant. The model was applied to WR 147 in Pittard et al. (2006), where only the radio emission was considered, and to WR 140 in Pittard and Dougherty (2006), where also estimations of the $\gamma$-ray fluxes have been given. In particular, the authors expected WR 140 to be detected by Fermi LAT after a 2 years all-sky survey. Interestingly, Pittard et al. (2006) also discussed the possibility of shock modification caused by the non-thermal particles. Their fits to the radio observations, consistent with their models, yielded best results with a hard spectral index $\sigma = 1.4$. This was proposed to be a possible consequence of shock modification at the WCR. Pittard and Dougherty (2006) noted, however, that the shock modification affecting the acceleration of electrons and the radio emission in the observed energy range would most likely produce a softer non-thermal distribution, and concluded that other processes were probably the cause for the hardness of the spectrum.

To date, the method developed by Reitberger et al. (2014a,b), and recently improved and applied to $\gamma^2$ Velorum (Reitberger et al., 2017), provides undoubtedly one of the most realistic models of particle acceleration and non-thermal emission from CWBs. It combines MHD simulations of the system to be studied with the solution of the transport equation for non-thermal electrons and protons. The MHD simulations include line-driven acceleration of the stellar winds (Lamers and Cassinelli, 1999), the gravitational attraction of the stars, and a consistent interaction between their winds and their magnetic fields (see also Kissmann et al. (2016) and Section 3.1). The most recent model also includes radiative braking of the stellar winds due to the radiation field of the companion stars. Concerning this aspect, it is interesting to mention that the shape of the WCR for $\gamma^2$ Velorum obtained including radiative braking is clearly closer to what was observed in the X-ray band (Henley et al., 2005) than in previous models (see Figure 1.5). The transport equation for the accelerated particles also includes, besides advection, diffusion, adiabatic cooling, and acceleration, energy losses due to IC synchrotron and bremsstrahlung emission, as well as losses by Coulomb scattering and inelastic nucleon-nucleon collisions. The obtained distributions of electrons and protons are used for computing the non-thermal $\gamma$-ray emission from the system. The results suggest that the detected $\gamma$-rays are likely of hadronic origin ($\pi^0$ decay). In fact, efficient $\gamma$-ray production via IC scattering is inhibited by the strong IC losses of electrons in the stellar radiation fields already, which lower the maximal energy the electrons can reach. In a short discussion, also considering the flux in the radio band, Reitberger et al. (2017) further claim that lower IC losses and higher magnetic fields at the WCR, and in turn higher synchrotron losses, could produce non-thermal fluxes consistent with the observations.

A similar approach has been adopted by Balbo and Walter (2017), who employed the HD simulations of $\eta$ Carinae by Parkin et al. (2011). They determine the maximal energy reachable by the particles in each cell of the simulation, based on the strength of the local magnetic field, assumed to be a dipole generated by the most massive star. From this, they obtain the $\gamma$-ray emission and compare it to the observations of the Fermi LAT, to find a good match for a surface magnetic field of the star of 500 G. Despite the interesting results presented, that work still suffers from some of the limitations of previous studies: a prescription is needed for both the magnetic field at the WCR and the injection efficiency, i.e. the fraction of thermal

---

5The test-particle result yields $\sigma \geq 2$, and $\sigma = 2$ is the result for strong shocks (see Section 2.1).

6This lies within the range of possible magnetic field strengths given by Walder et al. (2012).
Figure 1.5: Flow velocities of $\gamma^2$ Velorum as modelled by Reitberger et al. (2017). The opening half-angle of the shock-cone for “method A” (without radiative braking) is $\theta \approx 24^\circ$ while it is $\theta \approx 72^\circ$ for “method B” (including radiative braking). The observed value is $\theta \approx 85^\circ$. Figure adapted from Reitberger et al. (2017).

particles which get accelerated, although the authors do not provide details concerning the latter.

Some further comments are in order. As far as the magnetic field is concerned, the study of Kissmann et al. (2016) showed that magnetic fields on the order of magnitude of $\approx 100$ G can play a crucial role on the acceleration and maximal velocities reached by the stellar winds, which in turn has an effect on the shape of the WCR. This highlights the importance of a realistic model of CWBs, including the effect of the large-scale magnetic fields.

Another remark regards the injection efficiency, which is a key component of the models including particle acceleration. In the vast majority of models of CWBs, the injection efficiency is parametrized by an “injection parameter”. The injection efficiency is commonly set “by hand”, either to values which, being within a reasonable range, allow to fit the observational data, or to values which ensure that the energy density and the momentum flux of the cosmic rays (CRs) are negligible compared to those of the background plasma. In fact, the injection efficiency does not only control the strength of the non-thermal radiation from CWBs, directly affecting the densities of the accelerated particles. It also determines (and its determined by) the dynamical importance of the accelerated particles for the shock structure. The nonlinear backreaction in the case of efficient acceleration at collisionless shocks has been studied mainly in the context

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7Here and in the following, we use “cosmic rays” as synonym for “accelerated particles”.
8In some studies, focused on providing prediction of fluxes from still undetected CWBs, the injection efficiency has been used for parametrizing the results (e.g. Reimer et al. (2006)).
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of supernova remnants. A selection of works will be briefly reviewed in Sections 2.2 and 2.2.1.

From the review above, it is apparent that CWBs can accelerate electrons to relativistic energies, and that protons might be the dominant parent population of particles producing $\gamma$-rays (due to $\pi^0$ production and subsequent decay). Mainly thanks to HD and MHD simulations of the considered systems, the models of particle acceleration at CWBs have become more and more realistic over the years. Nevertheless, in all of the methods used for modelling the acceleration of particles and the production of non-thermal radiation in CWBs, the rate at which particles are injected into the acceleration process is determined by an “injection parameter”. Such an approach is certainly useful for understanding which configurations of the system are more favourable for efficient $\gamma$-ray production, or which component (hadronic or leptonic) is most likely responsible for the detected emission. However, the open question of what is the reason for the lack of detection of non-thermal high-energy emission from most CWBs is left unsolved. In particular, it cannot be inferred if and how this is connected with the injection and the acceleration efficiency. Moreover, in the approaches used to study CWBs, the backreaction of the accelerated particles on the winds and on the WCR is completely neglected. Keeping this in mind, we will review in the next section the basics of particle acceleration at nonrelativistic, collisionless shocks, initially neglecting and then including the backreaction of the accelerated particles (in particular protons) on the background plasma at the shock.
Chapter 2

Particle acceleration at nonrelativistic shocks

In the previous chapter we have mentioned that DSA is thought to be taking place at the shocks of the WCR of CWBs. In this chapter, we will describe in more detail the mechanism of DSA. In doing so, we will provide the theoretical background needed for a comprehension of the phenomenon, together with the fundamental equations, which will be also referred to in the next chapters. In Section 2.1 we consider the case neglecting the backreaction of the CRs on the background plasma, while in Section 2.2 we review the main features of nonlinear DSA. Similarly to what has been done in the previous chapter concerning CWBs, we also review a selection of numerical approaches used for modelling nonlinear Fermi acceleration.

2.1 First order test-particle Fermi acceleration

The first analytical works concerning particle acceleration at shock fronts date back to the late 1970s. In fact, within a couple of years, several scientific articles were published aiming at developing a theory which could explain the origin and the acceleration processes of the cosmic rays detected at the Earth (e.g. Axford et al. (1977); Krymskii (1977); Bell (1978)). Two different approaches were employed, leading to the same results. It is worth to briefly introduce both of them, in order to better understand the robustness of the result, keeping in mind, however, that the accelerated particles are assumed to have no influence on the background plasma.

2.1.1 Microscopic approach

Following Bell (1978), let us consider an infinite one-dimensional space, with a parallel shock placed at the coordinate \( x = 0 \) in the shock frame, i.e. the reference frame where the shock is at rest. Choosing \( u > 0 \), the region where \( x < 0 \) (\( x > 0 \)) is upstream (downstream) of the shock. We make use of the transport equation for particles in a small energy range, which is given by:

\[
\frac{\partial n(t, x)}{\partial t} + u \frac{\partial n(t, x)}{\partial x} = \frac{\partial}{\partial x} \left[ D(x) \frac{\partial n(t, x)}{\partial x} \right],
\]

(2.1)
where \( n(t, x) \) is the particle density, \( D(x) \) is the spatial diffusion coefficient, and \( u \) is the speed of the plasma flow.

In the steady-state scenario, Equation (2.1) can be integrated upstream or downstream to give:

\[
 n(t, x) = A + B \exp \left[ \int_0^x \frac{u}{D(x')} dx' \right]. 
\]

(2.2)

Under the condition

\[
 \int_0^x \left[ \frac{1}{D(x')} \right] dx' \to \pm \infty \quad \text{for} \quad x \to \pm \infty ,
\]

(2.3)

which is a reasonable assumption, in order to obtain a finite solution one needs \( B = 0 \) for the downstream region. Therefore,

\[
 n(x) = n(0) = \text{const} 
\]

(2.4)
downstream of the shock. The flow of particles advected away from the shock, downstream, is thus \( u_2 n(0) \), where the subscript \( 2 \) indicates the downstream region. Assuming an isotropic distribution of velocities, the total flux of the upstream particles with speed \( v \) crossing the shock can be calculated to be \( \frac{1}{4} n(0) v \) (half of the particles have positive velocities, and the average particle speed in the \( x \)-direction is \( v_x = 1/2 \)). By dividing the flux of particles advected downstream by the total flux through the shock (in the given, small energy range), one obtains the probability for a particle crossing the shock to leave the system downstream:

\[
 \eta = \frac{4u_2}{v} .
\]

(2.5)

This corresponds to a probability of completing a cycle from upstream to downstream and back of:

\[
 P = 1 - \frac{4u_2}{v} .
\]

(2.5)

The (isotropic) scattering of charged particles due to Alfvén waves (i.e. the scattering centres) is elastic in the reference frame of the waves. For the sake of simplicity, we assume that the scattering centres move with the velocity of the plasma (corresponding to a high Alfvén Mach number).

\[
 \text{Let us consider a particle crossing the shock from upstream to downstream with energy } E_k, \text{ and returning upstream after scattering in the downstream region. The energy of the particle can be derived by performing the Lorentz transformations between the local reference frames (upstream and downstream), and by making use of the conservation of the particle energy at the scattering events in the local flow frames:}
\]

\[
 E_{k+1} = E_k \left( \frac{1 + v_{k0}(u_0 - u_2)}{1 + v_{k2}(u_0 - u_2)} \cos \theta_{k0}/c^2 \right) .
\]

(2.6)

Herein, \( c \) denotes the speed of light, \( u_0 \) is the flow velocity in the upstream region, while \( v_{k0} \) and \( v_{k2} \) are the velocities of the particle crossing the shock from upstream to downstream, and

\[1\text{A non-negligible difference between the plasma flow velocity of the scattering centres, as seen from the shock frame, could change the velocity difference between the upstream and downstream local frames (or introduce a contribution from second order Fermi acceleration), but it would not affect the validity of the result.}\]
from downstream to upstream, respectively, making the corresponding angles \( \theta_{k0} \) and \( \theta_{k2} \) with the shock normal. The quantities \( v_{k0}, v_{k2}, \theta_{k0}, \) and \( \theta_{k2} \) are all measured in the upstream flow frame. If one considers a particle with energy \( E_i \) such that its speed is \( v \approx c \), the energy gained by the particle after a significant number of cycles \( l \) is given, on average, by:

\[
\ln \left( \frac{E_l}{E_i} \right) = \frac{4}{3} \ln \left( \frac{u_0 - u_2}{c} \right) \left[ 1 + \mathcal{O} \left( \frac{u_0 - u_2}{c} \right) \right].
\]  (2.7)

Furthermore, for the probability of a particle to do \( l \) cycles, recalling Equation (2.5), we can write:

\[
\ln P_l = l \ln \left( 1 - \frac{4u_2}{c} \right) = - \left[ \frac{3u_2}{u_0 - u_2} + \mathcal{O} \left( \frac{u_0 - u_2}{c} \right) \right] \ln \left( \frac{E_l}{E_i} \right),
\]  (2.8)

where in the last step, we employed Equation (2.7). If \( N_i \) particles are injected with energy \( E_i \), the number of particles completing \( l \) cycles and reaching an energy \( E_l \) will be (neglecting the term \( \mathcal{O}[(u_0 - u_2)/c] \) in Eq. (2.8)):

\[
N_l = P_l N_i = N_i \left( \frac{E_i}{E_l} \right)^{-\frac{3u_2}{u_0 - u_2}}. 
\]  (2.9)

Therefore, the differential energy spectrum assumes the form of a power-law:

\[
N(E)dE \propto E^{-\sigma}dE,
\]  (2.10)

where

\[
\sigma = \frac{2u_2 + u_0}{u_0 - u_2} + \mathcal{O} \left( \frac{u_0 - u_2}{c} \right) = \frac{r + 2}{r - 1}. 
\]  (2.11)

In the last step we employed the definition of the compression ratio \( r = u_0/u_2 \), and the approximation \( \mathcal{O}[(u_0 - u_2)/c] = 0 \). As a result, for example, for a strong shock with \( r = 4 \), the differential energy spectrum has a spectral index \( \sigma = 2 \). The same result can be obtained with a macroscopic approach, which is outlined in the next section.

### 2.1.2 Macroscopic approach

Also here, we consider parallel shocks of infinite extent. Following Drury (1983), we write the transport (diffusion-convection) equation for the isotropic part of the distribution function \( f(t, x, p) \) in the local plasma frame:

\[
\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = \frac{\partial}{\partial x} \left( D \frac{\partial f}{\partial x} \right) + \frac{1}{3} \frac{\partial u}{\partial x} \frac{\partial f}{\partial p} + \frac{1}{p^2} \frac{\partial}{\partial p} \left( p^2 \kappa \frac{\partial f}{\partial p} \right).
\]  (2.12)

Herein, \( u \) is the background flow velocity, \( D(x, p) \) is the diffusion coefficient in space, and \( \kappa \) is the diffusion coefficient in momentum space. The second term on the left-hand side represents advection of particles by the background flow. On the right-hand side, the first term represents diffusion in space, the second term represents adiabatic heating or cooling, and the last term represents diffusion in momentum space due to the random velocities of the scattering centres.
The latter is, in fact, the second-order acceleration mechanism originally proposed by Fermi (1949). At strong shocks, this second-order process is usually negligible as compared to the first-order acceleration. Let us therefore consider the equation without diffusion in momentum space. Then, on either side of the shock, where \( \partial u / \partial x = 0 \), the steady-state equation to be solved is:

\[
\frac{u_i}{\partial x} \frac{\partial f(x, p)}{\partial x} = \partial f(x, p) \left( \frac{\partial f(x, p)}{\partial x} \right),
\]

where the index \( i \) takes the value 0 for \( x < 0 \) (upstream) and 2 for \( x \geq 0 \) (downstream).

Using again the condition (2.3), together with \( f(x, p) \to f_0(p) \) for \( x \to -\infty \), and \( f(x, p) \) finite downstream, one can find the solution:

\[
f(x, p) = \begin{cases} 
  f_0(p) + g_0(p) \exp \int_0^x \frac{u_x}{B_x} dx' & \text{if } x < 0, \\
  g_2(p) = f_2(p) & \text{if } x \geq 0.
\end{cases}
\]

An equation relating the generally arbitrary function \( g_0(p) \) with \( f_0 \) and \( f_2 \) can be found by assuming that the density jump of the background thermal plasma does not affect the particle distribution of the energetic particles. This gives

\[
f_0(p) + g_0(p) = f_2(p).
\]

At this point, Drury (1983) considers the full distribution \( F(x, p, \mu) \) (\( \mu \) is the cosine of the pitch angle) and equates also the anisotropic part of the distribution, proportional to \( \partial f / \partial x \). Also employing Eq. (2.15), the resulting differential equation is:

\[
(r - 1) \frac{\partial f_2}{\partial p} = 3r(f_0 - f_2),
\]

with solution

\[
f_2(p) = a p^{-a} \int_0^p p'^{a-1} f_0(p') dp' + b p^{-a},
\]

where

\[
a = 3r/(r - 1)
\]

and \( b \) is an integration constant. Following Jones and Ellison (1991), we set \( b = 0 \) in order to allow normalization, since there is no low-energy cutoff for the homogeneous term. Assuming that \( f_0(p) \propto p^{-a+\delta} \) for \( p > p_0 \) and zero for \( p < p_0 \), \( p_0 \) being the “injection momentum”, from Equation 2.17, we obtain:

\[
f_2(p) \propto p^{-a} \left( \frac{p_0^\delta - p_0^\delta}{\delta} \right).
\]

In the case of injection of thermal particles,\(^3\) \( \delta < 0 \), \( f_0(p) \) is steeper than \( p^{-a} \). The term \( p_0^\delta \) at the numerator in Equation (2.19) dominates, and the distribution function is:

\[
f_2(p) \propto p^{-a}.
\]

\(^2\)For the details of the derivation we refer the reader to Drury (1983).

\(^3\)In the thermal leakage model, the injection momentum \( p_0 \) is a multiple of the “thermal momentum” \( p_{\text{th}} = \sqrt{2mk_BT} \). Therefore, the distribution function (i.e. the Maxwell-Boltzmann distribution) is steeply decreasing with increasing momentum.
2.1. FIRST ORDER TEST-PARTICLE FERMI ACCELERATION

In order to better compare with the differential particle spectrum in Equation (2.10), we can exploit the isotropy of \( f(p) \), and integrate \( f_2 \) of Equation (2.20) to obtain the differential particle spectrum \( N_2(p) = 4\pi p^2 f_2(p) \):

\[
N_2(p)dp \propto 4\pi p^2 \rho^{-\alpha} dp \propto \rho^{-\alpha} dp,
\]

(2.21)

with \( \alpha = (r + 2)/(r - 1) \).

For later reference, we also define the differential flux of particles:

\[
J(p)dp = vN(p)dp \propto v \rho^{-\alpha} dp.
\]

(2.22)

In terms of the kinetic energy \( E \) this corresponds to:

\[
J(E)dE \propto (E^2 + 2E mc^2)^{-\alpha/2}dE.
\]

(2.23)

This means that \( J(E) \propto E^{-\alpha/2} \) in the nonrelativistic regime and \( J(E) \propto E^{-\alpha} \) in the relativistic regime.

The results shown above have been derived for parallel shocks. In the next section we provide the equations for oblique shocks relevant for the next chapters.

2.1.3 Acceleration at oblique shocks and further remarks

Here, we present the case of particle acceleration at oblique shocks, i.e. shocks with an inclined magnetic field with respect to the shock normal, which lies in the \( x \)-direction.

Considering shocks where the magnetic field and the flow velocity are parallel to each other, but not with respect to the shock normal, Bell (1978) showed that:

- the probability of return to the shock for a relativistic particle is given by

\[
P = 1 - 4\frac{u_{2x}}{c},
\]

(2.24)

where \( u_{2x} \) is the \( x \)-component of the plasma velocity, and \( c \) is the speed of light.

- also for oblique shocks, the spectral index of the non-thermal distribution of energetic particles depends on the compression ratio, as specified by Eq. (2.11).

In addition to what has been considered in the previous sections, in this more general configuration, we also provide the expression for the acceleration time, i.e. the time needed for a particle to reach a certain energy, which will constitute a reference for the validation of the code described in Chapter 3. Recall that all quantities vary only in the \( x \)-direction, and that the background fields are uniform in the upstream and downstream regions (but not at the shock discontinuity). The mean acceleration time to the momentum \( p \) is then given by (e.g. Drury (1983)):

\[
\tau_a(p) = \frac{3}{u_{0x} - u_{2x}} \int_{p_x}^{p} \left( \frac{D_0}{u_{0x}} + \frac{D_2}{u_{2x}} \right) \frac{dp'}{p'}.
\]

(2.25)

\(^4\)A vast range of shock configurations can be brought to this arrangement by means of a de Hoffmann-Teller transformation (de Hoffmann and Teller, 1950).
Herein, $p_i$ is the initial momentum of the particle, and $D_0$ and $D_2$ are the spatial diffusion coefficients in the $x$-direction (i.e. normal to the shock) for the upstream and downstream regions, respectively. These are given by (e.g. Jones and Ellison (1991)):

\[
D(x, p) = D_{\parallel}(x, p) \cos^2 \theta_B(x) + D_{\perp}(x, p) \sin^2 \theta_B(x),
\]

\[
D_{\parallel}(x, p) = \xi \frac{p}{qB(x)} \frac{v}{3},
\]

\[
D_{\perp}(x, p) = \frac{\xi}{(1 + \xi^2)} \frac{p}{qB(x)} \frac{v}{3},
\]

with $D_{\parallel}$ and $D_{\perp}$ being the diffusion coefficients parallel and perpendicular to the magnetic field lines, respectively. Here, $q$ is the charge of the particle, and the factor $\xi$ is a parameter relating the mean free path and the gyroradius of the particle:

\[
\lambda_{\text{mfp}} = \xi r_g,
\]

where the gyroradius is defined as $r_g = p/(qB)$.\(^5\)

This parametrization is a convenient choice, which “hides” (and simplifies) the microphysics of the interaction of particles and scattering centres into $\xi$. Eq. (2.26) is written with a general dependence on $x$, for later reference. In the particular case of uniform upstream and downstream regions, the angles $\theta_B(x)$ of the magnetic field with respect to the shock normal can be denoted by $\theta_{B0}$ and $\theta_{B2}$. Ellison et al. (1995) combined Eqs. (2.25) and (2.26), obtaining, for a given shock (expressed in terms of the kinetic energy $E$ of the particle):

\[
\tau_a(E) = \frac{\xi}{q B_0} \frac{E - E_i}{u_{0x} - u_{2x}} \left( \frac{1}{u_{0x}} \cos^2 \theta_{B0} + \frac{\sin^2 \theta_{B0}}{1 + \xi^2} \right) + \frac{1}{u_{2x}} \cos \theta_{B2} \left( \cos^2 \theta_{B2} + \frac{\sin^2 \theta_{B2}}{1 + \xi^2} \right).
\]

Concluding this section, we draw the attention of the reader to two important points. First, in both the microscopic and the macroscopic approaches, the results have been derived in the limit of particle velocities $v \gg u_x$. The energy range relevant for the injection of the thermal particles in the acceleration process is not included, and, therefore, no conclusion about the injection efficiency can be drawn.

Second, and partially connected with the first point, the treatments did not include any backreaction of the accelerated particles on the background plasma. In cases of efficient particle acceleration, this effect should be included in realistic models. This will be the subject of the next section.

### 2.2 Nonlinear Fermi acceleration

The possibility that the pressure of the accelerated particles at a shock could have an influence on the shock structure itself has been already noted in the first works modelling the actual

\(^5\)More correctly, if $\zeta$ is the angle between the momentum vector and the magnetic field, the gyroradius is $r_g = p \sin \zeta/(qB)$. However, in the literature of the field, the gyroradius is defined as a more general quantity, without the dependence on $\zeta$.\]
acceleration mechanism of particles at shocks (e.g. Axford et al. (1977, 1982), Eichler (1979), Achterberg et al. (1984)). For reviews concerning different aspects of nonlinear DSA, we refer the reader to, e.g., Bell (2013, 2014), or Malkov and Drury (2001). In this section, we will briefly review the main characteristics of a modified shock. The idea is that, if particle acceleration is sufficiently efficient, the momentum and energy fluxes of the high-energy particles streaming against the incoming plasma flow become non-negligible, when compared to the bulk flow momentum flux. As a result, a shock precursor forms, where the thermal plasma upstream of the shock is gradually slowed down before what is commonly defined as the subshock (see Figure 2.1 (a)). This is an MHD shock, i.e. a discontinuity satisfying the standard MHD shock jump conditions (Eqs. (2.39)). In this case, the total compression ratio,\(^6\)

\[
 r_{\text{tot}} \equiv \frac{u_{0x}}{u_{2x}} = \frac{\rho_2}{\rho_0},
\]

can become much larger than the limit of 4 obtained for non-modified MHD shocks. The compression ratio at the subshock, on the other hand, becomes smaller. This has the effect of lowering the rate at which the suprathermal particles are injected into the acceleration process. Moreover, since the more energetic particles can stream further upstream, they effectively “see” increasing compression ratios. The spectrum of the distribution function of the accelerated particles becomes, therefore, softer than in the non-modified case at low energies \((r_{\text{sub}} < 4)\) and harder at high energies \((r_{\text{tot}} > 4)\) (see Figure 2.1 (b)). The cosmic rays

---

\(^6\)Here and in the following, we use the indices 0, 1 and 2 for quantities far upstream, directly upstream and downstream of the subshock, respectively, unless otherwise specified.
also trigger plasma waves, turbulence, and instabilities. In fact, these constitute the scattering centres necessary for DSA. The importance of such a process for shock acceleration was first pointed out by Bell (1978), who derived it by using the results of Skilling (1975a,b,c), concerning the interaction between particles and Alfvén waves, in the context of collisionless shocks. In particular, the resonant-streaming instability (RSI) was considered, which is caused by the gradient (upstream of the shock) of the accelerated particle pressure. The process produces Alfvén waves in resonance with the particle gyromotion. The idea was further developed in the context of non-linear DSA by McKenzie and Völk (1982) (see Eqs. (2.33) and (2.34), and Appendix A). The magnetic turbulence generated by the backstreaming charged particles during the acceleration process can also have an effect on the shock structure (Caprioli et al., 2009b). Therefore, in the following, we will review the relevant equations for shocks, including the turbulence pressure. In our work, we will include only the effect of the resonant-streaming instability, motivated by the relative ease of treatment. Even if other instabilities might become important, or even dominant and more efficient at amplifying the ambient magnetic field, the choice of considering only RSI has been made in several studies in the literature (e.g. Amato and Blasi (2005); Amato and Blasi (2006); Caprioli et al. (2010a, 2011)). We adopt the same approximation as a first step in the combined approach developed in this work, and leave the possibility of including other kinds of instabilities for future developments. We note that the microphysics and the exact physical mechanisms initiating the Fermi acceleration mechanism is the subject of intensive studies (e.g. Marcowith et al. (2016) and references therein).

Let us suppose that the only spatial dependence of the background fields (flow velocity $u$, magnetic field $B$, density $\rho$, and temperature $T$) is in the $x$-direction. The starting point are Maxwell’s equations and the MHD conservation laws in the presence of Alfvén waves and cosmic rays. The latter read:

$$\rho u_x = \text{const},$$

$$\rho u u_x + \left(p_g + \frac{B^2}{2\mu_0} + p_w + p_c\right) \hat{n} - \frac{B_x B}{\mu_0} = \text{const},$$

$$u_x \left\{ \frac{1}{2} \rho u^2 + \frac{\gamma}{\gamma - 1} p_g + \frac{B^2}{\mu_0} \right\} + F_w + F_c - \frac{B_x (B \cdot u)}{\mu_0} = \text{const}.\quad (2.30c)$$

Herein, $\hat{n}$ is the unit vector normal to the shock, $\mu_0$ is the permeability of free space, $\gamma$ is the adiabatic index, $p_g = nk_BT$ is the thermal pressure of the plasma, where $T$ is its temperature, $n$ is the particle density, and $k_B$ is the Boltzmann constant. The subscripts $x$, $y$ or $z$ indicate the $x$-, $y$- or $z$- components of a vector. Furthermore, the quantities related to the accelerated protons are the energy flux $F_c$ (see Eq. (2.33)), and the pressure

$$p_c = \frac{4\pi}{3} \int_{p_{\text{min}}}^{p_{\text{max}}} dp \ p^3 v(p) f(p),$$

where $v(p)$ is the speed of a proton of momentum $p$. The pressure term associated with the Alfvén waves is $p_w = (\delta B)^2/(2\mu_0)$, where $\delta B$ is the magnetic field amplitude of the waves. The energy flux $F_w$ includes the kinetic energy flux and the $x$-component of the Poynting vector.
associated with the Alfvén waves:

\[ F_w = \frac{1}{2} \rho (\delta u)^2 u_x + \frac{1}{\mu_0} \left\{ (B \times \delta u + \delta B \times u) \times \delta B \right\} \cdot \hat{n}, \quad (2.32) \]

where \( \delta u \) is the velocity change of the plasma due to the Alfvén waves.

McKenzie and Völk (1982) derived, in their Appendices A and B, the equations for the energy flux of cosmic rays, and the equations describing the generation and growth (or damping) of Alfvén waves, including adiabatic and streaming-instability effects. These read:

\[ \frac{dF_c}{dx} = (u - v_A') \frac{dp_c}{dx} + \bar{Q}, \quad (2.33) \]

\[ F_c = \frac{\gamma_c}{\gamma_c - 1} (u - v_A) p_c - \frac{\bar{D}}{(\gamma_c - 1)} \frac{dp_c}{dx}, \]

and

\[ \frac{dF_w}{dx} = u \frac{dp_w}{dx} + v_A \frac{dp_c}{dx} - \bar{L}, \quad (2.34) \]

respectively. In Eq. (2.33), \( \bar{D} \) is an effective diffusion coefficient for the cosmic ray momentum density, and \( \bar{Q} \) represents any other possible additional energy losses or gains for the cosmic rays. Any additional energy gains or losses for the Alfvén waves are represented by \( \bar{L} \) in Eq. (2.34).

The adiabatic index for CRs, \( \gamma_c \), is (e.g. Caprioli et al. (2009a)):

\[ \gamma_c = 1 + \frac{p_c}{E_c} = 1 + \frac{1}{4} \int_{p_{\text{min}}}^{p_{\text{max}}} \frac{dp}{4\pi p^2} \int \frac{dE}{E} \int \frac{f(p)}{E^2}, \quad (2.35) \]

where \( E(p) \) is the energy of the non-thermal protons, i.e. \( E(p) = (\Gamma(p) - 1) m_p c^2 \), with the Lorentz factor \( \Gamma(p) \) for a proton of momentum \( p \). By taking the divergence of the energy equation (Eq. (2.30c)) and employing Eqs. (2.33), (2.34), and the particle and momentum flux conservation equations (Eqs. (2.30a) and (2.30b)), McKenzie and Völk (1982) derived the “thermodynamic form” of the energy equation:

\[ \frac{u\rho p^\gamma}{(\gamma - 1)} \frac{d}{dx} \left( \frac{p_{\gamma}}{\rho} \right) = \bar{L} - \bar{Q}. \quad (2.36) \]

If \( \bar{L} = \bar{Q} = 0 \), corresponding to the case where CRs and Alfvén waves exchange energy only between each other, the background plasma is adiabatically heated in the precursor and Eq. (2.36) yields \( \rho p^\gamma = \text{const} \). Even if a certain degree of heating of the thermal plasma due to dissipation of the magnetic turbulence may be expected, the magnitude of such a mechanism is not known. Several models (analytical and semi-analytical) treat this effect either by assuming that the growth of magnetic turbulence due to the accelerated protons is entirely dissipated, producing non-adiabatic heating of the background plasma (e.g. Berezhko and Ellison (1999); Völk et al. (1984)), or by introducing yet another parameter in the equations, describing the strength of turbulent heating (e.g. Caprioli et al. (2008, 2009b); Vladimirov et al. (2008)). In their treatment, Berezhko and Ellison (1999) found that the effect of turbulent heating was to substantially decrease the shock modification and the total compression ratio. At the same
time, the acceleration efficiency changes only slightly compared to the case without non-adiabatic heating. Later studies, including also the possibility of strong magnetic turbulence, indicated that only with very high dissipation the shock modification is appreciably (but not dramatically) reduced. Furthermore, Vladimirov et al. (2008) found that, despite the increased efficiency of injection of particles in the acceleration process in the presence of wave dissipation, the overall acceleration efficiency changed only slightly. Based on those results, in our approach we assume adiabatic heating of the background plasma in the precursor.

With the discussed set of equations, the expressions relating the magnetic field, the flow velocity, and the density along \( x \), assuming that the background magnetic field lies in the \( x-z \) plane, can be found to be:

\[
\begin{align*}
  u_x(x) &= \frac{\rho_0 u_{0x}}{\rho(x)}, \quad (2.37a) \\
  u_y(x) &= u_{0y}, \quad (2.37b) \\
  u_z(x) &= u_{0z} + \left( \frac{B_z(x) - B_{0z}}{\mu_0} \right) \frac{B_{0x}}{\rho_0 u_{0x}}, \quad (2.37c) \\
  B_x(x) &= B_{0x}, \quad (2.38a) \\
  B_z(x) &= \left( \frac{M_{A0x}^2 - \cos^2 \theta B_0}{U_x(x)M_{A0x}^2 - \cos^2 \theta B_0} \right) B_{0z}. \quad (2.38b)
\end{align*}
\]

Here, we introduced the normalized flow speed in the \( x \)-direction, \( U_x(x) \equiv u_x(x)/u_{0x} \). The electric field is \( E = -\hat{u} \times \hat{B} \), and it is entirely due to the motion of the plasma in the magnetic field. In all of our setups, \( \hat{u} \) is (almost) perfectly parallel to \( \hat{B} \), and the electric field is therefore small.

For strong turbulence, \( \delta B/B > 1 \), the definition of a background magnetic field becomes questionable. In such cases, we consider \( \hat{B}(x) \) just as the field determining the direction of propagation of the Alfvén waves.

As a common practice, analogous to the test-particle case, it is assumed that the distribution function of the accelerated particles is constant between directly upstream and downstream of the MHD shock (i.e. the subshock). Therefore, the CR terms do not appear in the shock jump conditions, which become (see, e.g., Scholer and Belcher (1971) and Decker (1988)):

\[
\begin{align*}
  [\rho u_x]^2 &= 0, \quad (2.39a) \\
  \left[ \rho u u_x + \left( p_y + \frac{B^2}{2\mu_0} + p_w \right) \hat{n} - \frac{B_z \hat{B}}{\mu_0} \right]_1^2 &= 0, \quad (2.39b) \\
  \left[ u_x \left( \frac{1}{2} \rho u^2 + \frac{\gamma}{\gamma-1} p_y + \frac{B^2}{\mu_0} \right) + F_w - \frac{B_x (B \cdot \hat{u})}{\mu_0} \right]_1^2 &= 0, \quad (2.39c) \\
  [B_z]^2 &= 0, \quad (2.39d) \\
  [\hat{n} \times (\hat{u} \times \hat{B})]^2 &= 0. \quad (2.39e)
\end{align*}
\]
Here, the notation $r_s$ denotes the difference between downstream and upstream quantities. 

When solving the system of Eqs. (2.39), Scholer and Belcher (1971) used the transmission and reflection coefficients of Alfvén waves incident on a shock given by McKenzie and Westphal (1969), and obtained a third-order equation for the compression ratio $r = \rho_2/\rho_1 = u_{1x}/u_{2x}$ equivalent to:

$$a_3 r^3 + a_2 r^2 + a_1 r + a_0 = 0,$$

(2.40)

with coefficients

$$a_3 = [(\gamma - 1)(1 + \lambda) M_{A1x}^2 + \gamma \beta_1 \cos^2 \theta B_1] \cos^2 \theta B_1$$
$$a_2 = \left\{ (2(1 + \lambda) - \gamma(1 + \cos^2 \theta B_1 + \lambda)] M_{A1x}^2 - [1 + \lambda + \gamma(2\beta_1 + 1 + \lambda)] \cos^2 \theta B_1 \right\} M_{A1x}^2$$
$$a_1 = \left\{ (\gamma - 1) M_{A1x}^2 + \gamma(1 + \lambda + \cos^2 \theta B_1 + \beta_1) + 2 \cos^2 \theta B_1 \right\} M_{A1x}^4$$
$$a_0 = - (\gamma + 1) M_{A1x}^6.$$

Herein, $\theta B_1$ is the angle between the shock normal and the magnetic field directly upstream of the shock, $\lambda = (\delta B_1/B_1/2)$, and $\beta = \rho g 2 \mu_0 / B^2$. The quantity $M_{A1x} = u_{1x}/v_A$, with the Alfvén speed $v_A = B/\sqrt{\mu_0 \rho}$, is the Alfvén Mach number (here in the $x$-direction) directly upstream of the subshock. It is the analogue for Alfvén waves of the sonic Mach number, $M = u/c_s$, where $c_s = \sqrt{\gamma \rho_g / \rho}$. In the limit without magnetic field disturbance $\lambda = 0$, Eq. (2.40) reduces to Eqs. (11) of Decker (1988). The temperature downstream is given by the relation:

$$\frac{T_2}{T_1} = \frac{1 \rho g_2}{r \rho g_1} = \frac{1}{r[(\gamma + 1) - (\gamma - 1)]} \left\{ (\gamma + 1) r - (\gamma - 1) + (\gamma - 1) \frac{M_{A1x}^2 (r - 1)^3}{(M_{A1x}^2 - r \cos^2 \theta B_1)^2} \frac{(p_{B1} + p_{w1})}{p_{g1}} \right\}.$$

(2.41)

This equation can be obtained with the same approach as used by Vainio and Schlickeiser (1999), except using the conservation laws and transmission and reflection coefficients of Alfvén waves for the case of oblique shocks given by Scholer and Belcher (1971) (see Appendix B).

We have now provided the necessary theoretical background concerning DSA. In the next section, we will introduce several numerical techniques employed for the study of the acceleration process.

### 2.2.1 Review of simulations of nonlinear DSA

Here, we briefly give an overview of different numerical approaches which have been used to study particle acceleration at shocks with nonlinear effects, reviewing some of their strengths and weaknesses.

The study of the microphysics of shock formation and injection of particles into the Fermi process is most realistically accomplished with (full) particle in cell (PIC), and hybrid PIC.

---

7This is true after correcting for a typo in Decker (1988): the term $\cos^2 \delta_1$ should always be multiplied by $M_{A1}^2$ in their equations (11a)-(11c).
simulations (e.g. Gargaté and Spitkovsky (2012), Caprioli and Spitkovsky (2014a) for dedicated simulations; Tskhakaya et al. (2007) for a review of the PIC method). The reason lies in the low number of approximations applied. The numerical method can be roughly summarized as follows. At each time-step, the positions and velocities of the particles (e.g. ions, protons, electrons, positrons) are used to determine the electromagnetic fields on the grid points of the computational box. These fields are in turn used to compute the forces acting upon the particles and let them move self-consistently to the next time-step. Full PIC simulations are computationally very demanding, especially when simulating plasmas of ions (protons) and electrons. In fact, they must resolve the time- and length-scales of the lightest species (e.g. electrons) while being able to simulate time and space intervals sufficiently large for the heaviest species (e.g. protons) to (i) produce the magnetic turbulence providing the scattering centres, (ii) be scattered multiple times, and (iii) be accelerated via the Fermi mechanism. The time scales to be resolved are typically expressed in terms of the plasma frequency of the considered species $\sigma$:

$$\omega_{p\sigma} = \sqrt{\frac{n_{\sigma} q_{\sigma}^2}{\epsilon_0 m_{\sigma}}} ,$$

(2.42)

where $n$ is the particle density, $q$ is the charge of the particle, $m$ is its mass, and $\epsilon_0$ is the vacuum permittivity. The ratio of the time scales to be resolved for electrons to those for protons is, therefore, $\sqrt{m_e/m_i} \approx 1/43$. This computational challenge is partially side-stepped by using a reduced proton-to-electron mass ratio. The results of the first PIC simulation showing evidence for both proton and electron acceleration were presented by Park et al. (2015). It was obtained in a 1D setup, with a reduced proton-to-electron mass ratio of $m_p/m_e = 100$. Momenta of about $10^2 m_e c$ have been reached, and the non-thermal tail in the proton distribution extended only from $\approx 4 \times 10^2 m_e c$ to $\approx 7 \times 10^2 m_e c$.

The closest approximation to the full PIC model is a hybrid model, considering electrons as a fluid and protons as particles. This recipe allows to simulate the acceleration of ions to much larger energies, as compared to the full PIC method, because the smallest time-scale to be resolved is that associated with the ion (not electron) plasma frequency. The approach has been extremely valuable for studying instabilities in the nonlinear regime (e.g. Bell (2004)). An extensive study of the acceleration process at collisionless shocks has been conducted, for example, by Caprioli and Spitkovsky (2014a,b,c), who considered in particular three aspects: acceleration efficiency, magnetic field amplification, and the diffusion coefficient of protons at nonrelativistic shocks. It is interesting to note that those simulations show some of the features of nonlinear DSA described above, namely a decrease in the downstream temperature and a slowdown of the upstream flow. However, the concave shape of the non-thermal distribution function has not been observed. This can be attributed to the fact that, due to the computational costs, the maximal energies reached are below $10^3$ times the shock kinetic energy, $E_{sh} = 1/2 m_p v_{sh}^2$, where $v_{sh}$ is the upstream fluid velocity in the downstream frame. This energy corresponds to a Lorentz gamma factor for the most energetic protons of $\Gamma \approx 1.1$. For a comparison, typical Lorentz factors of high-energy protons accelerated in CWBs are expected to be on the order of $\Gamma \approx 10^2 - 10^4$ (e.g. Farnier et al. (2011); Reitberger et al. (2017))\footnote{Similar energies are reached in our Monte Carlo simulations of a typical CWB system, consisting of a B star, while protons in supernova...}, while protons in supernova...
remnants (SNRs) are expected to reach Lorentz factors as high as $\Gamma \approx 10^5 - 10^6$ (e.g. Bell (2014)). The existence of other processes responsible for limiting the effect of shock modification and reducing the concavity of the spectra cannot be excluded, also in light of the fact that no clear evidence of concavity has been found from observations of $\gamma$-ray-bright SNRs (see, e.g., Caprioli (2012) and references therein). However, as noted by Caprioli and Spitkovsky (2014a), the PIC simulations should reach the relativistic regime in order to be able to investigate this open question.

Approaches other than PIC have been developed, which allow to simulate the acceleration of particles up to such energies, and to model the shock modification due to the pressure of the ions accelerated to relativistic energies. In the following, we will give an overview of three methods, the results of which, applied to a benchmark case, have been compared by Caprioli et al. (2010b).

Kang and collaborators developed a code, which allows to follow the time evolution of modified shocks during the acceleration process (Gieseler et al., 2000; Kang and Jones, 2007; Kang et al., 2001). The method mainly consists of solving the transport equation for the accelerated protons (Eq. (2.12), without diffusion in momentum space), together with the hydrodynamic equations for the background plasma. At every time step, the shock position is determined, and a multi-level grid structure is defined, in order to be able to resolve the precursor and subshock transition with sufficient accuracy (Kang et al., 2001). The injection of protons into the acceleration process is modelled numerically by using an approximation for the transparency function.

The above-cited versions of the code, included in the comparative study of Caprioli et al. (2010b), considered only plane-parallel shocks. An adaptation to spherically symmetric shocks has been used by Kang and Jones (2006) and Kang et al. (2012a). The latter also considers the acceleration of electrons (including radiative losses), in test-particle approximation.

One of the first methods used for studying the acceleration of particles at shocks is the Monte Carlo method. Several authors employed it in the test-particle approach (e.g. Baring and Summerlin (2005); Baring et al. (1993); Baring et al. (1994); Ellison et al. (1995); Kirk and Schneider (1987); Ostrowski (1991); Summerlin and Baring (2011)). A technique including the effects of the backreaction of cosmic rays has also been developed (Bykov et al., 2014; Ellison and Eichler, 1984; Ellison et al., 2015; Vladimirov, 2009; Vladimirov et al., 2006). To our knowledge, currently, the most sophisticated Monte Carlo simulations are those presented by Bykov et al. (2014, 2017), which include several types of plasma instabilities, e.g. RSI and the non-resonant hybrid – or Bell – instability (Bell, 2004). Caprioli et al. (2010b) refer to Vladimirov et al. (2006), in their comparison of different models. The Monte Carlo method constitutes the core of the code developed for the project presented in this thesis and will be described in detail in Chapter 3. The nonlinear approach of Vladimirov et al. (2006) (in its original form developed by Ellison and Eichler (1984), see also Vladimirov (2009)) is entirely based on Monte Carlo simulations. For a given profile of the shock precursor,
the particle, momentum, and energy fluxes are measured at several positions, from the subshock to far upstream. The shock profile is then iteratively adjusted, until the fluxes are conserved throughout the shock. A distinctive feature of Monte Carlo methods is that there is no difference in the treatment of thermal and non-thermal particles. The non-thermal tail to the thermal distribution naturally develops as a consequence of repeated scatterings across the shock by a fraction of the thermal particles initially injected into the computational box. The other methods which allow to model nonlinear DSA up to high energies, i.e. that of Kang and collaborators (outlined above) and that of Amato and Blasi (2005) (see below) treat the thermal and non-thermal particles as two different components of the same system. The calculations for the non-thermal component relies on the assumption of isotropy of the distribution at all energies. The method of Vladimirov et al. (2006), on the contrary, can catch the effects of anisotropies in the low-energy regime, which may affect the injection efficiencies. The main approximations reside in the modelling of the scattering process and of the plasma instabilities. The latter are computed by considering the particle distributions including anisotropies. In a loose sense, the Monte Carlo technique is placed somewhere between the PIC technique and the semi-analytical techniques.

The last method we want to mention is that developed by Amato and Blasi (2005); Caprioli et al. (2009b) and successive works. It consists of a semi-analytical method for the calculation of the profiles of modified shocks in a steady-state approximation. Similarly to the Monte Carlo technique, the solution is found iteratively. It is based on the MHD equations and the transport equation for the protons. The injection efficiency is derived in the thermal leakage scenario, assuming a finite width of the order of a few gyroradii for the subshock transition layer. As opposed to the approach of Kang et al. (2001), this technique relies on the steady-state assumption. In fact, Kang et al. (2001) can follow the temporal evolution of the shock, while it propagates along the simulated region. Unfortunately, this translates to higher computational costs as compared to the procedure developed by Amato and collaborators. Owing to its speed of computation, in the last part of this PhD project, we decided to implement the latter semi-analytical method and adapt it, allowing it to work in combination with the Monte Carlo technique, and in oblique shock configurations. Therefore, more details of the model can be found in Chapter 3.

In these models, the phenomenon of magnetic field amplification (MFA) can also be included. The latter is caused by the above-mentioned magnetohydrodynamic instabilities and turbulence generated by the non-thermal protons (Caprioli and Spitkovsky, 2014b). MFA is at present the best explanation for the high magnitude of the magnetic field at SNR shocks (~ 0.1 – 1 mG, as compared to the typical interstellar magnetic field of ~ 1μG) inferred from the detection of very thin emission regions of the X-ray synchrotron radiation associated with accelerated electrons. The thickness of the filaments is consistent with the picture that the amplified magnetic field causes severe energy losses of the relativistic electrons (e.g. Ballet (2006); Morlino et al. (2010)). Besides increasing the synchrotron radiation losses, the amplified magnetic field exerts a pressure which, in case of efficient particle acceleration, influences significantly both the subshock and the overall compression ratio. Several kinds of instabilities have been included in the models over the years (see, e.g., Bykov et al. (2017)).

Concluding this chapter, we summarize the essential points. Diffusive shock acceleration is
an efficient mechanism at collisionless shocks, which can produce a non-thermal particle population, extending to relativistic energies. In the test-particle approximation, the non-thermal distribution is a simple power-law, with the spectral index depending on the compression ratio. In most cases, if particle acceleration is efficient, the pressure of the cosmic rays slows down the upstream plasma flow, forming a precursor before the MHD shock. We have reviewed different methods modelling DSA. The Monte Carlo method and the semi-analytical method of Amato and Blasi (2005) have been adapted and implemented in our code, as described in the next chapter. Finally, we note that Caprioli et al. (2010b) have found that the methods of Amato and collaborators, Kang and collaborators, and Ellison, Vladimirov and collaborators, yield solutions (i.e. shock profiles and particle distributions) for nonlinearly modified shocks in good agreement with each other. Some further discussion on this is conducted in Section 4.3.1.
Chapter 3

Numerical method

This chapter provides a description of the methods used in our model of particle acceleration in CWBs. Except for the MHD part, shortly described in Section 3.1, all the code was developed in the context of this thesis. The core of our approach, i.e. the Monte Carlo method, will be presented in Section 3.2. In Section 3.3.1 we will describe how we combine the (M)HD and the Monte Carlo simulations. The challenges of this approach will be discussed and provide a motivation for the development and use of the superimposed-cell (in the following, supercells, or SCs) system at the shocks, in our combined simulations. In Sections 3.3.2 and 3.3.3 we describe our implementation of particle splitting, and exemplify this method by tracking the paths of some split particles in the simulation box. The semi-analytical method for the calculation of nonlinear effects due to CRs (e.g. Amato and Blasi (2005)) and here adapted for our purposes of considering oblique shocks, is introduced in Section 3.4. Section 3.5 is devoted to the validation of the code.

Before illustrating the code developed in this PhD project, it is worth to briefly mention the main features of the MHD code used for obtaining realistic background conditions for the simulations presented in this thesis.

3.1 Magnetohydrodynamic simulations

The first step of the combined approach presented in this chapter consists of running MHD simulations for a CWB system. This is achieved by means of the code CRONOS, developed by Kissmann et al. (2018). For modelling the stellar wind of a star in the presence of a stellar magnetic field (assumed to be a dipole inside the star), the code solves the ideal MHD equations
on a Cartesian grid:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3.1}
\]

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \nabla \cdot (P \mathcal{I}) + \frac{1}{\mu_0} \mathbf{B} \times (\nabla \times \mathbf{B}) = \mathbf{f} \tag{3.2}
\]

\[
\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\nabla \times \mathbf{B}) \tag{3.3}
\]

\[
\frac{\partial e}{\partial t} + \nabla \left[ \left( e + \frac{B^2}{2\mu_0} + P \right) \mathbf{u} - \frac{1}{\mu_0} (\mathbf{u} \cdot \mathbf{B}) \mathbf{B} \right] = \mathbf{u} \cdot \mathbf{f} + \left( \frac{\rho}{m_H} \right)^2 \Lambda(T) \tag{3.4}
\]

Herein, \( \rho, \mathbf{u}, \mathbf{B}, \) and \( \mu_0 \) have their usual meaning, \( e \) is the total energy density, \( P \) is the thermal pressure, \( \mathcal{I} \) denotes the unit tensor, and \( m_H \) indicates the mass of the hydrogen atom. The radiative cooling function, \( \Lambda(T) \), models the cooling of the plasma due to line transitions, and for the simulations providing our background is taken from Schure et al. (2009). The term \( \mathbf{f} \) represents the external force densities, given by:

\[
\mathbf{f} = \rho \sum_i \left( -GM_{\ast,i} \frac{\mathbf{r}_i}{r_i^3} + \mathbf{g}^{\text{rad}, i} + \mathbf{g}^{\text{rad}, i} \right). \tag{3.5}
\]

Here, the index \( i \) can assume values 1 or 2, corresponding to the two stars, \( \mathbf{r}_i \) is the distance vector relative to star \( i \), \( \mathbf{g}^{\text{rad}, i} \) is the radiative line acceleration of ions, and \( \mathbf{g}^{\text{rad}, i} \) denotes the acceleration by stellar radiation scattering off free electrons (for details, see Kissmann et al. (2016) and references therein). The temperature is set to \( T_{\text{inf}} = 10^4 \) K at the beginning of the simulations. This also constitutes a lower boundary: the plasma of the winds is not allowed to cool (via adiabatic expansion) below this limit, mimicking photo-ionization heating. The distances from the stellar surface at which the magnetic field has the strongest influence on the acceleration of the stellar winds are typically small, as compared to the stellar separation in CWB systems. In order to capture the effect of the magnetic field on the stellar wind, the simulation is divided into two parts. First, the region in the vicinity of the star is simulated in a 2D spherical setup, assuming axial symmetry. These extend up to about 6 stellar radii. No rotation of the stars is considered. Second, the large-scale simulations of the CWB system are performed, employing the results of the first part for determining the wind flow near the stars. In all of the setups we used, the orbital motion of the stars is not considered. More precisely, the large-scale simulations are typically initialized as follows. The 2D simulations of the vicinity of the stellar surface for the two stars are mapped into the 3D Cartesian grid. The two stars are positioned in the computational domain, centrally in the \( y-z \) direction and at a determined distance, symmetrically with respect to the centre of the domain, in the \( x \)-direction. The simulation box is then divided into two regions, with the position of the boundary between them determined by the respective ram pressure (Eq. (1.2)). The cells outside the near-star solutions are initialized with the fields of the outermost cells of the 2D simulations. The solution from the near-star simulations is kept fixed up to 30 \( R_\odot \) above the stellar surface, while the rest of the computational domain, after the initialisation, is left free to evolve according to the MHD.
equations (3.4).
The results obtained from the simulations performed following the procedure described here,
which was developed by Kissmann et al. (2016), constitute the environment that will be used
in the combined approach for the study of proton acceleration in CWB systems. This allows to
model the influence of the stellar magnetic field on the wind acceleration and flow velocity, and
to obtain the large-scale magnetic field avoiding the use of ad hoc prescriptions, at any given
cell of the computational domain.
In the next section, we describe the Monte Carlo method for simulations of particle acceleration
at shocks, which is the core of the combined approach presented in this thesis.

3.2 Monte Carlo method

In this section we introduce the Monte Carlo approach, the core of which resembles that of
Ellison et al. (1995), further developed by Vladimirov (2009) and e.g. Bykov et al. (2014).\(^2\)
Here, we describe the simplest setup, since all the developments of the Monte Carlo part of our
code are based on this and only differ in the number of cells used and how the background is
initialized.
The computational box is divided in two regions: upstream and downstream of the shock. As
a common practice, we assume that the particles (protons, in all of our simulations) have a
Maxwell-Boltzmann distribution of velocities in the frame comoving with the local plasma flow,
with the temperature of the local background. The protons are injected into the upstream cell,
close to the shock surface (typically about one mean free path away, but the distance can be
varied). Naively, one could inject the particles by assigning the particle momenta isotropically
in the plasma frame, and simply performing a transformation to the shock frame. However,
as discussed by Vladimirov (2009), this procedure does not yield an isotropic distribution of
velocities (momenta) in the plasma frame, when measuring at positions close to the injection
location.\(^3\) This happens because, in Monte Carlo simulations like those described here, the
presence of particles at a certain position \(x\) is inferred by counting the crossing events of particles
through the surface at the considered position. This counting procedure, however, does not yield
a density, but a flux of particles. More specifically, the total flux of particles through a surface
(“detector”) is given by (the \(x\)-axis being perpendicular to the shock surface):

\[
\Phi = \sum_i v_{x,i} \left( \frac{u_0}{v_{x,i}} \right) w .
\]  
(3.6)

Herein, \(u_0\) is the flow speed, \(v_{x,i}\) is the \(x\)-component of the velocity of the particle crossing the
measurement surface (i.e. the shock), and the statistical weight is given by:

\[
w = n_0/N_p ,
\]  
(3.7)
\(^2\)Vladimirov (2009) and Bykov et al. (2014) study the nonlinear modifications of parallel shocks. Our approach
to model the backreaction is a combination of Monte Carlo simulations and the semi-analytical approach of, e.g.,
Amato and Blasi (2005), and will be discussed in Section 3.4.
\(^3\)As will be shown in Section 3.5, the scattering process in the simulations ensures that this anisotropy is
removed further downstream of the injection position.
where \( n_0 \) is the particle density and \( N_p \) is the number of particles injected. The quantities \( u_0 \) and \( w \) refer to the point where the particles are injected at the beginning of the simulation. The index \( i \) runs over all the crossing events of all the simulated particles. The contribution of each crossing event to the particle density must take into account that the simple counting yields a flux. Therefore, the particle density measured at the location of the detector is:

\[
n = \sum_i \left| \frac{u_0}{v_{x,i}} \right| w .
\]  

(3.8)

In other words, the naive injection procedure disregards the fact that the particles crossing the measurement surface with a lower velocity \( |v_{x,i}| \) must contribute more to the measured particle density. By considering this, Vladimirov (2009) derived the following prescription to obtain the correct distribution of the component of the particle velocity perpendicular to the measurement surface, in the shock frame:

\[
v_{sf,x} = \sqrt{(v^2_{\text{max}} - v^2_{\text{min}})Z + v^2_{\text{min}}} .
\]  

(3.9)

Herein, \( v_{\text{max}} = u_x + v_{\text{MB}} \), and \( v_{\text{min}} = u_x - v_{\text{MB}} \), where \( v_{\text{MB}} \) is the speed of the particle in the plasma frame, randomly selected using the Maxwell-Boltzmann distribution for the local temperature \( T \), and \( Z \) is a random number drawn from a uniform distribution between 0 and 1. In the oblique case, we transform the particle velocity to the frame comoving with the local (upstream) background plasma and with the axes parallel to those of the shock frame. We additionally assign a random direction to the velocity in the \( y-z \) plane, with magnitude \( v_{yz} = \sqrt{v^2_{\text{MB}} - v^2_x} \), where \( v_x \) is the \( x \)-component of the speed of the particle in the plasma frame.

After injection, we let each particle move using the Bulirsch-Stoer algorithm (Press et al., 1992). This technique for the integration of ordinary differential equations essentially consists of considering the solution to the integration over a time step \( H \) as a function of the parameter \( h \), i.e. the size of subintervals of \( H \). The integration from \( t \) to \( t + H \) is thus performed with an increasing number of subintervals (of decreasing size \( h \)) with a modified midpoint integration method, in order to find the value of the solution function for different values of \( h \). An extrapolation of the solution to \( h = 0 \) is then performed. If the required accuracy is not obtained, the number of substeps is increased, and a new extrapolation is performed, until either the requirements are met, or a maximum number of refinements has been reached. In the latter case, \( H \) is scaled and the procedure is repeated. For a fully detailed description of the different components of the algorithm, we refer the reader to Press et al. (1992).

In the simulations of particle acceleration, the particles are acted upon by the Lorentz force given by the background electromagnetic fields. After a time \( t_c \), exponentially distributed with a mean value \( \bar{t}_c = \xi r_g/v \), a scattering occurs (elastic in the frame of the local plasma flow). The new direction of the momentum vector is randomly determined at each scattering, mimicking strong magnetic turbulence.\(^4\) In most cases, we set \( \xi = 1 \), corresponding to Bohm diffusion.

\(^4\)The randomization of the direction of the momentum in one single event is also motivated by computational costs. Schemes closer to the physical case of a perturbed medium are commonly used to investigate the acceleration process at a single shock (e.g. Vladimirov (2009); Bykov et al. (2014)). Those techniques model the pitch-angle diffusion by letting the particle momentum change many times, by a smaller amount, within a mean free path.
This choice is supported by PIC simulations (Caprioli and Spitkovsky, 2014c). However, other scattering laws, with different values of $\xi$, as well as other dependences on the momentum can in principle be easily used.

In order to find the distribution function $f(p_k)$ for particles passing a surface of interest (with the shock normal parallel to the $x$-axis), we note that if $\Delta p_k$ is the width of the $k$-th momentum bin centred at momentum $p_k$, we have:

$$f(p_k) = \frac{1}{4\pi p_k^2 \Delta p_k} n(p_k) , \quad (3.10)$$

with

$$n(p_k) = \sum_{p \in \Delta p_k} \left| \frac{u_0}{v_{x,i}} \right| w . \quad (3.11)$$

Here, the index $i$ runs over all the crossing events of the particles having a momentum within the $k$-th momentum bin. The corresponding flux of particles is:

$$\varphi(p_k) = \sum_{p \in \Delta p_k} v_{x,i} \left| \frac{u_0}{v_{x,i}} \right| w . \quad (3.12)$$

The simulation of a particle is stopped and the particle removed from the system in three cases:

- when it reaches a distance
  $$x_D = 10 \frac{D}{u_2} \quad (3.13)$$
  downstream of the shock, where $D$ is the diffusion coefficient given by Eq. (2.26). Assuming an infinitely extended homogeneous downstream medium, as it is, effectively, for low-energy (thermal) particles, this choice corresponds to stopping the simulation for a particle when its probability to return to the shock is $\lesssim e^{-10}$ (Ostrowski and Schlickeiser, 1993);

- when it leaves the whole simulated box;\(^5\)

- when the number of scatterings experienced by the particle reaches a pre-set value, much greater than the expected mean number of scatterings needed to reach the highest possible energy in the system.

### 3.3 Combined (magneto-) hydrodynamic and Monte Carlo test-particle simulations

In this section, we describe how we combined the Monte Carlo approach with the MHD simulations for modelling particle acceleration in CWBs. We will present the challenges encountered and the solutions we adopted. We will also describe some useful features of the code, such as our

\(^5\)When doing simulations in the simple two-cells setup presented in this section, the cell size is $\Delta x \approx 30 \frac{D}{u_2}$, with the diffusion coefficient $D$ referring to the particles with $E = E_{\text{max}}$. 


implementation of particle splitting, and the tracking of the particles in the region of the CWB selected for the combined simulations. In the following, since the treatment of the background is the same in most aspects, both HD and MHD will be referred to as MHD, unless otherwise specified.

### 3.3.1 Background

In the previous section, where we introduced the basic setup for simulations of particle acceleration with the Monte Carlo method, the shock was considered as an infinite plane and the downstream flow did not change with the distance from the shock. In order to render the simulations more realistic, and to study particle acceleration specifically in CWBs, we now inject the particles into the plasma of models of typical CWB systems. More precisely, in the combined approach we use a snapshot of an MHD simulation of such a system, in an evolved state. This is consistent with the Monte Carlo approach yielding a steady-state solution. In practice, we assume that the snapshot represents the steady-state configuration of the CWB system. This is usually a good approximation for CWBs with large separation, and when the time scale for changes of the MHD background, and in particular of the shock conditions, is larger than the acceleration time of the most energetic particles in the system. In these cases, particle acceleration for different stellar separations, corresponding to different orbital phases, can be modelled to a good approximation with our approach. However, for some systems with strong eccentricity, the steady-state assumption may not be justified for the entire orbit, because at periastron the MHD conditions might change significantly over a time scale comparable to the acceleration time. In some cases, the WCR may be even temporarily disrupted, due to the catastrophic growth of instabilities triggered by efficient radiative cooling, as suggested by observations and modelling of η Carinae, WR 22 (Parkin and Gosset, 2011; Parkin et al., 2011), and other CWB systems (Midooka et al. (2019) and references therein). The treatment of similar rapidly changing conditions, as well as of large-scale MHD turbulence such as the Kelvin-Helmholtz instability possibly developing at the contact discontinuity, as shown in Section 4.2, is beyond the scope of this thesis.

**Shock location and orientation, shock transition.** The particles are injected directly upstream of the considered shock (see Section 3.2). Therefore, when using an extended region with a complex 3D MHD structure, the first step is to locate the shocks. This is achieved, in our code, by setting a threshold to the gradient of the temperature within the simulation box. The temperature gradient was found to be a good tracer of the shock front position by Reitberger et al. (2014a). This is because of the uniform temperature of the unshocked winds, caused by the lower boundary $T_{\text{inf}} = 10^4$ K (see Section 3.1). At the shocks, the plasma is heated up to temperatures $\gtrsim 10^7$ K. Knowing where the shocks are located is not sufficient to successfully run Monte Carlo simulations on the MHD background. In fact, in the MHD simulation results, the transition between upstream and downstream is about three cells wide, for numerical reasons only, as can be seen

---

6Little fluctuations are possible due to numerical heating, therefore motivating the use of a threshold for the temperature gradient.
in Figure 3.1 (see also e.g. Kissmann et al. (2018)). The diffusion length of thermal particles,

![Figure 3.1: Speed of the winds and temperature of the plasma in an interval including the WCR, as a function of the x-coordinate. The data is that used for the simulations presented in Sections 4.2, and 4.3.3. The coordinates (y,z) are (0,20), corresponding to the injection locations B1 and W1 of Table 4.5.](image)

on the other hand, is smaller than the size of a single MHD cell. If the particles were injected upstream of the shock transition, they would not “see” the whole shock as a discontinuity, but only a smaller jump of the background fields. As a consequence, as compared to the case of a sharp shock transition, the protons would be more efficiently advected far downstream and their probability to reach the shock (i.e. the cell boundary) again would decrease. This can be seen, for particles with velocity \( v \gg u_{2x} \), with the aid of Eq. (2.24). Indeed, the probability to return to the shock would decrease, since the ratio of the flow speed of the shock-transition cell, \( u_{2x} \), to the particle speed, \( v \), would increase. Fewer particles would be injected into the acceleration process, and both thermal and non-thermal particles would be more easily advected to the next cell boundary, where they would see another numerical weak shock, within the shock transition. Again, some particles would be accelerated at an artificial shock, much weaker than the actual one. By recalling that the width of the shock transition (\( \sim 3 \) cells) is a numerical effect and is not related to its physical size, it becomes clear that some rearrangement of the numerical background at the shocks is necessary.

For the first preliminary study, presented in Grimaldo et al. (2015), and in Section 4.1, we used a simplified approach: the fields of the cells of the Monte Carlo simulations were initialized with the values of the MHD cells, but three cells downstream of the beginning of the shocks, corresponding to the yellow squares in Figure 3.1, were skipped. To improve this very rough approach, which resulted in a resized WCR, our first strategy consisted of extrapolating the field
values of the cells upstream and downstream, within the shock transition region. This approach, however, is limited by the complication illustrated in Figure 3.2. The problem stems from the orientation of the cell surface, which is in general not the same as the orientation of the shock front in the MHD simulations. Since the discontinuity seen by the particles coincides with the cell surface, the orientation of the shock for the particles is not correctly reproduced. In the extreme cases, the x-component of the flow velocity changes sign, i.e. it can be positive (negative) upstream, and negative (positive) downstream. Under these conditions, the advection of the particles scattered on the two sides of the cell surface pushes them towards the shock. The number of thermal particles accelerated is thus greatly increased and hard spectra are produced. This is shown in Figure 3.2 (b). When the shock-transition layer of three cells is bypassed (by cutting or extrapolating the fields from upstream and downstream), but the cell boundary is not aligned with the actual shock surface, the distribution function can reach a momentum dependence as hard as \( f(p) \propto p^{-3} \) (solid line). Therefore, we developed a system of superimposed cells (supercells), set up at the shocks, with which we obtain a momentum dependence of the distribution function consistent with the local compression ratio. In the case shown in Figure 3.2 (b), the compression ratio is close to the maximum for strong shocks, i.e. \( r = 4 \). We note that

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.2}
\caption{(a) Schematic representation of an upstream and a downstream cell, together with the actual shock surface resulting from MHD simulations. On the Cartesian grid, the cell boundary, which divides upstream and downstream, is in general not aligned with the shock surface. Reproduced from Grimaldo et al. (2017a), with the permission of AIP Publishing. (b) Comparison of the distribution function of protons obtained at the same position along the shocks of the WCR, but with two different treatments of the numerical shock transition. The peak on the left corresponds to the thermal bulk flow through the measurement surface, while the spectrum at higher energy is produced by the accelerated particles. In these two examples, the particles were removed from the system as soon as they left the pair of upstream-downstream cells.}
\end{figure}
there are, in the MHD computational domain, other positions where the $x$-component of the flow velocity changes sign between two neighbouring cells (e.g. at the contact discontinuity close to the apex of the WCR). However, this does not produce artefacts in the final spectra. This is not a surprise, because there the divergence of the velocity is not as high as at the shocks, and because mostly particles which have already been accelerated at the shocks reach those cells. In the following, we will first describe how the supercells are initialized and then how they are used in the Monte Carlo simulations.

**Supercells system.** We start by initializing the cells of our simulation box by taking the values of the fields for a selected region of interest from the MHD simulations. We then locate the shock by means of the temperature gradient, as previously discussed, and we divide the cells in three categories:

- far upstream or downstream;
- directly upstream;
- directly downstream.

At every cell directly upstream, the orientation of the shock normal $\vec{n} = (n_x, n_y, n_z)$ is determined by taking the average

$$
\vec{n} = \frac{\vec{n}^{(2)} + \vec{n}^{(3)}}{2}
$$

where the positive or negative sign is used depending on the side of the WCR, so that the normal points towards the downstream region, and

$$
\begin{align*}
n_x^{(l)} &= \frac{1}{|\vec{n}^{(l)}|} 
&= \frac{i_{SF}(j_0 - l, k_0) - i_{SF}(j_0 + l, k_0)}{2l} 
\quad \text{for } n_x^{(l)}

n_y^{(l)} &= \frac{1}{|\vec{n}^{(l)}|} 
&= \frac{i_{SF}(j_0, k_0 - l) - i_{SF}(j_0, k_0 + l)}{2l} 
\quad \text{for } n_y^{(l)}

n_z^{(l)} &= \frac{1}{|\vec{n}^{(l)}|} 
&= \frac{i_{SF}(j_0, k_0 - l) - i_{SF}(j_0, k_0 + l)}{2l} 
\quad \text{for } n_z^{(l)}
\end{align*}
$$

Herein, the coordinates $i_{SF}(j, k, j_0, k_0)$ are integer numbers indicating the shock cell (i.e. the last upstream cell before the shock transition) on the computational grid. The integer number $l$ assumes the values 2 and 3 in our approach. This can be considered as taking the average of the orientations of the planes passing through the shocks at distances of 2 and 3 cell lengths from the selected cell.

Once the shock orientation has been assigned to each cell marked as directly upstream, we set up the supercell system. We associate each cell directly upstream with a pair of cells of size $(2\Delta x)^3$ upstream, and $3\Delta x \times 2\Delta x \times 2\Delta x$ downstream, where $\Delta x$ is the size of a standard MHD cell (see Figure 3.3 (a)). We have chosen these dimensions aiming at achieving a good coverage of the shocks and the shock transition with the SCs, while maintaining a local character for the SC system, and averaging the background only over a small volume of the simulated region.

The background in the upstream SC is obtained by averaging the fields of the cells marked
CHAPTER 3. NUMERICAL METHOD

Figure 3.3: (a) Schematic representation of the supercell system along the shock delimiting the WCR on the left side. In order to avoid confusion, only three supercell pairs are shown, but in the simulations every cell directly upstream of the shock on the standard Cartesian grid is associated with its own supercell pair. (b) Illustration of the method used for the initialization of the background of the downstream supercells, which results from a weighted average of the fields within a distance $\Delta x$ from the point $3\Delta x$ downstream of the centre $x_c$ of the upstream shock-front cell, in the direction normal to the shock front ($\Delta x$ is the size of a standard cell). The curvature of the WCR with respect to the cell sizes is exaggerated for display purposes; supercell sizes are $(2\Delta x)^3$ upstream, and $3\Delta x \times 2\Delta x \times 2\Delta x$ downstream. Reproduced from Grimaldo et al. (2017a), with the permission of AIP Publishing.

as directly upstream, within a cube of size $3 \times 3 \times 3$ cells, centred on the cell associated with the supercell pair to be initialized. Also the shock orientation is averaged over the same cells. As far as the downstream cells are concerned, we employ the method used by Reitberger et al. (2014a) for the calculation of the compression ratio. As illustrated in Figure 3.3 (b), we locate a point at a distance $3\Delta x$ downstream from the centre of the original cell directly upstream, in the direction pointed by the shock normal. The background of the downstream supercell is then obtained by averaging the fields of the cells within a distance $\Delta x$ from that point, with weight

$$w_C = 1 - \frac{d_C}{\Delta x},$$

where $d_C$ is the distance of the centre of a cell from the considered downstream point. The background vector fields of the SCs upstream and downstream are then rotated, such that the shock surface is oriented like the cell boundary (in other words, the shock normal is parallel to the normal to the cell boundary between upstream and downstream supercells). After selecting the injection position (directly upstream cell) in the MHD background of the CWB system, we inject the particles in the associated upstream SC, at the centre of the local SC frame in the $y$ and $z$ directions, and at a distance $\varepsilon = k\lambda_{mfp,th}$ from the shock, where $\lambda_{mfp,th}$ is the mean free path.
3.3. MHD AND MC TEST-PARTICLE SIMULATIONS

Figure 3.4: Schematic representation of a particle passing from upstream to downstream, through a pair of upstream and downstream supercells. When a particle enters a cell marked as directly upstream, its position $x_{\text{init}}$ in the computational domain is recorded, so that, when leaving the regime of the current supercell pair, the new position in the normal background is found by adding the displacement vector $\vec{d}$ to the recorded coordinates. $S$ is the non-rotated reference frame, $\text{SC}$ is the rotated reference frame used in the supercell regime. Reproduced from Grimaldo et al. (2017a), with the permission of AIP Publishing.

for the thermal particles (see Eq. (2.27)), and $k$ is an arbitrary constant. In our simulations, we use $k = 1$. The corresponding position, both in the supercell, $\mathbf{r}_{\text{init}}^{\text{SC}} = (x_{\text{init}}^{\text{SC}}, y_{\text{init}}^{\text{SC}}, z_{\text{init}}^{\text{SC}})$, and in the standard background, $\mathbf{r}_{\text{init}} = (x_{\text{init}}, y_{\text{init}}, z_{\text{init}})$, is calculated and saved for later use. The Monte Carlo simulation of the particle then proceeds in a two-cells set-up, as described in Section 3.2 (in this case with the upstream and downstream SCs), but with a notable difference: since the SCs are embedded in the standard MHD background grid, when a particle crosses a cell boundary which is not at the interface between the upstream and the downstream SCs, the simulation is not stopped. Instead, the displacement vector of the particle in the SCs from the injection to the point where it leaves the two-cells system is found (using the previously saved position):

$$d^{\text{SC}} = \mathbf{r}_{\text{new}}^{\text{SC}} - \mathbf{r}_{\text{init}}^{\text{SC}}$$

and rotated to the standard frame:

$$\mathbf{d} = R^{-1}d^{\text{SC}}.$$  

Herein, $R$ is the rotation matrix allowing to pass from the Cartesian frame $S$ to the local SC frame (see Figure 3.4). The new position in the Cartesian grid is then easily found by adding the displacement vector to the previously saved position: $\mathbf{r}_{\text{new}} = \mathbf{r}_{\text{init}} + \mathbf{d}$. At this point, the particle can be (i) in a cell marked as directly upstream, (ii) in a cell marked as directly downstream, or (iii) far upstream or downstream. In the first two cases, a new SC pair containing the position of the particle is searched for. For case (i), finding the appropriate cells is straightforward, since every cell directly upstream is associated with its own SCs pair. For case (ii), the situation is
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more complex. In fact, some positions downstream are included in more than one downstream SC. Hence, the upstream SC minimizing the distance of its centre to the particle is chosen. When passing from one supercell pair to another, the distance of the particle from the shock can vary, due to the discretization of the shock position in the MHD Cartesian grid. Aiming at limiting the effect of the numerical spatial discretization on the probability for a particle to return to the shock, we put the particle in the new supercell pair at the mean distance from the shock:

$$\varepsilon_{SC} = \frac{\varepsilon_{SC}^{init} + \varepsilon_{SC}^{new}}{2},$$

(3.19)

where $\varepsilon_{SC}^{init}$ is the distance from the shock in the supercell pair just left by the particle and $\varepsilon_{SC}^{new}$ is the distance from the shock in the supercell pair just entered by the particle, the position of the new supercell being determined as described above. The price to pay for averaging the distance from the shock in the SC system, while keeping the particle at the same position in the standard MHD computational box, is to give up a fixed position of the shock in the standard grid coordinates. Recall, however, that the shock transition is up to 3 cells wide, therefore the precise location of the shock is not well defined within that transition layer anyway.

In the cases when a particle upstream (downstream) of the shock enters a new supercell pair, but the coordinates in the new frame correspond to a downstream (upstream) position, we first try to average the distances (with sign) from the shock, similar to what has been just described. If the particle coordinate is still downstream (upstream), we put it upstream (downstream), at a distance $\varepsilon_{SC} = \min(10 \, r_g, \Delta x)$. This allows to keep the particle on the “right” side, at a reasonable distance from the shock, at the same time limiting the artificial shift in position to at most one half of the supercell size. We note that with the parameters of the system studied here, no such artefacts or apparent inconsistencies have been found in the final simulations using the extended computational box.

In the case of a particle exiting the SC pair and ending up far upstream or far downstream, its momentum is simply transformed to the non-rotated standard frame, and the simulation is continued. The removal of particles downstream of the shock, at the distance $x_D$ (Eq. (3.13)), is used only when the particles are in a SC pair, in order to avoid simulating the advection of low-energy particles which have a negligible probability to return to the shock or to reach the contact discontinuity. The simulation of a particle is otherwise continued until the limit on the number of scatterings has been reached, or the particle leaves the whole region simulated in the combined approach using the MHD background.

Summarizing, the simple injection of particles into the MHD background, using the Cartesian grid, can cause two types of artefacts. First, the thermal particles might not be accelerated (or the efficiency might be very low) due to the 3-cells wide shock transition in the MHD simulations. Second, due to the inclination of the shock front with respect to the cell boundary surface, the direction of the background fields with respect to the shock normal can differ substantially from the correct configuration. This can produce very hard spectra with no physical meaning. The introduction of the SC system allows to obtain a sharp shock discontinuity, and to remove the artefact of hard spectra, as shown in Figure 3.2 (b). By construction, the shock-jump conditions are not strictly fulfilled, because the fields of the supercells result from averaging of the fields of the MHD background cells. However, of course, the MHD simulations are based on the
conservation of fluxes between the cells of the Cartesian grid. We chose this approach in order to be more consistent with the large-scale MHD background. An alternative method consists in using the upstream conditions of the supercells to calculate the downstream fields by means of the shock jump conditions. A comparison of the particle spectra obtained with the two solutions can be found in Section 3.5.2.

**Magnetic field.** In Grimaldo et al. (2015) the plasma background was based on HD simulations. There, we determined the strength (but not the topology) of the magnetic field directly upstream of the two shock fronts by following the approximation formulated by Usov and Melrose (1992) (see Eq. (1.6)) using the surface magnetic field of the star on the same side of the WCR as the considered shock. At the shocks, we applied the MHD shock-jump conditions (Eqs. (2.39) with \( F_w = 0 \) and \( p_w = 0 \)) to obtain the field in the cells directly downstream. Inside the WCR, we adopted an approach similar to that of Pittard and Dougherty (2006): starting from the first cells downstream, we assumed the magnetic field to be proportional to the thermal energy density of the underlying plasma (Eq. (1.8)). The fields on either side of the WCR were thus scaled from the shock fronts up to the contact discontinuity. There, the magnetic field was also discontinuous, assuming the same surface magnetic field for the two stars. Later MHD simulations confirmed that the field strengths can differ by a considerable amount on the two sides of the contact discontinuity (see Section 4.3, and Kissmann et al. (2016)). The direction of the magnetic field was assumed to be parallel to the plasma velocity.

In later test-particle simulations (Grimaldo et al., 2017a), we used the fields from the MHD simulations for the background in the standard cells, including the magnetic field. The latter was determined in the supercells by averaging between standard cells, using the same method described above.

### 3.3.2 Parallel particle splitting

In order to improve statistics at higher energies, the technique of particle splitting is employed (e.g. Jones and Ellison (1991); Ostrowski and Schlickeiser (1993)).

Our Monte Carlo code is based on parallel programming, using the Message Passing Interface library Open MPI. The 3D background is loaded in a shared memory domain, allocated employing inter process communication (IPC).\(^7\) Our implementation of particle splitting, explained in the following, aims at better exploiting the parallelization, improving the statistics of the results and reducing the waiting time of the CPUs. In the following, we describe the steps of the simulation, including particle splitting, with the aid of Figure 3.5.

A certain number of particles \( N_p \) (e.g. 10 or 100) is assigned to the *working-array* of each thread. They are injected one by one into the simulation box and their position and momentum evolve as described above. If a particle reaches a momentum \( p_a \) such that

\[
(a(p_a) - 3) \log \left( \frac{p_a}{p_R} \right) \geq \log \zeta_p
\]

in the downstream plasma frame, its statistical weight is halved, and the particle is copied to an array of split particles (split-array). In Eq. (3.20), the reference momentum \( p_R \) is initially

\(^7\)For this implementation, I adapted some code by Felix Niederwanger.
the particle momentum at the first shock-crossing, and assumes the new value \( p_R = p_s \) when the particle is split. The factor \( \zeta_p > 1 \) can be adjusted for improving the statistics and the performance of the simulations, while the spectral index \( a(p) \) of the distribution function \( f_1 \), directly upstream of the shock, is given by:

\[
a(p) = -\frac{d \log f_1(p)}{d \log p}.
\] (3.21)

The condition of Eq. (3.20) corresponds to splitting the particle at a momentum such that, for a distribution function described by a power-law \( f_1(p) \propto p^{-a(p)} \), the ratios of the particle densities in the appropriate bins, as defined by Eqs. (3.10)-(3.11), are \( n_1(p_R)/n_1(p_s) \approx \zeta_p \). This scheme can help in maintaining the number of split particles within reasonable ranges, especially when the shock is strongly modified and the spectral index changes with momentum. For the test-particle Monte Carlo simulations, the value of \( a(p) \) is kept at the constant value given by Eq. (2.18).

After the splitting, the simulation of the original particle is continued, until it is either split again, or one of the conditions for removal are met. In the latest version of the parallel splitting implementation (used in Grimaldo et al. (2019)), once a thread finishes to simulate the total number of particles initially assigned to it, it checks if other threads are “lagging behind” and still have to simulate some particles. If this is the case, it takes one of those particles and simulates its history. Again, when finished, the thread checks if there are any protons initially assigned to another thread which can be simulated. As soon as there are no particles left from the initial set, a function checks how many particles have been copied to the split-array. If the number of split particles in any thread is less than \( N_p \), the particles with the highest statistical weights in the split-array are split again, until every empty slot is filled, and the particles are copied to the working-array. This procedure is denoted as Weighted split in Figure 3.5. At this point, each thread has again \( N_p \) particles in the working-array, and a new iteration of block B0 can start.

The described procedure aims at (i) reducing the waiting times of the threads, by distributing the load to other threads, when possible, and (ii) rationally splitting the particles, in order to avoid situations in which, for a given energy range, some simulated particles have a much smaller statistical weight than others.\(^8\) This can result in a waste of computation time, since the contribution to the spectra by the particles with small statistical weight can be “hidden” by the contribution of a particle with higher statistical weight. The iterations follow one another until no more particles are left in the split-array at the end of one iteration. In the first iteration, in which the particles are injected at the shocks with the Maxwell-Boltzmann distribution, new particles are injected until in each thread \( N_p \) of them have been split (see box First iteration of block B0? in the lower part of Figure 3.5). The total number of particles injected in the simulation, \( \mathcal{N}_p \) in Eq. (3.7) is thus usually larger than \( N_p \) multiplied by the number of threads. In such a way, as opposed to splitting particles from the split-array, each particle starting the second iteration has different “initial conditions”. These are the particles actually injected into the acceleration process.

Many particles reaching high energies will thus share at least one part of their history, since they all “descend” from the particles being split in the first iteration. In order to reduce possible

\(^8\)A different version of “weight-based” particle splitting has been used by Ostrowski and Schlickeiser (1993).
biases from one single run of the simulation from the injection to the end, especially in the simulations on the extended MHD background, we introduced a higher level of iterations, i.e. we repeat the execution of block B1 (see Figure 3.5)– typically 10-15 times – and we average the spectra.
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Figure 3.5: Flow chart of block B1. The whole block (from Start to End), which includes the iteration block B0, is iterated typically 10-15 times.
3.3.3 Particle tracking

A useful feature of the code is the possibility to track a selection of particles during the simulation. In particular, when they cross a cell surface, we record their energy, the number of scatterings and the time from the first shock-crossing. This allows to visualize their paths, and to learn where they are accelerated (or possibly lose energy). An example is given in Figure 3.6. The tracking of particles can be helpful for identifying the origin of possible spectral features and to discriminate between physical effects and artefacts (see the discussions in Section 4.3, and in Chapter 5).

![Figure 3.6](image)

Figure 3.6: Tracks of a selection of protons, split from track 1, in the simulation box. Figures from Grimaldo et al. (2017a) and related poster contribution.

3.4 Semi-analytical method for nonlinear DSA and Monte Carlo simulations

As mentioned in Section 2.2, the idea that the cosmic-ray pressure at collisionless shocks may change the shock structure is not new. We also introduced the underlying equations, including the CR pressure and the pressure of Alfvén waves. Motivated by the results of our test-particle simulations of particle acceleration in CWBs (see Section 4.2), we decided to implement a method including local modifications of the shocks due to the pressure of the accelerated protons. Aiming at modelling the effect of the backreaction of cosmic rays at parallel shocks of SNRs, Am-
ato and Blasi (2005) and Caprioli et al. (2009b) (and related articles) developed a semi-analytical method solving the transport equation for the accelerated particles at the shock iteratively, until the energy and momentum fluxes are conserved, from far upstream to downstream of the subshock. We adapted their work, in order to be able to also simulate oblique shock configurations. Furthermore, as described later in this section, we use a different approach for the determination of the injection efficiency, based on Monte Carlo simulations, instead of using an injection parameter. The procedure described below is used for the determination of the nonlinearly modified background in the supercell selected for the injection of the protons in the simulations combining MHD and Monte Carlo simulations, and semi-analytical calculations. Caprioli et al. (2009b) accounted for the possibility that the scattering centres move in the plasma frame with the Alfvén speed calculated using the background magnetic field. They did not find a strong discrepancy between the effective compression ratio and the MHD compression ratio for the typical parameters of SNRs. For the sake of simplicity, we do not include this effect in our model, even though it might have an influence on the strength of shock modification, at positions along the shocks delimiting the WCR where the Alfvén Mach number is small. For a discussion on the topic we refer the reader to e.g. Caprioli (2012) and references therein.

In the model adopted here, the background conditions are determined by the velocity $u$, the density $\rho$, the temperature $T$, and the magnetic field $B$. We assume that all the considered quantities change locally only in the $x$-direction (i.e. in the direction of the shock normal), and that $v_A \ll u$. The steady-state transport equation is then given by:

$$u(x) \frac{\partial f(x,p)}{\partial x} = \frac{\partial}{\partial x} \left[ D(x,p) \frac{\partial f(x,p)}{\partial x} \right] + \frac{du(x,p)}{dx} \frac{\partial f(x,p)}{\partial p} + Q(x,p), \quad (3.22)$$

where $f(x,p)$ is the isotropic part of the distribution function of the accelerated particles, and the diffusion coefficient is given by Eq. (2.26). The source term, which accounts for the injection of particles in the acceleration process, is given by (e.g. Blasi (2002)):

$$Q(x,p) = \frac{\eta \rho \gamma_1}{4\pi m_p p_{inj}^3} \delta(p - p_{inj}) \delta(x), \quad (3.23)$$

where $m_p$ is the proton mass, $\delta$ is the Dirac delta distribution, $p_{inj}$ is the injection momentum, and $\eta$ is the injection efficiency (see below for more details concerning these last two terms). A very good approximation of the solution to Eq. (3.22) is given by (Amato and Blasi, 2005):

$$f(x,p) = f_1(p) \exp \left\{ -\frac{a(p)}{3} \int_{-\infty}^0 dx' \frac{u(x')}{D(x',p)} \right\}, \quad (3.24)$$

where

$$f_1(p) = \frac{\eta \rho \gamma_1}{4\pi m_p p_{inj}^3} \frac{3 \rho_{tot}^3}{\rho_{tot}^3 U_{px}(p) - 1} \exp \left[ -\int_{p_{inj}}^p \frac{dp'}{p'} \frac{3 \rho_{tot}^3 U_{px}(p')}{\rho_{tot}^3 U_{px}(p') - 1} \right]. \quad (3.25)$$

is the distribution function immediately upstream of the subshock, and $a(p)$ is the power law index given by Eq. (3.21). Here and in the following sections, velocities and pressures indicated with capital letters are normalized by $u_0x$ and $\rho_0u_0^2x$, respectively. The mean velocity of the
3.4. SEMI-ANALYTICAL METHOD

scattering centres (of the plasma) seen by a particle of momentum \( p \) is:

\[
\mathbf{u}_p(p) = \mathbf{u}_1 - \frac{1}{f_1(p)} \int_{-\infty}^{0} \frac{d\mathbf{u}(x)}{dx} f(x,p) \, dx .
\]  
(3.26)

Similarly, for the magnetic field we define:

\[
\mathbf{B}_p(p) = \mathbf{B}_1 - \frac{1}{f_1(p)} \int_{-\infty}^{0} \frac{d\mathbf{B}(x)}{dx} f(x,p) \, dx .
\]  
(3.27)

Accordingly, the mean electric field, as seen by a particle of momentum \( p \), is:

\[
\mathbf{E}_p(p) = \mathbf{E}_1 - \mathbf{u}_p(p) \times \mathbf{B}_p(p) .
\]

The momentum flux conservation equation (Eq. (2.30b)), normalized by the kinetic momentum flux, reads:

\[
1 + P_{g0} + P_{B0} = U_x(x) + P_g(x) + P_w(x) + P_B(x) + P_c(x) .
\]  
(3.28)

Here, \( P_g \) is the thermal pressure of the plasma, \( P_w \) is the pressure associated with the Alfvén waves produced by the resonant-streaming instability (see Section 2.2), \( P_B \) is the background magnetic field pressure due to the \( z \)-component of the field, and \( P_c \) is the pressure of the accelerated protons. Considering only adiabatic heating in the precursor, one has:

\[
P_g(x) = \frac{U_x^{-\gamma}(x)}{\gamma M_0^2 x} ,
\]  
(3.29)

where \( M_0^2 = \rho_0 u_{0x}^2 / (\gamma p_{g0}) \). The \( z \)-component of the magnetic field exerts a pressure:

\[
P_B(x) = \frac{B_z^2(x)}{2\mu_0 \rho_0 u_{0x}^2} ,
\]  
(3.30)

where \( B_z \) can be found using Eq. (2.38b). This pressure term is present only if the shock is not strictly parallel, and is usually negligible in the precursor. However, as we will see in Section 4.3, it has an influence on the jump conditions at the subshock and on the total compression ratio in the case of efficient particle acceleration, especially in the absence of magnetic field amplification. The term \( P_w \), the pressure due to Alfvén waves, is given by (see Appendix A for a brief derivation):

\[
P_w(x) = \frac{U_x^{-\frac{3}{2}}(x)}{4M_{0x}} \left[ \left( 1 - U_x^2(x) \right) \cos \theta_{B0} \right] .
\]  
(3.31)

In order to find the nonlinearly modified shock profile, we proceed as illustrated by Caprioli et al. (2009b), but using the equations adapted for the case of oblique shocks. We first set the compression ratio at the subshock, \( r_{\text{sub}} \), and therefore the total compression ratio \( r_{\text{tot}} \) (see below for more details concerning this point). A scheme of the algorithm is shown in Figure 3.7. In the first iteration we set \( u_{px}(p) = u_x(x) = u_{1x} \). Starting with a different value, e.g. \( u_{0x} \) does not affect the final result. The magnetic field, the wave pressure and the diffusion coefficient are calculated according to Eqs. (2.38b), (3.31) and (2.26). We compute \( f_1(p) \) using Eq. (3.25), which in turn allows to compute \( P_c, \) i.e. \( P_c(x) \) at the subshock, according to:

\[
P_c(x) = \frac{4\pi}{3\rho_0 u_{0x}^3} \int_{p_{\text{min}}}^{p_{\text{max}}} dp \, p^3 v(p) f(x,p) .
\]  
(3.32)
Figure 3.7: Scheme of the algorithm used for the calculation of the nonlinearly modified shock profile at a fixed sub-shock compression ratio $r_{\text{sub}}$. The indices at the exponent indicate the equation used for the respective calculation. The numbers of the arrows indicate the step within the single iteration.
At this point, we calculate the pressure of the accelerated particles also with Eq. (3.28), and we find

\[ K = P_{cl}^{(3.28)} / P_{cl}^{(3.32)} , \]

where the bracketed exponent indicates the equation used for the computation. This allows us to normalize \( f_1(p) \) and obtain

\[ f_1^*(p) = K f_1(p) , \]

so that the momentum flux between far upstream and the subshock is conserved. This normalized distribution function is used to calculate \( f(x,p) \) by means of Eq. (3.24), and \( P_c \) by means of Eq. (3.32). Finally, the velocity profile \( U_x(x) \) can be obtained using Eq. (3.28), which allows to find \( B(x) \) and \( P_w(x) \), and in turn the diffusion coefficient \( D(x,p) \) using Eqs. (2.38b), (3.31) and (2.26), respectively. A new iteration is then started by calculating \( u_{px}(p) \) by means of Eq. (3.26). In order to achieve faster convergence, we average the flow profile between iteration \( n \) and \( n-1 \), before computing \( B(x) \), \( D(x,p) \) and \( u_{px}(p) \). A similar solution has also been used by Amato and Blasi (2005) (private communication). We stop the cycle when \( K \) does not change more than a specified amount between consecutive iterations. At this point, we check the value of \( K \): if it is within a 15\% tolerance interval around 1, an acceptable solution has been found, otherwise a new \( r_{sub} \) is used and the procedure is repeated. Since the injection efficiency is higher for stronger shocks, the compression ratio at the subshock is increased if \( K > 1 \) (i.e. if the cosmic ray pressure required for energy and momentum flux conservation is greater than the pressure calculated by means of the distribution function and Eq. (3.32)), while it is decreased if \( K < 1 \).

Due to the statistical nature of the Monte Carlo simulations, some fluctuations in the injection efficiency are unavoidable, at every cycle with \( r_{sub} \) fixed, and a tighter tolerance range would require very high statistics, which in turn would require unreasonable computation times. As discussed in Chapter 4, we found that there is a dramatic improvement concerning momentum and energy flux conservation when employing the nonlinear approach, as compared to the test-particle setup. A tighter constraint on the tolerance range would be only a minor correction. Moreover, the uncertainties in the microphysics of acceleration for shocks where the ions reach energies well above their rest mass, as well as the possible development of other instabilities (e.g., the Bell instability), would make it unlikely to improve the reliability of the results by tightening the convergence criteria.

Eq. (2.40) allows us to compute the flow velocity and magnetic field downstream, when combined with Eqs. (2.38b) and (2.37c), once the conditions directly upstream of the subshock are known. In order to find \( r_{tot} \), we numerically solve Eq. (2.40) keeping \( r = r_{sub} \) fixed and employ the relation \( U_{1x} = r_{sub}/r_{tot} \). In this way, knowing the far upstream conditions and \( r_{sub} \), we can determine the background directly upstream and downstream of the subshock. At this point, the only missing ingredient is the fraction \( \eta \) of particles being injected into the acceleration process. Caprioli et al. (2009b) use the formula:

\[ \eta = \frac{4}{3\sqrt{\pi}} (r_{sub} - 1) \psi^3 e^{-\psi^2} . \]

They consider a Maxwell-Boltzmann distribution with the temperature of the shocked plasma and assume that the particles with momentum \( p_{mj} \geq \psi p_{th,2} \), with \( p_{th,2} = \sqrt{2m_p k_B T_2} \), are
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injected into the Fermi acceleration. This approach aims at modelling the thickness of the shock, assuming that particles with gyroradii smaller than the shock thickness can only be advected away from the shock and will not contribute to the non-thermal tail of the particle distribution function. Values of the injection momentum factor \( \psi \approx 2 - 4 \) are usually chosen. Blasi et al. (2005) showed that, for example, \( \psi \approx 2 \) corresponds to a shock thickness \( \lambda_{sh} = r_{g,2}^{th} \), and \( \psi \approx 3.25 \) corresponds to \( \lambda_{sh} = 2r_{g,2}^{th} \), where \( r_{g,2}^{th} \) is the gyroradius of a particle with momentum \( p_{th,2} \).

In our approach, we do not make use of any assumption for the injection parameter. Instead, we determine \( \eta \) by means of Monte Carlo simulations. As mentioned in Section 2.2.1, with the Monte Carlo method a fraction of the particles scattered isotropically and elastically in the plasma frame are naturally injected into the acceleration process. For the determination of \( \eta \), which is then used in the semi-analytical calculations, we proceed as follows. At the beginning of the first cycle associated with the first guess for the compression ratio \( r_{sub} \), we roughly estimate the injection efficiency as follows. We initialize the background for Monte Carlo simulations with the parameters of the subshock (i.e. \( u_1, B_1 \), etc., upstream and \( u_2, B_2 \), etc., downstream). We then inject the particles upstream, close to the shock, and estimate \( \eta \) as \( \eta = N_{ret}/N_p \), where \( N_{ret} \) is the number of particles recrossing the shock from downstream to upstream, and \( N_p \) is the total number of injected particles.\(^9\) Using the so obtained injection efficiency, we calculate a new \( \psi \) which satisfies Eq. (3.35), and a new \( p_{nij} = \psi p_{th,2} \). We then find the modified shock solution for the current \( r_{sub} \) employing the semi-analytical method described above. Finally, in order to obtain a more accurate estimate for the injection efficiency, and in turn for the density of the non-thermal population, which is essential for obtaining an energy-conserving solution, we run Monte Carlo simulations in the modified background, letting particles reach momenta \( p \approx 100 p_{nij} \). The particle density obtained from the Monte Carlo runs is then compared, at the momentum \( p = 10 p_{nij} \), to the particle density obtained from the semi-analytical calculations, in order to find a corrected \( \eta \) and the respective \( K \). The comparison is done at \( 10 p_{nij} \) in order to avoid the low-energy part of the spectrum after the thermal peak, which shows some oscillations, and the cutoff at the end of the distribution. An even more accurate estimation would require to simulate the spectra up to higher energies, since there can be a difference in the slopes, up to momenta of \( p \approx m_pc \), of the non-thermal distributions obtained with the Monte Carlo technique as compared to the ones obtained with the semi-analytical method (see Figure 3.24 (a)). This discrepancy, ascribed to different treatments of the transition between thermal and non-thermal particles, was also found in Caprioli et al. (2010b). It has been shown in the same work that the spectra at high energies (i.e. above momenta \( p \approx m_pc \)) are in good agreement. For the purposes of the work presented in this thesis, the possible gain in accuracy in the determination of the normalization of the non-thermal distributions does not justify the related increase of the computation times.

For the Monte Carlo simulations we use a two-cells setup (upstream and downstream), similar to that introduced in Section 3.2. The shock modification is taken into account by using the momentum-dependent averaged quantities \( u_p(p), B_p(p) \): when a particle of momentum \( p \) is

\(^9\)A different estimation (educated guess) of the value of the injection parameter at the beginning of the calculation does not affect the final results, due to the more precise determination of the appropriate \( \eta \) used once the solution for a certain \( r_{sub} \) has been found, as described below.
in the upstream cell, we use the background fields $u_p(p)$, $B_p(p)$, given by Eqs. (3.26) and (3.27), and the corresponding $E_p(p)$. Owing to the spatial dependence of the magnetic field, the diffusion coefficient varies with the distance from the subshock (see Eq. (2.26)). This is still true if, following Caprioli et al. (2009b), the amplified magnetic field is used in Eq. (2.26), i.e. when using $B(x) = \delta B(x) \equiv \sqrt{2\mu_0 P_u(x)\rho_0 u_0^2}$ in that equation. In order to obtain the mean diffusion coefficient for a particle of momentum $p$, we employ an effective $B_{\text{eff}}(p)$, oriented like the computed $B_p(p)$, but with a magnitude $|B_{\text{eff}}(p)| = \max(|B_p(p)|, \delta B_p(p))$, when making use of the magnetic field amplification due to resonant-streaming instability. Here, 

$$
\delta B_p(p) = \delta B_1 - \frac{1}{f_1(p)} \int_{-\infty}^{0} \frac{d\delta B(x)}{dx} f(x, p), \tag{3.36}
$$

and $B_p$ is given by Eq. (3.27). The maximum is used in order to ensure that the magnetic field used for the diffusion coefficient is not smaller than the background field, which is used for the test-particle simulations. In this way, the gyroradius of a particle in the Monte Carlo simulations is the same as the gyroradius in the expression for the diffusion coefficient (Eq. (2.26)). Accordingly, we use the appropriate electric fields, as well as mean scattering times. Choosing such a diffusion coefficient appears reasonable, considering results from PIC simulations. In fact, Caprioli and Spitkovsky (2014c) found that, for strong shocks, the energetic particles experience Bohm diffusion in the magnetic field amplified predominantly by the non-resonant hybrid instability.

The full combination of MHD simulations together with the nonlinear semi-analytical method and Monte Carlo simulations proceeds as follows. The background is initialized in the selected computational domain as described in Section 3.3. A position along the shock fronts is then selected for injection of particles in the system. The upstream fields of the corresponding SC pair are then used as the far upstream conditions, and a modified-shock solution is found as described in this section. The particles are thus injected into the supercell with modified background, embedded in the selected MHD domain. As long as the particles are in the nonlinearly modified supercell, the simulation is carried out as described in this section, while it proceeds as described in Section 3.3 otherwise. We note that the procedures applied when a particle leaves a supercell pair, possibly involving a shift in the position of the shock front, cannot affect the results for local nonlinear modifications. In fact, the nonlinear shock profile is calculated separately, only for a single supercell pair at a time (still not embedded in the extended Cartesian grid). We stress that, with the parameters of the system studied here, no artefacts or apparent inconsistencies have been found in the final results of simulations using the extended computational box, neither in the test-particle approach, nor when local feedback is considered. Even in the (in our opinion, unlikely) case in which our method, including possible shifts in the SC positions, would influence the simulations in a hidden way, the conclusions drawn in Section 4.3.3, comparing the test-particle results to those with local shock modification, would not be affected. In fact, the way particles are moved in the extended computational box, and the assignment of coordinates in the supercells, is exactly the same for the two cases. Thus, although other solutions might be worth being investigated, we stick to this implementation for the studies presented in this thesis.
This section concludes the description of the computational method. Before presenting the results, we show in the next section the tests carried out for the validation of the code.
3.5 Code Validation

In this section, we validate the code by reproducing results in simple setups, which either have an analytical solution or have been used in other studies, with which we can compare the results. As described above, the code developed during this PhD project includes Monte Carlo simulations, the iterative semi-analytical method for the calculation of a modified shock profile, and a combination of them with each other and with the MHD simulations from CRONOS. First, we consider the Monte Carlo part.

3.5.1 Monte Carlo

Isotropy of velocities in the plasma frame. The first step of a simulation, after background initialization, is the injection of the particles into the simulation box. Vladimirov (2009) obtained the correct distribution of velocities needed at injection, for ensuring that their distribution in the plasma frame, as measured close to the injection point, is isotropic. In Figure 3.8 we verify the isotropy of the angular distribution of particles $g(\mu)$ measured in the plasma frame at three different distances downstream of the injection position, namely very near ($x_m = 10^{-5} r_g$), near ($x_m = r_g$), and far downstream ($x_m = 100 r_g$). The normal to the measurement surface is parallel to the flow velocity. The test is shown for a background plasma with $u_0 = 10^5$ m s$^{-1}$, $T_0 = 1.15 \times 10^5$ K, $n_0 = 5 \times 10^5$ m$^{-3}$, corresponding to a Mach number $M_0 = 2.5$. The magnetic field, of strength $B_0 = 5 \times 10^{-10}$ T, is dynamically unimportant, since the magnetic pressure is much lower than the thermal pressure. The particles ($6 \times 10^4$) have been injected with a kinetic energy $E = k_B T$ in the plasma frame. Figure 3.8 (a) shows the angular distribution $g(\mu)$ obtained when naively injecting particles by isotropizing their velocities in the plasma frame. Similar to what was found by Vladimirov (2009), the distribution is not isotropic in the plasma frame, when measured very close to the injection position, while it becomes isotropic far downstream. Additionally, it can be seen that, by virtue of the scattering of the particles in the fluid, the distribution is already almost isotropic at a distance $x_m = r_g$ from the injection position. From Figure 3.8 (b), which shows the distribution measured at the same distances as in Figure 3.8 (a) but with the prescription by Vladimirov (2009), it can be seen that our code can reproduce those results and that both the injection and the scattering process ensure isotropy of particle velocities in the plasma frame (see also Section 3.2). This is also confirmed by Figure 3.9, which shows the angular distribution of particles for a flow velocity (and magnetic field) oriented at an angle $\theta = 60^\circ$ with respect to the normal to the measurement surface. In this case, the speed of the plasma has been increased to $u_0 = 2 \times 10^5$ m s$^{-1}$, in order to keep $M_0 = 2.5$.

For high Mach numbers, i.e. when the thermal speed is much smaller than the plasma flow speed, the anisotropies very close to the injection position are negligible even when using the naive injection algorithm. This is because the weight $1/v_x$ used when measuring the distribution of particles crossing a measurement surface (e.g. Eq. (3.8)) does not change much in the shock frame, for different $\mu$’s in the plasma frame. Therefore, in typical unmodified shocks of CWBs, the difference between the naive and the correct injection procedure is not appreciable. In modified shocks, the local Mach number close to the subshock can become much smaller than the unmodified one, and the difference may become important.
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Figure 3.8: Angular distribution of particles in the plasma frame, for obliquity $\theta = 0^\circ$ with respect to the normal to the measurement surface, measured at different distances from the injection position, as indicated in the legend. (a) Naive injection procedure. (b) Injection procedure described by Vladimirov (2009).

Figure 3.9: Angular distribution of particles in the plasma frame, for obliquity $\theta = 60^\circ$ with respect to the normal to the measurement surface, measured at different distances from the injection position, as indicated in the legend. (a) Naive injection procedure. (b) Injection procedure described by Vladimirov (2009).
3.5. CODE VALIDATION

Standard test-particle DSA solutions. In order to validate the Monte Carlo simulations in the simple test-particle setup, we compare the results obtained with our code to the expectations from analytical calculations. In Figure 3.10 (a) we show the distribution functions, in the shock frame, of the particles accelerated at shocks with Mach number \( M_{0x} = 2.5 \) (cases A, B, and C of Table 3.1). In Figure 3.10 (b), the spectra for high Mach numbers \( M_{0x} = 384 \) are presented (cases D, E, and F of Table 3.1). While high-Mach-number shocks are typically found in non-modified models of CWBs, the backreaction of the accelerated particles can significantly reduce \( M_0 \), motivating the interest for the low-Mach-number configurations. The tests shown proof these two cases, at different obliquities. From both Figures 3.10 (a), and (b), it can be seen that the non-thermal distributions resulting from our test-particle simulations nicely match the theoretical predictions.

In Figure 3.11 the mean times needed for the accelerated particles to reach a certain kinetic energy are shown and compared with the theoretical predictions (Eq. (2.28)). In all cases, which have considerably different parameters amongst each other, we find excellent agreement.

This concludes the validation of the simple Monte Carlo part of our approach. In the following, we will consider the system of superimposed cells at the shock fronts.

Figure 3.10: Non-thermal distribution functions of protons, multiplied by \( [p/(m_p c)]^4 \), for the test cases summarized in Table 3.1. The straight reference lines indicate the theoretical expectations for the slopes of the spectra (cf. Eq. (2.11)). (a) Shocks with Mach number \( M_x = 2.5 \), similar to the parameters used for the test of isotropy (Figures 3.8, 3.9). (b) Strong shocks \( (r \approx 4) \) with parameters similar to unmodified conditions at CWBs.
3.5.2 Superimposed cells on MHD background

Here we want to focus on a particular aspect of the initialization of the supercell system, namely the determination of the shock orientation. Moreover, we will briefly discuss the differences between the determination of the downstream background by means of averaging of the MHD
3.5. CODE VALIDATION

fields and by employing the shock jump conditions, Eqs. (2.39). In Section 3.3.1 we have explained the reasons for introducing the supercell system in the simulations combining the MHD modelling of CWBs and the Monte Carlo technique for particle acceleration. In Figure 3.2 (b), we displayed the distribution functions obtained in the absence and in the presence of the supercells, highlighting that the latter case yields more physical results. Aiming at testing the procedure used for the determination of the shock orientation, we will start by analytically prescribing the shape of the WCR. We will thus compare the orientation of the shock normal obtained analytically with that obtained as described in Section 3.3.1. The shock orientation for a selection of slices of the WCR resulting from the MHD simulations will be shown, in order to be able to estimate the uncertainties in the model used for the simulations of particle acceleration. We will also show the results of simulations with injection at different positions, selected in order to estimate the effects of the uncertainties in the shock orientation on the final spectra of accelerated particles.

For the first test presented here, we used an analytical prescription for the background, so that the region recognised as WCR by the shock tracking routine is enclosed between two paraboloids with symmetry axis along the x-direction (see Figure 3.12). The paraboloids have been chosen so as to resemble the shape of the WCR resulting from the MHD simulations.

The position of the shock on the left (B shock) is described by the equation

\[ x = s^{B}(y, z) \equiv -\frac{y^2}{80} - \frac{z^2}{68} - 1 , \]  

while the position of the shock on the right (WR shock) is described by

\[ x = s^{WR}(y, z) \equiv -\frac{y^2}{295} - \frac{z^2}{240} + 7 . \]  

The coordinates of the cells on the grid, i.e. integer numbers, have been used in place of the real coordinates. This explains the truncated form of the paraboloids, visible in Figure 3.13. The shape of the shocks parallel to the x-z (x-y) plane at a given y (z) coordinate, together with the polar (azimuthal) angles of the local normal to the shocks, are shown in Figures 3.14 and 3.15 for the B shock and the WR shock, respectively. The orientation of the shock normal obtained by means of the procedure described above (green crosses in the plots) are in fairly good agreement with the analytical result (light blue line). The analytical unit vector normal to the paraboloids is:

\[ \hat{n} = \frac{\nabla S(x, y, z)}{|\nabla S(x, y, z)|} , \]  

where \( S(x, y, z) = \pm [x + s(u, z)] \), with the positive sign for the B shock, and the negative for the WR shock, in order to keep the normal pointing in the downstream direction.

Some oscillations, caused by the discrete jumps of the shock position, are visible especially in Figure 3.15 (b). There, the largest deviations of the reconstructed orientation from the analytical result are \( \approx 5^\circ \). When considering the orientation of the shock surfaces obtained from the MHD simulations (Figures 3.16 - 3.19), the comparison with an analytical reference is not possible. It
Figure 3.12: Analytical model of the WCR used for code validation. The shocks are paraboloids described by Eqs. (3.37) and (3.38).

can be seen, however, that the polar and azimuthal angles of the shock normal obtained with Eq. (3.14) have values close to what can be estimated by inspection of the corresponding slices of the shocks (magenta crosses). The strongest oscillations are visible in Figure 3.17 (a), and are \( \lesssim 12^\circ \) from peak to peak, consistent with the tests using the analytical functions for modelling the shape of the shocks. The pronounced protrusion in Figure 3.16 (a), on the contrary, is a real feature of the surface of the WCR.

Due to the discretization of the computational domain and to the oscillations in the orientation obtained with the presented method, there exist differences between the spectra obtained for neighbouring cells. In order to estimate the impact of the discrete position of the shocks, and of the oscillations in the obtained orientation of the shock normal, we compared the proton spectra obtained by injecting the particles at two neighbouring cells separated by a discrete jump of the shock front position in the \( x \)-direction (Figure 3.20), and at the two cells marked by the red points in Figure 3.17 (Figure 3.21). The two cells have been selected because they correspond to a minimum (\( \theta = 90^\circ \)) and a maximum (\( \theta \approx 102^\circ \)) in the oscillation of the reconstructed polar angle of the shock normal. Both, test-particle and nonlinear simulations have been carried out.
The strongest differences are found in the test-particle spectra for the case of cells separated by a discrete jump in the shock position. The differences in the spectral indices are on the order of a few percent. The corresponding nonlinear results are very close to each other (see Figure 3.20). The non-thermal proton spectra for the two cells with a difference in the shock orientation of \( \approx 12^\circ \), plotted in Figure 3.21, are almost indistinguishable (compare the solid lines with the dashed lines). The difference in the position of the thermal peaks in the nonlinear results is caused by the difference in the component of the flow velocity in the direction perpendicular to the shock normal far upstream. The \( x \)-component is reduced by the pressure of the accelerated particles, so that the velocity in the \( z \) direction determines the kinetic energy of the bulk flow in the shock frame.

Finally, we compare the particle spectra at the shocks when the downstream conditions are obtained by the averaging procedure described in Section 3.3.1 to those resulting when employing the shock jump conditions. Figure 3.22 shows the differences of the spectra with proton injection at the same position as for Figure 3.21. The non-thermal distributions obtained by averaging the fields of the MHD simulation downstream are up to \( \approx 3 \) times higher than those found when employing the shock-jump conditions. This is likely attributable to the further deceleration of the plasma flow downstream of the shock, close to the equatorial plane, in the WCR of the MHD simulations, which yields smaller advection velocities than for the case of using the shock jump conditions. In Figure 3.23, the difference of the spectra with particle injection at the same neighbouring cells as for Figure 3.23, separated by a discrete jump of the shock front position in the \( x \)-direction, is shown. The differences between the two approaches are more evident here. For both injection positions, the non-thermal distributions obtained by employing the shock-
jump conditions are close to a power law $f(p) \propto p^{-a}$, with spectral index $a = 4$. The distribution functions at the shocks resulting from initializing the downstream supercell with the averaged fields of the MHD simulation are steeper, with spectral indices $a \approx 4.2$ and $a \approx 4.3$. For the examples shown, the protons were injected at the B shock, at a considerable distance from the apex of the WCR.\footnote{More precisely, the injection position corresponds to Position B6 introduced in Section 4.3.3.} There, steeper spectra can be expected, considering the high oblique velocities in the WCR, which result from the complex interaction of the winds of the stars with each other and with the radiation fields of the stars.\footnote{For example, the WR-star radiation field can further accelerate the B-star wind via line-driven acceleration, as discussed, e.g., by Reitberger et al. (2014b).} The correct test-particle solution would likely lie between the two results: the low-energy part of the spectrum might be closer to that obtained with the jump conditions, while the high-energy range can be expected to be that of the averaged solution, due to the larger diffusion coefficient of the associated particles. For our simulations we use the averaging procedure, aiming at being more consistent with the large-scale MHD background.

We note that the difference between the test-particle and the nonlinear results is in all cases of about two orders of magnitude (or more). Also in light of this, the current approximation is sufficient for semi-quantitative investigations, especially if focussing on the possible causes for the elusiveness of CWBs in the $\gamma$-ray band. We leave the refinement and optimization – needed for quantitative comparisons to observational data of specific systems – to future developments (see also the discussion in Chapter 5).
Figure 3.15: Profiles of the WR shock of the analytical model of the WCR, for the $y = 0$ plane (a) and the $z = 0$ plane (b), and respective theoretical orientations and numerical approximations obtained as described in the text.
Figure 3.16: Profiles of the B shock of the MHD model used in the simulations presented in Sections 4.2 and 4.3, for the $y = 0$ plane (a) and the $z = 0$ plane (b), and respective numerical approximation of its orientation obtained as described in the text.

Figure 3.17: Same as Figure 3.16, but for the WR shock. The red points indicate the cells used for injection of protons producing the spectra of Figure 3.21.
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Figure 3.18: Profiles of the B shock of the MHD model used in the simulations presented in Sections 4.2 and 4.3, for the $y = 0$ plane (a) and the $z = 500$ plane (b), and respective numerical approximation of its orientation obtained as described in the text.

(a) (b)

Figure 3.19: Same as Figure 3.18, but for the WR shock.

(a) (b)
Figure 3.20: Proton spectra obtained by injecting particles at two neighbouring cells of grid-coordinates \((i,j,k) = (i_{SF}[j_0,k_0], j_0, k_0)\), and \((i,j,k) = (i_{SF}[j_0,k_0 - 1], j_0, k_0 - 1)\). The two cells are separated by a discrete jump in the \(x\)-direction: \(i_{SF}(j_0,k_0) - i_{SF}(j_0,k_0 - 1) = 1\). Both the results in the test-particle approach and those including nonlinear shock modification are shown. The reference lines are power-laws corresponding to distribution functions \(f(p) \propto p^{-a}\), with spectral index \(a = 4.2\) (upper line), and \(a = 4.3\) (lower line).
Figure 3.21: Proton spectra (in the shock frame) obtained by injecting particles at the WR shock, at the two cells marked by the red, filled points in Figure 3.17. The test-particle results are almost indistinguishable. The different positions of the bulk flow peaks of the nonlinear solutions are attributable to a larger (≈ 2.5 times) z-component of the flow velocity when the polar angle of the shock normal is \( \theta = 102^\circ \), as compared to the cell where \( \theta = 90^\circ \). In both cases, the z-component becomes larger than the x-component of the flow velocity, therefore determining the kinetic energy of the bulk flow in the shock frame.
Figure 3.22: Proton spectra obtained by injecting particles at the WR shock, at the two cells marked by the red, filled points in Figure 3.17. The results of the simulations applying the averaging procedure described in Section 3.3.1 and of those employing the shock-jump conditions for initializing the downstream supercells are shown.
Figure 3.23: Proton spectra obtained by injecting particles at two neighbouring cells of grid-coordinates $(i, j, k) = (i_{SF}[j_0, k_0], j_0, k_0)$, and $(i, j, k) = (i_{SF}[j_0, k_0 - 1], j_0, k_0 - 1)$. The two cells are separated by a discrete jump in the $x$-direction: $i_{SF}(j_0, k_0) - i_{SF}(j_0, k_0 - 1) = 1$. The results of the simulations applying the averaging procedure described in Section 3.3.1 and of those employing the shock-jump conditions for initializing the downstream supercells are shown. The reference lines are power-laws corresponding to distribution functions $f(p)p^{-a}$, with spectral index $a = 4.2$ (upper line), and $a = 4.3$ (lower line).
### 3.5.3 Semi-analytical method for nonlinear DSA

Here, we summarize the results of our calculations, and compare them to four examples of Caprioli et al. (2009b), where only parallel shocks were considered (see Table 3.2). The results of the semi-analytical calculations in combination with the Monte Carlo simulations, used to obtain the injection efficiency (last two rows of Table 3.2) will be discussed in the next section. For all cases, the particle density is \( n_0 = 0.5 \times 10^6 \text{ m}^{-3} \), the magnitude of the magnetic field is \( B_0 = 5 \times 10^{-11} \text{ T} \), the plasma speed upstream, in the shock frame is \( u_0 = 5.9 \times 10^6 \text{ m s}^{-1} \), and the injection momentum factor is set to \( \psi = 3.7 \), as in the reference paper. The results for Mach numbers \( M_0 = 500 \) and \( M_0 = 50 \) are shown, which correspond to temperatures \( T_0 = 10^4 \text{ K} \) and \( T_0 = 10^6 \text{ K} \), respectively. As mentioned in Section 2.2, our treatment differs to some extent from the one in Caprioli et al. (2009b), since we do not consider the possible nonzero velocity of the scattering centres in the plasma frame. Nonetheless, the results for the case of a strictly parallel shock are in good agreement with those of Caprioli et al. (2009b), despite the “loose” convergence criteria and the slightly different approach, as mentioned above. Our results for oblique configurations will be presented in Chapter 4.

#### Table 3.2: Comparison of the solutions of this work, with the semi-analytical results of Caprioli et al. (2009b) (first four rows). Only parallel shocks are considered, i.e. \( \theta_B = 0^\circ \). The quantities \( S_{\text{sub}} \) and \( S_{\text{tot}} \) are the effective compression ratios, when the scattering centres move with the Alfvén speed in the plasma frame. Recall that our implementation does not account for this possibility (Section 3.4). The last two rows are the results of the approach using Monte Carlo simulations for the determination of the injection efficiency. All the other calculations have been performed with \( \psi = 3.7 \).

<table>
<thead>
<tr>
<th>( M_0 )</th>
<th>( r_{\text{sub}} )</th>
<th>( r_{\text{tot}} )</th>
<th>( S_{\text{sub}} )</th>
<th>( S_{\text{tot}} )</th>
<th>( p_{\text{max}} )</th>
<th>( T_2 )</th>
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<tbody>
<tr>
<td>500</td>
<td>3.58</td>
<td>112.1</td>
<td>3.43</td>
<td>108.7</td>
<td>0.24</td>
<td>0.88</td>
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<tr>
<td>500</td>
<td>3.84</td>
<td>9.22</td>
<td>3.79</td>
<td>9.12</td>
<td>1.17</td>
<td>126.5</td>
<td>Yes</td>
</tr>
<tr>
<td>50</td>
<td>3.76</td>
<td>16.6</td>
<td>3.70</td>
<td>16.4</td>
<td>0.59</td>
<td>42.3</td>
<td>No</td>
</tr>
<tr>
<td>50</td>
<td>3.84</td>
<td>8.44</td>
<td>3.79</td>
<td>8.36</td>
<td>1.14</td>
<td>154.8</td>
<td>Yes</td>
</tr>
<tr>
<td>500</td>
<td>3.5</td>
<td>118</td>
<td></td>
<td>0.25</td>
<td>0.78</td>
<td>No</td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>3.8</td>
<td>9.8</td>
<td></td>
<td>1</td>
<td>110</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>3.7</td>
<td>18.0</td>
<td></td>
<td>0.6</td>
<td>36</td>
<td>No</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>3.8</td>
<td>9.0</td>
<td></td>
<td>1</td>
<td>135</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>2.4</td>
<td>17</td>
<td></td>
<td>1</td>
<td>5.1</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>2.2</td>
<td>15</td>
<td></td>
<td>1</td>
<td>10</td>
<td>Yes</td>
<td></td>
</tr>
</tbody>
</table>

The results of the approach combining Monte Carlo simulations for the determination of the injection efficiency and the semi-analytical method for obtaining a modified shock solution (SA-MC) are presented in the last two rows of Table 3.2 and in Figure 3.24 (a). Owing to a higher...
injection efficiency found from the Monte Carlo simulations as compared to the prescription of Caprioli et al. (2009b) with $\psi = 3.7$ (see also Sections 4.3.1 and 4.3.2), the shock modification is more pronounced, i.e. the difference between the subshock- and total compression ratios of the modified solution and the test-particle result ($r \approx 4$) for strong shocks is higher. The curves of the semi-analytical calculations in Figure 3.24 (a), obtained after determining $\eta$ with the SA-MC approach as described above, and the distributions resulting from the full Monte Carlo simulations with the calculated modified background, are in good agreement. The discrepancy, highest for the oblique shock with $\theta_{B0} = 60^\circ$, is smaller than a factor of 4. This is much smaller than the differences (typically of two orders of magnitude) that we have found between test-particle and nonlinear results, as mentioned in the previous section and further discussed in Section 4.3.3. The difference between the spectral shape of the semi-analytical calculation and the Monte Carlo particle distributions is predominantly in the nonrelativistic regime. As already mentioned, a similar feature has also been found in Caprioli et al. (2010b).

In order to obtain a Monte Carlo non-thermal spectrum consistent with the semi-analytical calculations, the determination of the injection efficiency by means of the Monte Carlo technique is necessary. This is apparent in Figure 3.24 (b). The solid lines, resulting from the SA-MC approach, are in good agreement with each other. On the contrary, the thin, dashed line (semi-analytical spectrum) and the thick, dashed line (Monte Carlo spectrum obtained with the same modified background solution of the thin, dashed spectrum) differ by almost three orders of magnitude. The reason is that the injection efficiency of the Monte Carlo simulations is higher than that obtained with $\psi = 3.7$. When the shock modification is computed with $\psi = 3.7$, the compression ratio at the subshock is not sufficiently low and the regulation of the acceleration efficiency due to the less modified flow profile is too mild for the Monte Carlo simulations. The differences in the injection efficiencies are further discussed in the second part of the next chapter.
Figure 3.24: Non-thermal distribution functions of protons, multiplied by $[p/(m_pc)]^4$, at the position of the subshock of nonlinear shocks including the effect of RSI. (a) Results from the approach employing Monte Carlo simulations and semi-analytical calculations, for three different obliquities. The curves labelled “Monte Carlo” (thick) are the spectra from the full Monte Carlo simulations after the determination of the nonlinear modification of the shock. The curves labelled “semi-analytical” (thin) are the solutions obtained with the iterative method described in the text, with Eq. (3.25). Figure from Grimaldo et al. (2019). (b) Comparison between the Monte Carlo spectra referred to modified shock solutions derived with different injection efficiencies. For the solid lines, the injection efficiency has been obtained by means of Monte Carlo simulations, while for the dashed lines the injection momentum factor has been set to $\psi = 3.7$. The parallel shock results are shown.
Chapter 4

Results

The outcomes of the first runs combining Monte Carlo and HD simulations have been presented in Grimaldo et al. (2015). In Section 4.1 we will briefly summarize those preliminary results. In Section 4.2, adapting the work of Grimaldo et al. (2017a), we present the outcomes of the combination of MHD and Monte Carlo simulations of particle acceleration in CWBs. Those results, obtained in the test-particle approach, constitute the motivation for the further developments of the code, presented in the following Section 4.3.

The parameters of the stars of the CWB system used for the combined simulations were the same in all cases presented here and are listed in Table 4.1. The system consists of a B star and a WR star. The stellar separation and the treatment of the magnetic field are the only differences between the (M)HD models of the CWB systems, and will be specified in the next sections.

Table 4.1: Stellar and stellar-wind parameters of a typical colliding-wind binary system, as, e.g., in Kissmann et al. (2016). $M_*$ is the stellar mass, $R_*$ the stellar radius, $T_*$ the effective temperature, $L_*$ the luminosity, $\dot{M}$ the mass loss rate, $v_\infty$ the terminal velocity of the wind, and $B_*$ the surface magnetic field.

<table>
<thead>
<tr>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>30</td>
<td>20</td>
<td>23000</td>
<td>$10^8$</td>
<td>$10^{-6}$</td>
<td>4000</td>
<td>100</td>
</tr>
<tr>
<td>WR</td>
<td>30</td>
<td>10</td>
<td>40000</td>
<td>$2.3 \times 10^5$</td>
<td>$10^{-5}$</td>
<td>4000</td>
<td>100</td>
</tr>
</tbody>
</table>

4.1 Combined hydrodynamic and Monte Carlo test-particle simulations

In this section, we present the first results that were obtained from Monte Carlo simulations on a HD background of a CWB system (see Table 4.1). Recall that, since the HD background contains no information about the magnetic field, the latter was initialized as described in Section 3.3.1, using a surface magnetic field of 100 G for both stars. The separation of the stars in the
system was set to $R = 720 \, R_\odot$. The flow speed in the equatorial plane of the HD simulation used for the background can be seen in Figure 4.1. The blue square highlights the selected region used in the Monte Carlo simulations, which consists of $(60 \times 60 \times 60)$ cells. The particles were injected upstream of the shocks, along the imaginary line connecting the two stars. The relatively small size of the simulation box and the injection position ensured that the shocks had only small obliquities. This was necessary, because the supercell method had not been developed yet. The details concerning the background initialization have been already given in Section 3.3.1. Following Ellison et al. (1995), the simulations were carried out with the factor $\xi = 3$, relating mean free path and particle gyroradius. The normalized differential fluxes of the protons at the shocks, resulting from the Monte Carlo simulations, are displayed in Figure 4.2. The dashed and dotted lines represent the best fits to the non-thermal tails of the Monte Carlo simulations with the energy dependence given in Eq. (2.10). The obtained spectral indices are $\sigma_B = 1.9$ for the B-side shock, and $\sigma_{WR} = 1.8$ for the WR-side shock. The difference between the two spectral indices can be ascribed to slightly different compression ratios on the two sides of the WCR. In fact, in the considered region, we found $r_{WR} \gtrsim r_B \gtrsim 4$, where $r_{WR}$ and $r_B$ are the compression ratios of the shock on the WR-side and on the B-side, respectively. In other words, in our simulations, two populations of particles are present – one on either side of the WCR – and produce different spectra. This is also visible when looking at the position of the

![Figure 4.1: Plasma flow speed map, from HD simulations, of the colliding wind binary system used for the combined approach presented in this section. The bow-shaped region containing plasma with smaller speed between the B star (left) and the WR star (right) is the WCR, delimited by two shocks. The blue square highlights the region selected for the Monte Carlo simulation. Figure from Grimaldo et al. (2015).](image-url)
4.1. HD AND MC TEST-PARTICLE SIMULATIONS

Figure 4.2: Normalized differential fluxes of protons towards the inner part of the WCR. The particles were injected at the shocks on the B-side (B shock) and on the WR-side (WR shock) of the WCR. The spectra were recorded at the corresponding shock front. The change of the slopes at \( \approx 10^9 \text{ GeV} \) is caused by the transition from the nonrelativistic to the relativistic regime. Figure from Grimaldo et al. (2015).

thermal peaks of the spectra, which are not coincident, owing to different flow velocities.

The possibility that distinct populations of particles could be produced at the WCR of binary systems, depending on the side of the WCR where they are accelerated has already been discussed in models of both CWBs (Bednarek and Pabich, 2011) and binaries consisting of a massive star and a pulsar (Bednarek, 2011). Although the argument of the authors was focused on the maximal energies, the underlying idea was that the accelerated particles could have different spectral features due to different conditions at the shocks on the two sides of the WCR. Also in light of this, the result presented in Grimaldo et al. (2015) is not surprising. Nonetheless, it confirmed the capability of our approach to catch the differences in the shock conditions of realistic backgrounds, even if the simulations were still limited in the size of the considered region and in the statistics at higher energies. Further developments of the CRONOS code, which allowed to simulate CWBs including the magnetic field component laid the foundations of the work presented in the next section.¹

¹The developments we refer to here were performed by Ralf Kissmann and, together with the related results, they have been presented in Kissmann et al. (2016).
4.2 Combined magnetohydrodynamic and Monte Carlo test-particle simulations

In this section, we adapt and present the results of Grimaldo et al. (2017a). The stellar separation in the considered system is $R = 1440R_\odot$, while we kept the other parameters of the stars unchanged with respect to the simulations presented in the previous section (see Table 4.1). This corresponds to one of the example systems studied by Kissmann et al. (2016), with a clear influence of the magnetic field on the wind flow, but also a well defined WCR, with a low degree of turbulence. The regions investigated in the Monte Carlo simulations consist of $(x \times y \times z) = (151 \times 81 \times 151)$ cubic cells of dimension $(3.9 R_\odot)^3$, and are highlighted by the yellow squares in Figure 4.3.

The particles were injected upstream of the shock fronts, at different positions along the WCR, on the $x$-$z$ plane, namely at $z = 40 R_\odot$, $z = -420 R_\odot$, and $z = 420 R_\odot$. The simulations were carried out assuming Bohm diffusion, i.e. with $\xi = 1$ in Eq. (2.27). As mentioned in Section 3.4, this choice is supported by the analysis of PIC simulations (Caprioli and Spitkovsky, 2014c).

The difference as compared to the system used in the previous section (Figure 4.1) is apparent.

Figure 4.3: Plasma flow speed in the $x$-$z$ plane used as background for the Monte Carlo simulations. The WCR is clearly visible between the B star (left) and the WR star (right). The yellow squares highlight the regions used for the test-particle Monte Carlo simulations.

As discussed by Kissmann et al. (2016), the acceleration of the wind of the B star is distinctly affected by the presence of the stellar magnetic field. The speed of the plasma is higher at the poles and gradually decreases towards the equatorial plane. On the lower half of the MHD computational box, some plasma turbulence develops, driven by the Kelvin-Helmholtz instability (see also Figure 4.12). However, since we use a snapshot of the MHD simulations, we
cannot follow the temporal evolution and the motion of these instabilities. Therefore, from our simulations we cannot estimate the importance of this turbulence on the acceleration and the advection of particles, and on their probability to return to the shocks. According to Reitberger et al. (2017), the MHD turbulence inside the WCR can cause moderate fluctuations in the $\gamma$-ray emission from WCR (Figure 8 of that work). The turbulence in that case, however, was much stronger than in the system considered here, and we do not expect significant deviations of our results due to such effects.

The spectra of the fluxes resulting from our simulations can be seen in Figure 4.4. The magnetic field on the WR-side of the WCR is weaker, which causes a difference of up to two orders of magnitude in the maximal energy reached by the particles injected on the WR-side ($E_{\text{max}}^{\text{WR}} \approx 10^{11}$ eV), compared to the energy reached by the particles injected on the B-side ($E_{\text{max}}^{\text{B}} \approx 10^{12} - 10^{13}$ eV). Moreover, the compression ratio is in general higher on the B-side, which results in harder spectra.

In Grimaldo et al. (2017a) we estimated the injection efficiencies for the system through the ratio of the particle densities in the non-thermal tail, $n_{\text{NT}}$ to the total densities $n_{\text{TOT}}$ (integrating the Monte Carlo spectra over the appropriate intervals):

$$\varepsilon = \frac{n_{\text{NT}}}{n_{\text{TOT}}}.$$  \hspace{1cm} (4.1)

We obtained considerable differences for the ratios $\varepsilon$ along the WCR, as summarized in Table 4.2. Our results indicate that the change in injection efficiency along the WCR may indeed be relevant when modelling non-thermal emission from CWB systems. However, the simulations were obtained in the test-particle approach. For all the considered injection positions, the ratio between the momentum flux due to the non-thermal tail to that of the entire distribution was $\approx 1$. In other words, the injection efficiencies obtained with the test-particle Monte Carlo method are so high that the backreaction of the accelerated particles cannot be neglected. This motivated further developments of the code, the results of which are presented in the next section.

<table>
<thead>
<tr>
<th>$z$ [$R_\odot$]</th>
<th>Side of WCR</th>
<th>$\sigma$</th>
<th>$\varepsilon$</th>
<th>$E_{\text{cutoff}}$ [GeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>40 B</td>
<td>1.9</td>
<td>0.26</td>
<td>$10^4$</td>
<td></td>
</tr>
<tr>
<td>WR</td>
<td>2.0</td>
<td>0.16</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>420 B</td>
<td>2.2</td>
<td>0.09</td>
<td>$10^4$</td>
<td></td>
</tr>
<tr>
<td>WR</td>
<td>2.2</td>
<td>0.08</td>
<td>$10^2$</td>
<td></td>
</tr>
<tr>
<td>420 B</td>
<td>1.9</td>
<td>0.16</td>
<td>$2 \times 10^3$</td>
<td></td>
</tr>
<tr>
<td>WR</td>
<td>2.1</td>
<td>0.13</td>
<td>$10^2$</td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER 4. RESULTS

Figure 4.4: Normalized spectra of fluxes through the shock fronts for test particles (protons) injected at (a) \( z = 40 \, R_\odot \), (b) \( z = -420 \, R_\odot \), and (c) \( z = 420 \, R_\odot \). The dashed curves were obtained by fitting Eq. (2.23) to the data. In the blue box we show the plasma’s background speed in a cut through the numerical domain at \( y = 0 \). The B star is on the left, the WR star on the right. The bow-shaped region, closer to the B star and bent around it, is the WCR. The smaller, yellow boxes represent the sections used for the Monte Carlo simulations. Reproduced from Grimaldo et al. (2017a), with the permission of AIP Publishing.
4.3 Nonlinear combined magnetohydrodynamic and Monte Carlo simulations

The goal of the PhD project has been to develop more accurate models of particle acceleration in CWBs, with a particular focus on the injection and acceleration efficiencies. Having this in mind, we extended the code, to allow for the computation of local nonlinear modifications of the shock at the injection position. Mainly due to its moderate computational costs, we decided to implement the method developed by Amato and Blasi (2005) and Caprioli et al. (2009b), adapting it to our purposes and combining it with the Monte Carlo simulations, as described in Chapter 3.

In this section, we will present the results of Grimaldo et al. (2019), enriched with further comments on several aspects of the model. We will first discuss the dependence of the magnetic field strength – and, in turn, of the diffusion coefficient – on the distance from the subshock. This will be done by setting the far upstream parameters to values typical for conditions of SNR and CWB shocks. Also the injection momentum factor, and in turn the injection parameter (Eq. (3.35)), will be set to determined values (e.g., \( \psi = 3.7 \) or \( \psi = 3.1 \)), and the corresponding solutions will be found with the semi-analytical method, similarly to what was done by Caprioli et al. (2009b). In addition, we will also consider different obliquities, as outlined in Section 3.4, and determine the injection efficiency by means of the Monte Carlo approach. We will then show and discuss the respective distribution functions of the accelerated protons. Finally, we will apply the method combining MHD, semi-analytical and Monte Carlo simulations to the typical CWB system with parameters summarized in Table 4.1, comparing between the test-particle results and those including the backreaction of the non-thermal protons.

The additional material in Sections 4.3.1 and 4.3.2 is intended to give an overview of the effects of the backreaction of the accelerated protons in the different setups of our models. The modified shock solutions alone, in the simple setup not embedded in the extended MHD background, can be found with limited computational costs. This is particularly true when the injection parameter is prescribed, and not derived from the Monte Carlo simulations. Therefore, in principle, it could have been an option to perform a parameter study, letting the calculations run with tighter convergence criteria than those used in Grimaldo et al. (2019) and Section 4.3.3. However, we use the same criteria because, besides being more consistent with the other presented results, it is sufficient to catch the important aspects of the model.

4.3.1 Magnetic field and diffusion coefficient

Here, we consider the models which include the backreaction of the non-thermal protons in the cases either including or not including the resonant-streaming instability, and either by setting the injection momentum factor to \( \psi = 3.7 \) or to \( \psi = 3.1 \), or by employing the Monte Carlo technique for the determination of the injection efficiency. For an easier comparison, we chose the high-Mach-number case of Caprioli et al. (2009b), which is more relevant for our purposes. We further considered another set of parameters, closer to the typical parameters obtained from the MHD simulations of the CWB system of Table 4.1. The background magnetic field at the shock was set to be close to the maximum of the MHD results, on the B-side of the WCR \( (B_0 = 10^{-5} \)
T), and the particle density was set to \( n_0 = 10^{13} \text{ m}^{-3} \). The temperature far upstream is in all cases \( T_0 = 10^4 \text{ K} \). The Mach numbers are \( M_0 \approx 503 \) for the SNR parameters, and \( M_0 \approx 384 \) for the CWB parameters, while the Alfvén Mach numbers are \( M_{A0} \approx 383 \), and \( M_{A0} \approx 65 \) for the SNR and the CWB parameters, respectively. An additional set of calculations has been performed using the same conditions far upstream as those considered for typical SNRs, with the exception of a higher magnetic field, \( B_0 = 3 \times 10^{-3} \text{ T} \), which translates to an Alfvén Mach number \( M_{A0} \approx 64 \). The shock parameters and the results of the calculations are summarized in Tables 4.3 and 4.4. Unlike the work of Caprioli et al. (2009b), we mainly focus on the cases with same maximal momentum of CRs when considering and when not considering the effect of RSI. However, for the sake of completeness, we also list the results for the parameters as in Table 3.2, but with different shock obliquities (Models B1-B3 of Table 4.3).

In Figure 4.5 we show an example of how the magnetic field varies with the distance from the subshock, for three different shock obliquities, and the parameters in the first section of Table 4.3, similar to the article of Caprioli et al. (2009b). While being obviously constant in the case of a parallel shock, the background magnetic field changes with the distance from the subshock when \( \theta_{B0} \neq 0 \). This is due to the increase in \( B_z \), as the upstream flow is slowed by the CR pressure (Eq. (2.38b)). The change of \( B(x) \) is stronger if the effect of RSI is not taken into account (solid line of Figure 4.5). In fact, for \( \theta_{B0} = 30^\circ \) and \( \theta_{B0} = 60^\circ \), \( B(x) \) acts similarly to \( \delta B(x) \) in the parallel case: the presence of the magnetic field pressure generally raises the compression ratio at the subshock and lowers the total compression ratio. The ratio of the magnetic field strengths directly upstream of the subshock to far upstream, \( B_1/B_0 \), is \( \approx 11 \) for \( \theta_{B0} = 30^\circ \), and \( \approx 10 \) for \( \theta_{B0} = 60^\circ \). When RSI is included, \( \delta B(x) \) is clearly the dominant component, for all the three considered obliquities. For \( \theta_{B0} = 30^\circ \) the ratio of the turbulent magnetic field directly upstream of the subshock to the far upstream background field, \( \delta B_1/B_0 \), is \( \approx 27 \), and it is \( \approx 17 \) for \( \theta_{B0} = 60^\circ \). In our model, the diffusion coefficient is directly affected by the change of \( B(x) \) if RSI is not taken into account, and indirectly also when RSI is part of the model, due to the change of direction of the magnetic field (due to the increase of \( B_z \)), which causes the diffusion coefficient parallel to the shock to change (see Eq. (2.26)).

The variation of the magnetic field with the distance from the subshock for parameters resembling CWB shocks, with stronger magnetic fields and lower Alfvén Mach numbers than for Figure 4.5, is shown in Figure 4.6. The parameters are listed in the first section of Table 4.4. A comparison with Figure 4.5 highlights a similar qualitative behaviour. However, the change in the magnetic field strength is significantly lower, for both the background magnetic field and the magnetic field associated with the Alfvén waves. This is only partially ascribable to the different \( p_{\text{max}} \). An important factor is the strength of the magnetic field and, in turn, of its pressure: a lower field amplification is sufficient to have an effect on the shock modification, and to yield a solution conserving the energy and momentum fluxes. Examples of shocks with a similar Alfvén Mach number, \( M_{A0} \approx 65 \), but with parameters more similar to the environment in SNRs or CWBs are shown in Figure 4.7 (a) and (b), respectively. The maximal momentum is, in both cases, \( p_{\text{max}} = 1.1 \times 10^6 \text{ GeV/c} \). The ratio \( B_1/B_0 \) for (a) and (b), without considering RSI, is \( \approx 3.5 \). When considering the effect of RSI, \( \delta B_1/B_0 \) is \( \approx 5 \) for case (a) and \( \approx 6 \) for case (b). The comparison with the results shown in Figure 4.5 highlights the importance of the magnetic field strength. We note that a similar dependence of magnetic field amplification on \( B_0 \) (and
on $M_{A0}$ has been found in other works (e.g. Vladimirov (2009)). Consistently, we find that smaller Alfvén Mach numbers correspond to a smaller increase in the magnetic field strength from far upstream to the subshock, also for the cases without RSI, but with a non-vanishing $B_z$.

In Figures 4.8 (a), (b), we compare the profiles of $B(x)$ from calculations with the pre-set $\psi = 3.7$ to those from calculations where the injection efficiency has been determined with Monte Carlo simulations. The parameters are close to those of CWBs, and are summarized in the first and third sections of Table 4.4. Only the case $\theta_{B0} = 30^\circ$ is shown. The stronger shock modification for the SA-MC approach (which can also be seen when comparing the results of Models A2 with D1, A4 with D2, and A6 with D3 in Table 4.3) is reflected in the spatial profiles of the magnetic field strength. Both $B(x)$ and $\delta B(x)$ are lower by a few, close to the subshock, when $\psi = 3.7$, as compared to the SA-MC approach. The background field $B(x)$ barely changes from far upstream to the subshock in this case. From $r_{\text{sub}}$ and $r_{\text{tot}}$ of Model F4 of Table 4.4, it can be seen that the shock is only very slightly modified. A comparison with Model H4 of Table 4.4 highlights the stronger shock modification obtained with the SA-MC approach. In fact, due to a rather high injection efficiency derived from the Monte Carlo simulations, the total compression ratio is higher ($r_{\text{tot}} = 8.5$) and the subshock compression ratio is lower ($r_{\text{sub}} = 2.7$) for the SA-MC approach, as compared to the case with $\psi = 3.7$ ($r_{\text{tot}} = 5.1$, $r_{\text{sub}} = 3.9$).

The higher injection efficiency obtained with the Monte Carlo simulations and, in turn the stronger shock modification, are most likely attributable to two underlying assumptions. These represent an idealization of the system and provide extremely favourable conditions for DSA, i.e: (i) the scattering is efficient for all particles, and (ii) the subshock is infinitesimally thin. In other words, all of the particles see the shock as a sharp discontinuity. As will be shown in Section 4.3.3, even under these assumptions, the acceleration efficiency obtained by considering the backreaction of the accelerated protons can be lower than what has been estimated in previous studies of CWBs. Further considerations support the use of the Monte Carlo approach in our study.

As mentioned in Chapter 2, Caprioli et al. (2010b) compared three different methods used in the literature for modelling the nonlinear shock modification. These include a version of the Monte Carlo method (Vladimirov et al., 2006) and a version of the semi-analytical method (Caprioli et al., 2010a). In order to match the results in their test case, they set $\psi = 3.1$. This, in the thermal leakage picture of the semi-analytical model, corresponds to a shock transition width of about two gyroradii of the downstream thermal protons (see also Section 3.4). This lies well within the reasonable range for the parameter. Therefore, we decided to run the calculations for the cases tested with the SA-MC approach also setting $\psi = 3.1$. In Figure 4.8 (c) we illustrate the results, comparing again with the SA-MC approach for shock obliquity $\theta_{B0} = 30^\circ$. Interestingly, the curves of $B(x)$ and $\delta B(x)$ for the $\psi = 3.1$ case are very close to those of the SA-MC approach. A look at the last two sections of Table 4.4 confirms that the strength of shock modification is very similar in the two cases (see also the last two sections of Table 4.3). This will be further discussed in the next section, with the aid of the distribution functions of the non-thermal protons obtained for the same shocks.
Table 4.3: Parameter sets and nonlinear shock results for the cases discussed in Sections 4.3.1 and 4.3.2, with upstream speed $u_0 = 5.9 \times 10^6$ m s$^{-1}$, temperature $T_0 = 10^4$ K, and particle density $n_0 = 5 \times 10^5$ m$^{-3}$. The Mach number is $M_0 \approx 503$. The calculations for which the injection efficiency has been determined via Monte Carlo simulations are indicated by “MC” in the column for $\psi$.

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<th>$M_{A0}$</th>
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<th>$r_{\text{sub}}$</th>
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4.3.2 Distribution functions

We start this section by considering the cases with parameters typical for SNR shocks, without considering RSI. The corresponding distribution functions of the non-thermal population of protons obtained by means of the semi-analytical approach alone (Models A1, A3 and A5 of Table 4.3) are shown in Figure 4.9 (a). A trend towards lower densities of accelerated particles is apparent when the shock obliquity increases. This happens despite the (slight) increase of the compression ratio at the subshock, and is an effect of the presence of a non-zero $z$-component of the magnetic field, and the associated pressure: Eqs. (2.38) and (3.30) imply that the decrease in the $x$-component of the plasma velocity results in an increase in $B_z$, and in turn in $P_B$. At the subshock, the equation for the compression ratio resulting from the shock-jump conditions (Eq. (2.40)) must hold, resulting in a lower $r_{\text{tot}}$: the additional magnetic pressure reduces the overall compressibility of the plasma. The reduced compression ratio translates to a shift downwards
4.3. NONLINEAR MHD MC SIMULATIONS

Table 4.4: Parameter sets and nonlinear shock results for the cases discussed in Sections 4.3.1 and 4.3.2, with upstream speed \( u_0 = 4.5 \times 10^6 \text{ m s}^{-1} \), temperature \( T_0 = 10^4 \), and particle density \( n_0 = 10^{13} \text{ m}^{-3} \). The Mach number is \( M_0 \approx 384 \), and the Alfvén Mach number is \( M_{A0} \approx 65 \) in all the considered cases. The calculations for which the injection efficiency has been determined via Monte Carlo simulations are indicated by “MC” in the column for \( \psi \).

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<th>( T_2 )</th>
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of the distribution function of non-thermal protons, as can be seen, for example by evaluating \( f_1(p) \) (Eq. (3.25)) at the momentum \( p = p_{\text{inj}} \). Note that the downstream temperature is also affected by \( P_B \): as expected from Eq. (2.41), it increases when passing from shock obliquities of \( 0^\circ \) to \( 60^\circ \).

For similar shock configurations, but with finite pressure of the magnetic turbulence, i.e. \( P_w \neq 0 \), the particle density at the injection momentum \( p_{\text{inj}} \) increases with increasing obliquity, due to the increasing compression ratio \( r_{\text{tot}} \) and the decreasing downstream temperature. Nevertheless, the decrease of \( p_{\text{inj}} \) (caused by the lower \( T_2 \)), combined with the spectral slope of \( f_1 \propto p^{-q} \), is such that the distribution functions at momenta \( p \geq p_{\text{inj,0}} \) (\( p_{\text{inj,0}} \) being the injection momentum for \( \theta_{B0} = 0^\circ \)) are lower for higher obliquities. This results in an overall shift of the curves...
Figure 4.5: Magnitudes of the background and RSI magnetic fields upstream, as a function of the distance from the subshock, normalized by $r_{g,c}$. The shock parameters are listed in the first section of Table 4.3 (Models A1-A6). $B(x)$ is the absolute value of the background magnetic field. (a) Shock obliquity $\theta_{B0} = 0^\circ$; (b) Shock obliquity $\theta_{B0} = 30^\circ$; (c) Shock obliquity $\theta_{B0} = 60^\circ$.

The nonlinear modification for the shocks obtained by employing the Monte Carlo simulations downwards for more oblique cases in Figure 4.9 (b).²

²Recall that the distribution function $f_1$ is multiplied by $[p/(m_pc)]^4$, i.e., loosely speaking, Figure 4.9 shows the particle density of the bin $\Delta p$ multiplied by $p/(m_pc)$. 
for the determination of the injection efficiency is stronger than that for the solutions obtained by fixing the injection momentum factor $\psi = 3.7$. As discussed in the previous section, this is caused by higher acceleration efficiencies resulting from the Monte Carlo method, as compared to the cases with $\psi = 3.7$. This can be seen in the semi-analytical non-thermal spectra shown in Figure 4.10 (a). The stronger shock modification translates to lower $p_{\text{inj}}$ in the SA-MC approach. However, the different strengths of shock modification for the two approaches also result in different spectral indices, especially at low momenta, and the discrepancies between the distribution functions obtained with the two approaches rapidly decrease with increasing momentum. Close to $p_{\text{max}}$, these discrepancies are less than a factor of $\approx 2$.

For parameters closer to those of CWB shocks, Figure 4.10 (b) shows a more pronounced discrepancy between the spectra obtained with $\psi = 3.7$ and those resulting from the SA-MC approach (Table 4.4, Models F2, F4, F6, and H2, H4, H6, respectively), also in the relativistic regime. This is consistent with what was found in the previous section (see Figure 4.8 and related discussion). Accordingly, the distribution functions obtained with $\psi = 3.1$ lie much closer to those derived with the SA-MC approach, as can be seen in Figure 4.11 (b).

As a last example, the spectra in Figure 4.11 (a), which shows the results for parameters typical for SNRs (last two sections of Table 4.3), show a similar trend when compared to Figure 4.10 (a). From the comparison of the distribution functions obtained with different injection and acceleration efficiencies, it can be seen that if the acceleration efficiency (and, in turn, the pressure of the relativistic CRs) is high, the high-energy part of the spectra is very similar even amongst the results for considerably different injection efficiencies (see Figures 4.10 and 4.11). In fact, in those cases – e.g. Figure 4.10 (a) and Figure 4.11 (a)– the conservation laws (Eqs. (2.30)) limit the distribution functions at high energies. However, the acceleration efficiency can be lower than this upper limit, as can be seen in Figure 4.10 (b): the low injection efficiencies of the cases with $\psi = 3.7$ result in distribution functions which stay well below those obtained with the high injection efficiencies of the Monte Carlo simulations.

As a final remark, we note that for the case of a strictly parallel shock ($\theta_{B0} = 0$) with parameters typical of CWBs and without magnetic field amplification (Model H1 of Table 4.4), the acceleration efficiency obtained with the Monte Carlo simulations is so high that we did not find a solution. The injection momentum $p_{\text{inj}}$ was very close to (at some iterations even below) the peak of the Maxwell-Boltzmann distribution downstream, used in the semi-analytical calculations. Recall that we inject the particles upstream of the shock, with an isotropic Maxwell-Boltzmann distribution of temperature $T_1$ in the local (upstream) plasma frame. With the shock parameters of Model H1, our procedure fails at combining the Monte Carlo simulations and the semi-analytical calculations. However, this limiting case is not expected to be of physical interest. Indeed, by inspection of the other calculations with $\theta_{B0} = 0$ and no additional effect of RSI included, it becomes apparent that the total compression ratio becomes uncomfortably high and not compatible with the observations. It should be kept in mind, however, that a combination of the two methods is not always successful.

The discussion above suggests that, as far as the acceleration efficiencies are concerned, i.e. how many particles are accelerated to the highest energies, the approach presented here, combining semi-analytical calculations and Monte Carlo simulations for the determination of the injection efficiency, yields reasonable results. Furthermore, due to the high injection efficiencies
obtained with our method, possible deviations of our model from the actual CWB systems appear to rather consist of higher acceleration efficiencies. Smaller injection efficiencies at the shocks of the actual CWBs may be caused by effects which are not modelled in the Monte Carlo simulations. Also in light of this, the conclusions drawn in the next section seem to be rather robust.

4.3.3 Application to a CWB system

In this section, we use the combined method (MHD, Monte Carlo and semi-analytical) to investigate the acceleration of protons in colliding-wind binaries. We include a comparison of the test-particle results with those including the backreaction of the non-thermal protons. An illustration of the plasma background for the Monte Carlo simulations is shown in Figure 4.12. The system is the same as in the previous sections, summarized in Table 4.1, with stellar separation \( R = 1440 \, R_\odot \). The regions used in the Monte Carlo simulations are different subregions of the MHD simulations, each consisting of \((x \times y \times z) = (201 \times 101 \times 101)\) cubic cells of dimension \((3.9 \, R_\odot)^3\).

After initializing the background as described in Section 3.3.1, we select 12 supercells where we inject thermal protons. The positions of these cells are summarized in Table 4.5 and, for those on the \(x\)-\(z\) plane, depicted in Figure 4.12. Recall that for the test-particle simulations we do not modify the background more than what is needed for setting up the supercells system and we simply let the particles move and scatter in the simulated region. Instead, for the simulations including the backreaction of the accelerated protons, we first find the nonlinearly modified background for the supercells where the protons are injected, as outlined in Section 3.4 and, once a solution is found, we start a simulation embedding the modified supercells into the same simulated region of the test-particle case. A self-consistent determination of the maximal energies to which the protons are accelerated in the CWB when backreaction is taken into account would require the modification of the MHD background of the entire WCR, together with the regions upstream of the shocks being modified by the pressure of the non-thermal protons. This is not possible with the approach presented in this thesis. As discussed in Section 4.2, test-particle simulations for the same system indicate that, due to the differences in the magnetic field strength on the two sides of the WCR (see Figure 4.12 (a)), the maximal energies of the accelerated protons can differ by an order of magnitude or more. Therefore, based on those results, the maximal momentum of the protons is set to \(10^2 \, m_p c\) on the WR-side and \(10^3 \, m_p c\) on the B-side of the WCR. This approximation does not take into account that some of the most energetic particles are also accelerated in cells different from the initial one, where the shock is modified. This, combined with the effect illustrated in Figure 3.24 (a) – i.e. steeper Monte Carlo spectra, in the nonrelativistic regime, as compared to the semi-analytical spectra – can lead to an overestimation (more often) or to an underestimation of the proton density at high energies from the semi-analytical calculation, as compared to the final Monte Carlo spectra. However, this does not considerably affect our conclusions.

In Figure 4.19 (a) we show the distribution functions \(f_1(p)[p/(m_p c)]^4\), obtained by injecting the protons close to the apex of the WCR, on the B-side, for both the test-particle and the nonlinear approach. Note the difference between the test-particle spectra obtained for injection at B1 and at B2. Whereas the spectral indices are very similar at small energies, they become
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Table 4.5: Modified shock parameters at different positions along the WCR. The WR star and the B star are located at coordinates $x_{WR} = (720, 0, 0)$ and $x_B = (-720, 0, 0)$, respectively. The definitions of the parameters are given in Section 3.4.

<table>
<thead>
<tr>
<th>Position</th>
<th>$(y, z)$ [$R_G$]</th>
<th>$r_{sub}$</th>
<th>$r_{tot}$</th>
<th>$T_2$ [$10^6$ K]</th>
<th>$M_{A0x}$</th>
<th>$P_{w1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>B1</td>
<td>(0, 20)</td>
<td>2.7</td>
<td>9.3</td>
<td>10</td>
<td>76</td>
<td>$1.8 \times 10^{-2}$</td>
</tr>
<tr>
<td>B2</td>
<td>(0, -20)</td>
<td>2.7</td>
<td>9.3</td>
<td>6.4</td>
<td>62</td>
<td>$1.7 \times 10^{-2}$</td>
</tr>
<tr>
<td>B3</td>
<td>(0, 420)</td>
<td>2.7</td>
<td>6.8</td>
<td>41</td>
<td>30</td>
<td>$2.2 \times 10^{-2}$</td>
</tr>
<tr>
<td>B4</td>
<td>(0, -420)</td>
<td>2.7</td>
<td>7.0</td>
<td>44</td>
<td>33</td>
<td>$2.3 \times 10^{-2}$</td>
</tr>
<tr>
<td>B5</td>
<td>(500, 420)</td>
<td>2.7</td>
<td>8.3</td>
<td>15</td>
<td>43</td>
<td>$2.9 \times 10^{-2}$</td>
</tr>
<tr>
<td>B6</td>
<td>(-500, -420)</td>
<td>2.7</td>
<td>8.4</td>
<td>15</td>
<td>45</td>
<td>$2.8 \times 10^{-2}$</td>
</tr>
<tr>
<td>W1</td>
<td>(0, 20)</td>
<td>2.6</td>
<td>80</td>
<td>0.32</td>
<td>$3.7 \times 10^4$</td>
<td>$1.1 \times 10^{-3}$</td>
</tr>
<tr>
<td>W2</td>
<td>(0, -20)</td>
<td>2.5</td>
<td>78</td>
<td>0.30</td>
<td>$3.0 \times 10^4$</td>
<td>$1.4 \times 10^{-3}$</td>
</tr>
<tr>
<td>W3</td>
<td>(0, 420)</td>
<td>2.7</td>
<td>33</td>
<td>0.80</td>
<td>$1.7 \times 10^3$</td>
<td>$6.1 \times 10^{-3}$</td>
</tr>
<tr>
<td>W4</td>
<td>(0, -420)</td>
<td>2.6</td>
<td>32</td>
<td>0.74</td>
<td>$1.5 \times 10^3$</td>
<td>$5.2 \times 10^{-3}$</td>
</tr>
<tr>
<td>W5</td>
<td>(500, 420)</td>
<td>2.5</td>
<td>34</td>
<td>0.51</td>
<td>$1.9 \times 10^3$</td>
<td>$4.6 \times 10^{-3}$</td>
</tr>
<tr>
<td>W6</td>
<td>(-500, -420)</td>
<td>2.7</td>
<td>33</td>
<td>0.53</td>
<td>$1.6 \times 10^3$</td>
<td>$6.9 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

notably different in the relativistic regime, where the B1 spectrum hardens, while the B2 spectrum softens. This is ascribable to different conditions downstream of the respective shocks. The particles which are sufficiently energetic to return to the shock from farther downstream at B1 are subject to a higher effective compression ratio, caused by the slowdown of the plasma approaching the contact discontinuity. The effect observed in the test-particle simulations is entirely due to the interaction of the stellar winds, and the geometry of the WCR. In the investigated scenario the downstream flow is slower than it would be for a shock of infinite extent downstream, calculated using the shock-jump conditions. Therefore, it is more likely for the particles to cross the shock again from downstream to upstream in our setup than it would be in a shock structure modelled according to the assumptions commonly made for (semi-) analytical works. We do not see, however, any appreciable effect of hardening of the spectra due to scattering of the particles between the upstream “colliding shock flows” on the two sides of the WCR, as modelled by Bykov et al. (2013). This is likely due to different background conditions at, and between, the shocks. Bykov et al. (2013) considered a completely symmetric set-up, and obtained a hard spectrum for the distribution function, namely $f_1(p) = (U_p(p))^3$. For energetic particles with $\lambda_{mfp} > L_{WCR}$, where $L_{WCR}$ is the width of the WCR, it should be possible to see this effect even without considering any modification due to the backreaction of the accelerated protons upstream of the shocks (i.e. with $U_p(p) = 1$). In the system presented here, however, the conditions on the two sides of the contact discontinuity are not equal. Particularly important is the difference in the magnetic field, which is much weaker on the WR-side. As a consequence, the particles accelerated at the B-side shock which manage to cross the contact discontinuity get much larger mean free paths and can therefore more easily escape the system from the WR-side of the WCR. This is exemplified in Figure 4.13, where the trajectory inside the WCR of a proton injected at B1 and reaching high energies can be seen. The change in gyroradius and mean free
path is clearly visible. Figure 4.13 (c) shows that the protons gain energy at the shock, and confirms that the supercell method used here does not produce artefacts when the particles pass from a supercell pair to the standard background, and vice versa.

In Figures 4.14-4.18 we present other examples of trajectories for protons injected at different positions. In particular, Figures 4.14 and 4.15 show the trajectories (and the momenta) of two particles injected at W1. Due to the lower magnetic field on the WR-side, the diffusion of the particles is higher as compared to the B-side. The protons accelerated at the WR-side shock usually do not reach sufficiently high energies to allow them crossing the contact discontinuity and reaching the B-side shock before they are advected out of the simulation box, as shown by the two examples in Figures 4.14 and 4.15.

We did not find any signature in the spectra related to scattering of protons between the two converging flows upstream of the shocks, nor between the two downstream flows separated by the contact discontinuity. As already pointed out in Grimaldo et al. (2015), this situation might change for different parameters of the system, for example if the magnetic field strength on both sides of the contact discontinuity were similar. Other factors might also play an important role, e.g. the width and the curvature of the WCR, or the distances between the stars and the shocks. Further studies are required, in order to better understand such effects (see also the outlook in Chapter 5).

As opposed to the B1 spectrum, the B2 spectrum does not harden, but instead it softens in the relativistic regime. The effect of advection in the WCR appears to be more pronounced for protons injected at B2 (slightly below the equatorial plane) than for injection at B1 (slightly above the equatorial plane), as shown in Figure 4.16. This is caused by the equatorial plasma flow of the B star which enters the WCR and flows downwards with relatively high velocities (for a discussion concerning the stellar winds and WCR structure in this and other systems, see Kissmann et al. (2016)). Even if some of the protons injected at B1 diffuse towards the equatorial plane and from there are advected downwards by the flow (see Figure 4.17), the probability of such an event is much lower than for particles starting from B2. The latter, when entering deeper into the WCR, are “forced” to reach the equatorial flow. The track in Figures 4.18 (c), (d) belongs to a particle which crosses the contact discontinuity, reaches the WR shock and gains further energy there, before leaving the system. We remark that we have observed similar types of proton trajectories only when analysing simulations close to the equatorial plane of the system, although we cannot exclude that the same may happen, less frequently, also farther away from the apex of the WCR. This is possibly caused by several factors, such as the thinner WCR, or the lower velocity of the background flow, and the smaller magnetic field allowing more particles with moderate energies to cross the contact discontinuity close to the equatorial plane. It should be noted that the magnetic dipoles of the stars in a CWB are not expected to be necessarily oriented as in the simulations presented here, and further investigations with different setups will certainly help in better understanding the effects on particle acceleration in CWBs of the stellar magnetic-field–wind interaction.

When comparing the test-particle spectra to those obtained with shock modification, shown in Figure 4.19 (a), the effect of the backreaction of the accelerated protons is clearly visible. The density of the non-thermal protons is reduced by up to more than three orders of magnitudes. The shock modification is stronger on the WR-side, as can be seen in Figure 4.19 (b) and in Table
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4.5: the “thermal peak” moves towards lower momenta, while the total compression ratio reaches much higher values on the WR-side. This is caused by the very high Alfvén Mach number on the WR-side. The Alfvén waves produced via the resonant-streaming instability considerably lower the value of \( r_{\text{tot}} \), but not as much as on the B-side of the WCR, where the pressure associated with the waves is up to about one order of magnitude larger (see Table 4.5). This is similar to what has been shown in Sections 4.3.1 and 4.3.2. In Figures 4.20 and 4.21 we show the test-particle and the nonlinear spectra for further positions. In all cases, the test-particle results strongly overestimate the acceleration efficiency, as was found in many studies of SNRs (e.g. Vladimirov (2009), Bykov et al. (2014), Amato and Blasi (2005), Kang et al. (2012b)). We note that these conclusions are not affected by the oscillations of the shock orientation, discussed in Section 3.5.2.

We now want to estimate the impact of backreaction on the \( \gamma \)-ray fluxes from CWB systems. The lack of detection of \( \gamma \)-rays from CWBs is well known. As mentioned in the introduction, up to now only \( \eta \) Carinae and \( \gamma^2 \) Velorum (WR 11) have been detected as \( \gamma \)-ray sources. In the model of Reimer et al. (2006), the dominant production mechanism for \( \gamma \)-rays in WR 140 and WR 147 was found to be inverse Compton scattering from relativistic electrons in the stellar radiation field. This picture might considerably change if particle acceleration is efficient and magnetic field amplification takes place, leading to a situation similar to what has been found by Reitberger et al. (2017), modelling WR 11. There, the inverse Compton losses in the strong radiation fields prevent the electrons from reaching sufficiently high energies for \( \gamma \)-ray production. The \( \gamma \)-ray emission is therefore likely of hadronic origin. In the same work it is further claimed that a stronger magnetic field and smaller inverse Compton losses would also yield \( \gamma \)-ray fluxes in agreement with observations.

Similarly to what was done in many works, Reitberger et al. (2017) use an injection parameter, fixing the injection efficiency on the acceleration process. There, in particular, the proton density at 1 MeV is set to \( n(E = 1 \text{MeV}) = \eta_{1\text{MeV}} n_0 \), with the injection parameter \( \eta_{1\text{MeV}} = 10^{-3} \), and \( n_0 \) the proton density of the background plasma. In Figure 4.22 we show the particle density for a selection of injection positions obtained with feedback, together with the non-thermal tails of the test-particle case, shifted in order to match the injection parameter of Reitberger et al. (2017). Amongst B1-B6 and W1-W6, we chose the positions corresponding to the highest densities at high energies in the test-particle case, close to the apex and far away from it, for each side of the WCR. It turns out that the particle densities obtained with the nonlinear approach are even lower than the shifted test-particle results, with \( \eta_{1\text{MeV}} = 10^{-3} \). Together with the spectral energy distributions of the particles, the \( \gamma \)-ray fluxes from a modified WCR will also change, but not necessarily in the same manner: the increased density in the WCR do to higher compression ratios will also have an effect, since hadronic collisions producing neutral pions will be more frequent there. In the following, we roughly estimate the \( \gamma \)-ray production for the model studied here, in the vicinity of the apex of the WCR, using as the target proton population the thermal particles downstream of the considered shock. At position B1, the ratio between the non-thermal proton density (Eq. (3.11)) in the model with the modified shock, \( n_{1p}^{\text{NL}}(60 \text{ GeV}) \), and the one in the test-particle approach, with \( \eta_{1\text{MeV}} = 10^{-3} \), \( n_{1p}^{\text{TP}}(60 \text{ GeV}) \), is \( n_{1p}^{\text{NL}}(60 \text{ GeV}) / n_{1p}^{\text{TP}}(60 \text{ GeV}) \approx 0.02 \). At an energy of 10 GeV (corresponding to a proton energy of \( E_p \approx E_\gamma/\kappa_{\pi^0} \approx 60 \text{ GeV} \), with the inelasticity factor for pion production
$\kappa_{\gamma} \approx 0.17$ (Aharonian and Atoyan, 2000)), the ratio between the $\gamma$-ray emissivities would be $q_{\gamma}^{\text{NL}}(10 \text{ GeV})/q_{\gamma}^{\text{TP}}(10 \text{ GeV}) \approx 0.07$. At the WR-side of the WCR, at position W2, the ratios of the densities of the non-thermal population at $\approx 6 \text{ GeV}$ is $n_{1}^{\text{NL}}(6 \text{ GeV})/n_{1}^{\text{TP}}(6 \text{ GeV}) \approx 0.06$, while the $\gamma$-ray emissivity in the case of a modified shock, due to the much larger compression ratio, would be higher than in the test-particle case: $q_{\gamma}^{\text{NL}}(1 \text{ GeV})/q_{\gamma}^{\text{TP}}(1 \text{ GeV}) \approx 2$. Despite being a limiting case, since the nonlinear compression ratio close to the apex on the WR-side reaches the highest values, this estimate highlights the non trivial modifications of the $\gamma$-ray fluxes due to nonlinear modifications of the shocks of the WCR in colliding-wind binary systems.

Another intriguing observable effect of proton acceleration in CWBs, even if highly speculative, might be the change of the opening angle of the WCR cone. Reitberger et al. (2017) found that modelling $\gamma^2$ Velorum with a strong coupling between the stellar winds, i.e. when the magnitude of the acceleration of the winds due to the radiation fields of the two stars depends on whether the wind plasma originated from the O star or from the WR star, yields an opening half-angle of the shock-cone $\approx 72^\circ$, i.e. closer to the observed value of $\approx 85^\circ$, as compared to the case when radiative braking is neglected ($\approx 24^\circ$). High-energy protons escaping the WCR from the O-side towards the WR-side, might slow down even further the wind of the WR star, and therefore contribute to a further increase of the shock-cone opening angle. Recall that, in our simulations, we observe that some of the protons from the B-side with higher energies eventually reach the contact discontinuity at the interface between the B-side and the WR-side downstream regions, and more easily escape on the WR-side.

The discussion above shows that a viable way to reconcile the theoretical predictions for $\gamma$-ray fluxes with the observations of CWBs in the radio and $\gamma$-ray bands, is to employ the widely accepted idea of the existence of a backreaction of the accelerated particles at collisionless shocks.

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3Employing a strong coupling may be justified, by the different composition of the winds belonging to the two stars.
Figure 4.6: Magnitudes of the background and RSI magnetic fields upstream, as a function of the distance from the subshock – normalized by $r_{g,c} = m_p c/(q B_0)$ – for conditions similar to those in CWBs (Models F1-F6 of Table 4.4). $B(x)$ is the absolute value of the background magnetic field. (a) Shock obliquity $\theta_{B0} = 0^\circ$; (b) Shock obliquity $\theta_{B0} = 30^\circ$; (c) Shock obliquity $\theta_{B0} = 60^\circ$. 
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Figure 4.7: Magnitudes of the background and RSI magnetic fields, as a function of the distance from the subshock – normalized by $r_{g,c}$ – upstream of shocks with obliquity $\theta_{B0} = 30^\circ$ and (a) parameters similar to those in Caprioli et al. (2009b), but with $B_0 = 3 \times 10^{-9}$ T (Models C3 and C4 of Table 4.3); (b) parameters similar to those resulting from MHD models of CWB, but with high maximal momentum of the particles, i.e. $p_{\text{max}} = 1.1 \times 10^6$ GeV/c (Models G3 and G4 of Table 4.4). $B(x)$ is the absolute value of the background magnetic field.
Figure 4.8: Magnitudes of the background and RSI magnetic fields upstream, as a function of the distance from the subshock – normalized by $r_{g,c}$ – for parameters close to typical CWB shocks, and inclination $\theta_{B_0} = 30^\circ$. (a) Background magnetic field for the case without RSI. Comparison between the calculations performed with the SA-MC approach and with $\psi = 3.7$ (Models F3 and H3 of Table 4.4). (b) Background and RSI magnetic fields for the case with RSI. Comparison between the calculations performed with the SA-MC approach and with $\psi = 3.7$ (Models F4 and H4 of Table 4.4). (c) Background and RSI magnetic fields for the case with RSI. Comparison between the calculations performed with the SA-MC approach and with $\psi = 3.1$ (Models H4 and I4 of Table 4.4).
Figure 4.9: Non-thermal distribution functions of protons, multiplied by $[p/(m_p c)]^4$, at the position of the subshock of the nonlinear shocks specified below, for three different obliquities. (a) Without magnetic field amplification due to resonant-streaming instability (Models A1, A3, A5 of Table 4.3). Figure from Grimaldo et al. (2019). (b) With the effect of RSI (Models A2, A4, A6 of Table 4.3). The result for the parallel shock without RSI is plotted as a reference.
Figure 4.10: Non-thermal distribution functions of protons, multiplied by \( \left[ \frac{p}{(m_p c)} \right]^4 \), at the position of the subshock of the nonlinear shocks specified below, obtained from Eq. (3.25) by employing the SA-MC approach as compared to fixing \( \psi = 3.7 \). Three different obliquities are shown. Magnetic field amplification due to RSI is included in all models. (a) Parameters of SNRs, with \( M_{A0} \approx 383 \) and \( p_{\text{max}} \approx 10^6 m_p c \) (Models A2, A4, A6, and D1-D3 of Table 4.3). (b) Parameters of CWBs, with \( M_{A0} \approx 65 \) and \( p_{\text{max}} \approx 10^3 m_p c \) (F2, F4, F6, and H2, H4, H6 of Table 4.4).
Figure 4.11: Non-thermal distribution functions of protons, multiplied by \( \left[ \frac{p}{(m_p c)} \right]^4 \), at the position of the subshock of the nonlinear shocks specified below, obtained from Eq. (3.25) by employing the SA-MC approach and by fixing \( \psi = 3.1 \). Three different obliquities are shown. Magnetic field amplification due to RSI is included in all models. (a) Parameters of SNRs, with \( M_{A0} \approx 383 \) and \( p_{\text{max}} \approx 10^6 m_p c \) (Models D1-E3 of Table 4.3). (b) Parameters of CWBs, with \( M_{A0} \approx 65 \) and \( p_{\text{max}} \approx 10^3 m_p c \) (Models H2, H4, H6, and I2, I4, I6 of Table 4.4).

Figure 4.12: \( x-z \) plane of the MHD simulation box and some selected injection positions (see Table 4.5). The B star is on the left, at \( x_B = -720 R_\odot \), the WR star is on the right, at \( x_{WR} = 720 R_\odot \). (a) Magnetic field strength. (b) Plasma speed. Figure from Grimaldo et al. (2019).
Figure 4.13: Track of a proton injected at B1 (see Table 4.5). The particle is accelerated at the shock, until it reaches and crosses the contact discontinuity, entering the region with lower magnetic field, and eventually crossing the WR shock and leaving the system. (a), (b) Two different 3D views of the track inside the computational box. The blue surfaces are the B shock (left) and the WR shock (right). (c) Proton momentum vs distance from the B shock.
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Figure 4.14: Two different views of the track of a proton injected at W1 (see Table 4.5). The highest momentum reached by the particle is \( \lesssim 0.1 \) times that of the particle shown in Figure 4.13.

Figure 4.15: Two different views of the track of a proton injected at W1 (see Table 4.5). As compared to the case shown in Figure 4.14, the proton enters more deeply into the WCR, but it cannot reach the B shock, and eventually leaves the system from the WR-side.
Figure 4.16: Two different views of the track of three protons reaching approximately the same maximal energy. Two were injected at B2, one at B1 (see Table 4.5). The advection due to the equatorial flow wedging into the WCR is apparent, for the particles injected at B2. The proton injected at B1 crosses the contact discontinuity and eventually leaves the system from the WR-side.

Figure 4.17: Example of a proton injected at B1 which diffuses downwards and is advected a long distance inside the WCR by the equatorial flow, and finally reaches the WR-side.
Figure 4.18: Tracks of two protons inside the WCR. (a), (b) Proton injected at B2 (see Table 4.5). The particle, after reaching the WR-side close to the bottom of the computational domain, interacts multiple times with the WR shock and leaves the system from the upper part of that side. (c), (d) Proton injected at B1, which reaches the equatorial flow and is advected downwards until it reaches the WR-side. There, it gains a considerable amount of energy upon multiple shock-crossings, until it leaves the system.
Figure 4.19: Proton distribution functions multiplied by \( \left[ \frac{p}{(m_p c)^4} \right] \), resulting from injection of particles at positions close to the apex of the WCR (see Table 4.5 and Figure 4.12 for more details), for the test-particle approach (thin lines) and for the nonlinear calculations (thick lines). (a) B-side of the WCR. (b) WR-side of the WCR. Figure from Grimaldo et al. (2019).

Figure 4.20: Same as Figure 4.19, but at positions farther away from the apex of the WCR (see Table 4.5 for more details). Figure from Grimaldo et al. (2019).
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Figure 4.21: Same as Figure 4.19, but at positions farther away from the apex of the WCR (see Table 4.5 for more details). Figure from Grimaldo et al. (2019).

Figure 4.22: Proton density spectra as a function of energy obtained by injecting particles at the shocks at four selected positions of the WCR. The thin lines are the test-particle Monte Carlo results, renormalized in order to match the condition $n_1(E = 1\text{MeV}) = 10^{-3} n_0$, where $n_0$ is the thermal proton density upstream of the unmodified shock. The thick lines are the nonlinear results. (a) Close to the apex of the WCR. (b) Farther away from the apex of the WCR (see Table 4.5 for more details). Figure from Grimaldo et al. (2019).
Chapter 5

Conclusions and outlook

In this work we have presented an approach combining magnetohydrodynamic simulations, a semi-analytical method for obtaining nonlinear solutions of modified collisionless shocks, and Monte Carlo simulations of proton acceleration. We have shown the path which led to the current state of the code and to the results published in Grimaldo et al. (2019). We have explained the various steps taken during a simulation, e.g. shock tracking, determination of shock orientation, initialization of a supercell system, etc. Furthermore, we have shown why we have also implemented a module for calculating local nonlinear shock modifications, conserving momentum and energy fluxes. In order to use the methods commonly applied to strictly parallel shocks to the broad variety of obliquities found along the wind-collision regions of colliding-wind binaries, we adapted the technique of Caprioli et al. (2009b) to the case where the shock normal and the magnetic field are not aligned. The approach makes use of the equations of conservation of energy and momentum fluxes, and the equation describing the evolution of the pressure due to the Alfvén waves in the shock precursor.

Motivated by the elusiveness of CWB systems in the γ-ray band, in conflict with the fluxes predicted by models in the literature (as discussed in Section 1.3), the aim of the project has been to provide an improved treatment of particle acceleration in CWBs. Of particular interest for us have been the injection and acceleration efficiencies in such systems. By applying our method to a model of a typical CWB, we showed that, similarly to what was found in studies of typical SNR shocks, the Monte Carlo test-particle results differ considerably from the nonlinear solutions: the test-particle approach greatly overestimates the injection efficiencies, which are dramatically reduced when energy and momentum conservation at the shock is fulfilled. Remarkably, we found that the injection and acceleration efficiencies at the shocks of CWBs may be lower than what is often assumed in approaches based on the transport equation for the accelerated particles, which assume that their backreaction on the background plasma can be neglected.

Another interesting aspect is that the results of our simulations support the hypothesis that two distinct populations of non-thermal protons can be produced at the two shocks delimiting the WCR of a CWB. This was obtained in the test-particle approximation, as described in Section 4.2. The maximal energies reached by the protons are different, depending on which side of the WCR they were injected. The existence of different populations has been proposed as a possible
cause for the appearance of two components, reaching different energies, in the \( \gamma \)-ray spectrum of \( \eta \) Carinae (e.g. Bednarek and Pabich (2011)). The specific model of CWB used in this thesis consists of a B star and a WR star, both with surface magnetic field \( B_\ast = 100 \text{ G} \), and separated by a distance of \( R = 1440 R_\odot \). In this case, the protons injected on the B-side, can reach energies of up to \( \approx 10 \text{ TeV} \), while on the WR-side the cutoff is in the range of 10-100 GeV. The difference in the maximum energies is ascribed to the different strengths of the magnetic fields at the two sides of the WCR: a stronger magnetic field corresponds to a higher maximum energy. Even in the more realistic case of different surface magnetic fields of the two stars, it seems unlikely that its magnitude be the same on the two sides of the WCR. For this to happen, at least in the test-particle approach, the right combination of \( B_\ast \) and of the distance of the WCR from the stars would have to be fulfilled. We note, however, that the difference in the magnetic field strengths might be reduced if the shock modifications were globally taken into account. In fact, as discussed in Section 4.3.1, the magnetic field is more strongly amplified when the background magnetic field is lower (and the Alfvén Mach number is larger). In our CWB model this happens on the WR-side. By construction, the shock modification obtained with our approach is only local. Therefore, we cannot confirm if, and by what amount, the difference of the magnetic field strength on the two sides of the contact discontinuity will be globally reduced.

We further tried to roughly estimate possible observational consequences of the results of our model. In this regard, we formulated the hypothesis, based on the results of Reitberger et al. (2017), that the magnetic field amplification due to the accelerated protons could increase synchrotron losses of the electrons accelerated at the shocks delimiting the WCR. This would reduce the maximal energy reached by the relativistic electrons, preventing them from efficiently producing \( \gamma \)-rays via inverse Compton scattering in the stellar photon fields. This might help to address the open question, mentioned in the introduction, of why non-thermal synchrotron emission has been observed by many CWB systems, while so far there has been no detection of \( \gamma \)-rays from those sources, with the only exception of \( \gamma^2 \) Velorum (\( \eta \) Carinae, detected as a \( \gamma \)-ray source, does not show any synchrotron emission in the radio domain, presumably due to synchrotron self-absorption).

From the discussion in Sections 4.3.1 and 4.3.2, it emerges that the Monte Carlo simulations probably set an upper limit to the efficiencies of injection into the Fermi process, due to the assumptions of efficient scattering for particles at all energies, and of infinitesimally thin MHD (sub-) shock transition. Under these assumptions, we obtained shocks strongly modified by the backreaction of the accelerated protons. This in turn regulates the overall acceleration efficiency. If microphysical mechanisms, i.e. other than the simple conservation of momentum and energy fluxes, are effective at reducing the injection efficiency, the shock modification would be reduced. The densities of the highest energy CRs would be approximately unchanged or even lower than what was found in Section 4.3.3. Such a situation might occur for example farther away from the apex of the WCR, where the shock obliquities can become larger than \( \approx 45^\circ \). The results of hybrid PIC simulations (Caprioli and Spitkovsky, 2014a) suggest that shocks with such high obliquities do not efficiently accelerate particles because of insufficient production of the magnetic turbulence responsible for the scattering of the charged particles. In our simulations, we implicitly assume that there is a pre-existing turbulence there, produced by the CRs accelerated at different positions, closer to the apex of the WCR. This is comparable, for example, to the
case considered by Takamoto and Kirk (2015).

We can summarize the results concerning particle acceleration in CWBs, which derive from the code and methods developed for this PhD project, in the following points:

- our simulations provide support for the hypothesis that different non-thermal populations are present in CWBs, due to the double-shock structure delimiting the WCR;
- if the scattering is efficient at the shocks, the backreaction of the accelerated protons on the background plasma cannot be neglected in CWBs, similarly to what is commonly accepted for particle acceleration at the shocks of SNRs;
- the number of particles accelerated to high energies, as obtained in models conserving energy and momentum fluxes in the shock precursor, can be lower than what has been supposed in previous models of $\gamma$-ray emission from CWBs.

In the following, we provide some prospects for possible future studies and developments based on the work done in this project. Needless to say, an optimization of the code, as far as the efficiency and resource management are concerned, would be advantageous, helping to increase the statistics and the number of injection points along the WCR. Also, it would further reduce possible size effects, e.g. particles might be accelerated to higher energies if the computational domain were larger, allowing for more shock interactions. Also the development of better tools for the analysis of particle trajectories inside the computational box would be desirable. Finally, we discuss more specific aspects which could be improved or further investigated.

**Scattering law.** Throughout the computational domain, we use the same dependence of the mean free path on the particle gyroradius. It might be worth to allow for a spatial change of the scattering law, in order to model physical processes which possibly have an influence on the strength and efficiency of the scattering process inside the WCR. For example, wave damping might increase the mean free path of the protons further downstream in the WCR and enhance the probability of scattering of particles between converging flows, similar to what was modelled by Bykov et al. (2013). Technically, a spatial dependence of the scattering law should be fairly easily achievable with the Monte Carlo method.

**Contact discontinuity.** The aspect we want to focus on, is connected to the point above and lies somewhere between the physics of the system and the technical details of the method combining Monte Carlo and MHD simulations. In principle, particles crossing the contact discontinuity multiple times might gain energy by scattering between the two converging (downstream) flows, even without reaching the shocks and the upstream regions on the two sides of the WCR. While writing this thesis, we have found some trajectories of protons, injected at the WR shock, which gain energy deep in the WCR (see Figure 5.1), even if the particle spectra resulting from our simulations did not show any particular feature attributable to such mechanism. Further investigations are needed in order to exclude that the acceleration is an artefact, similar to what has been discussed in Section 3.3.1. Since, as mentioned, there are some physical (geometrical) reasons for expecting acceleration across the contact discontinuity, disentangling the numerical and physical effects will probably be challenging. In any case, if artefacts are produced with
parameters of the system which differ from the one considered here, a solution similar to that adopted at the shocks (i.e. the supercell system) might be needed.

![Proton track](image1.png)

Figure 5.1: Two different views of the track of a proton injected at W2 (see Table 4.5). This particle gains energy far away from the shocks, deep inside the WCR.

**Shock orientation and related issues.** As seen in Sections 3.3.1 and 3.5.2, the orientation of the subshock is determined with a quite rough method and produces oscillations, along the shocks, of the azimuthal and polar angles of the shock normal. Implementing a smoothing procedure like, for example, Savitzky-Golay filtering (Press et al., 1992), could smooth the oscillations. Dedicated tests will be needed, in order to ensure that the filtering does not hide actual features of the shocks. The smoothing might have the attractive effect of minimizing the need to adjust the positions of the particles (or of the shock) when they enter a new supercell pair, and of reducing the differences in the spectra obtained with particle injection at neighbouring cells (see Section 3.3.1). A further, possible strategy allowing to reduce the latter might consist of injecting the particles at many neighbouring cells (e.g. a $3 \times 3$ “square”), in order to dilute the influence of the fluctuations of the background conditions in the single cells. This will increase the computational cost, especially when computing the nonlinear solutions. An improvement in the efficiency in finding the modified shock profiles is desirable.

**Nonlinear shock modification.** In our model, the treatment of the shock modification is considerably simplified. We use the transmission and reflection coefficients of McKenzie and Westphal (1969), who considered only linearly polarized Alfvén waves. Other kinds of turbulence are likely to develop and provide the scattering centres for the charged particles (e.g. Bell (2004), Caprioli and Spitkovsky (2014a)). Even if not considering these, the situation can become complicated. For example, Achterberg and Blandford (1986) built a considerably complex model,
based on the observation that the most relevant Alfvén waves in the context of shock acceleration are circularly polarized. The circularly polarized Alfvén waves produce several other kinds of waves downstream of the shock. These, in general, do not propagate parallel to the ambient magnetic field. Exploring if and how this and similar results can be included into our code has the potential to increase the realism of the model of oblique modified shocks, with clear benefits for models of particle acceleration in CWBs.

As a further remark, we note that the inclusion of a finite velocity of the scattering centres in the plasma frame could also be necessary for achieving a more self-consistent modelling of the acceleration process. Caprioli (2012) explored, in the context of SNRs, the possibility that the scattering centres move in the plasma frame upstream with velocities pointing away from the shock. When the Alfvén velocity was calculated with respect to the amplified magnetic field, the effect was an overall steepening of the spectra, caused by lower effective compression ratios. Using the amplified field for the determination of the speed of the scattering centres is a “phenomenological approach”, which permits to obtain CR spectra more similar to what can be inferred by observations of SNRs. In the context of CWBs, for some configurations with high magnetic field, the Alfvén Mach number referred to the background field alone may become sufficiently low for playing a non-negligible role in the regulation of the acceleration efficiency. Finally, an interesting point concerning the nonlinear modification of shocks in CWBs is related to the escape of some of the protons accelerated on the B-side of the WCR to the WR-side. The energies of these particles can be considerably higher than those of the protons accelerated on the WR-side. If the fluxes of CRs crossing the contact discontinuity and subsequently escaping is high enough, the pressure on the WR shock might have an influence on the flow profile, and in turn on the acceleration efficiencies. An *ad hoc* study would be certainly of interest.

**Properties of the background plasma.** In our simulations we considered only proton acceleration. The main component of the wind of a WR star, however, is helium. Considering the different species might cause some difference in the results. For example, the different magnetic rigidity, \( R = \frac{pc}{q} \), of helium ions as compared to protons might result in differences in both the maximal energies reached by the ions (e.g. Schure and Bell (2013)) and the extension of the precursor of nonlinear shocks (see Figures 4.5-4.8).

In addition to this, the work presented in this thesis opens more general questions, which appear to be worth further investigation, possibly by applying different methods (e.g. two fluid MHD simulations), for example:

- How does the backreaction of the protons accelerated on either side of the WCR modify its large-scale structure?
- What consequences on the WCR structure can have the escape of high-energy protons through the contact discontinuity?
- Would this escape trigger instabilities and further MFA, lowering the differences in the strength of the magnetic field between the two sides of the contact discontinuity?

\(^1\)Recall that \( p \) is the momentum of the ion, \( c \) denotes the speed of light, and \( q \) is the charge of the ion.
• How would all these possible modifications of the environment eventually affect particle acceleration in CWBs?

The work done for the PhD project presented in this thesis has led to the development of a code which, to our knowledge, models for the first time the actual process of particle acceleration in CWBs, allowing to simulate and follow the motion of individual particles in such environments. We have shown that, even at the current stage with much room for improvement, these simulations can be a valuable tool for the investigation of DSA in realistic astrophysical environments. An intrinsic limitation of the method is that it assumes a steady state of the system. This can still be a good approximation for systems with large separation, while for close systems this is not necessarily the case.

Other methods are more suited for modelling the emission of $\gamma$-rays and radio waves, e.g. those combining MHD simulations and the transport equation for the non-thermal particles (see Section 1.3). These can model the system and the acceleration of particles in a time-dependent manner. However, not only the background but also the non-thermal component can be described using only macroscopic quantities, such as densities and fluxes. The major strength of our approach is probably the complementarity with respect to those approaches. For systems where a steady state can be assumed, the results of the different methods can be compared to each other and strengthen the conclusions, or highlight possible differences ascribable to the approximations used. The results of the nonlinear calculations might help in constraining the injection parameter when modelling real systems and predicting their $\gamma$-ray emission. This, naturally in conjunction with experimental data, may lead to a more complete understanding of CWBs.

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2I would like to further dedicate this footnote to him, so that the sentences I dedicated him are between two and a half, and three.

3L’elenco completo, in ordine alfabetico: Luca, Luca, Marco, Marco, Matteo, Stefano, Tiziano e il dormiente Erik.
Appendices
Appendix A

Wave pressure

Here, we summarize the derivation of the expression for the pressure associated with the Alfvén waves in the case of an oblique shock. Following Caprioli et al. (2009b), we start from the stationary equation for growth and transport of magnetic turbulence which, for an oblique shock, reads:

\[
\frac{\partial F_w(k, x)}{\partial x} = u_x(x) \frac{\partial P_w(k, x)}{\partial x} + \sigma(k, x) P_w(k, x). \tag{A.1}
\]

Herein, \(F_w\) is the energy flux, \(P_w\) is the pressure, both per unit logarithmic bandwidth, \(\sigma\) is the growth rate of the energy in the magnetic turbulence. The latter has been derived by Skilling (1975c), and for the case of only backwards propagating waves, as assumed here and in many other works (e.g. McKenzie and Völk (1982), Kang and Jones (2007), Caprioli (2012)) it reads:

\[
\sigma(k, x) = \frac{\pi^2 m_p^2 \Omega_0^2 v_A}{B_0^2} 2\pi \int d\mu \ dp \ p^2 (1 - \mu^2) v^2 \hat{n}_B \cdot \nabla f(x, p) \delta(kp|\mu| - m_p \Omega_0), \tag{A.2}
\]

where \(\Omega_0 = qB_0/m_p\) is the nonrelativistic gyrofrequency, \(B_0\) is the (mean) background magnetic field, \(\hat{n}_B\) is the unit vector along \(B_0\), \(\nu_- = \pi \Omega_0 P_w/(4\gamma U_B)\) is the collision frequency of particles against waves moving backwards in the frame comoving with the plasma. In the latter expression, \(\Gamma\) is the Lorentz factor of the particle, while \(U_B = B_0^2/(2\mu_0)\) is the magnetic energy density of the background field. Integrating Eq. (A.1) over \(k\), and normalizing by \(\rho_0 u_{ix}\), yields:

\[
2U_x(x) \frac{dP_w(x)}{dx} = V_{Ax}(x) \frac{dP_e(x)}{dx} - 3P_w(x) \frac{dU_x(x)}{dx}, \tag{A.3}
\]

where \(V_{Ax}(x) = v_A(x) \cos \theta_B(x)/u_{0x}\). As discussed in Caprioli et al. (2009b), we can neglect \(P_B\), \(P_w\) and \(P_g\) in Eq. (3.28) in the precursor (but not at the subshock) with respect to the kinetic momentum flux and the pressure of the accelerated particles, if acceleration is efficient, and use \(P_e(x) \approx 1 - U_x(x)\). The solution of Eq. (A.3), assuming no wave pressure far upstream is:

\[
P_w(x) = U_x(x)^{-1} \left[ \frac{1 - U_x^2(x)}{4M_{A0x}} \right], \tag{A.4}
\]

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Appendix B

Pressure ratio

In this appendix, we derive the ratio $p_{g2}/p_{g1}$ of the plasma pressures downstream and upstream of the subshock. The derivation closely resembles that of Vainio and Schlickeiser (1999). The main difference is that we use the conservation laws for the case of oblique shocks, Eqs. (2.39) (Scholer and Belcher, 1971), and the transmission and reflection coefficients of Alfvén waves derived by McKenzie and Westphal (1969). We consider the configuration in which the background fields have no components in the $y$-direction and the shock is in the $y$-$z$ plane. The Alfvén waves, on the other hand, are linearly polarized, with components in the $y$-direction.

For the sake of convenience, we rewrite the conservation equations here:

\[
[rho]u_x \frac{2}{2} \frac{B}{mu_0} = 0 ,
\]

\[
[rho]u_x + \left( p_y + \frac{B^2}{2mu_0} + P_w \right) \hat{n} - \frac{B_x B}{\mu_0} \right)^2 = 0 ,
\]

\[
\left[ \frac{1}{2} \rho u_x^2 + \frac{\gamma}{\gamma-1} p_y + \frac{B^2}{\mu_0} + F_w \right] - \frac{B_x (B \cdot u)}{\mu_0} \right)^2 = 0 ,
\]

\[
B_1 \frac{2}{2} \frac{B}{mu_0} = 0 ,
\]

\[
[\hat{n} \times (u \times B)]^2 = 0 .
\]

Recall that $\hat{n}$ is the shock normal, the pressure of the Alfvén waves is

\[
P_w = \frac{(\delta B)^2}{2\mu_0} ,
\]

and the energy flux (kinetic and Poynting vector) is

\[
F_w = \frac{1}{2} \rho (\delta u)^2 u_x + \frac{1}{\mu_0} \{(B \times \delta u + \delta B \times u) \times \delta B \} \cdot \hat{n} .
\]

The quantities $\delta u$ and $\delta B$ are the changes in velocity and magnetic field, respectively, due to the Alfvén waves. For these, it holds (following from the conservation equations):

\[
B_1 \delta u_1 - u_1 \frac{2}{2} \delta B_1 - B_2 \delta u_2 - u_2 \delta B_2 = 0 ,
\]

\[
\rho_1 u_1 \delta u_1 - \frac{2}{2} \delta B_1 - \rho_2 u_2 \delta u_2 - \frac{2}{2} \delta B_2 = 0 ,
\]

\[
\rho_1 u_1 \delta u_1 - B_1 \frac{2}{2} \delta B_1 - \rho_2 u_2 \delta u_2 - B_2 \frac{2}{2} \delta B_2 = 0 .
\]
and
\[ \delta B_1 = \delta B^\pm, \]
\[ \delta B_2 = \delta B_2^+ + \delta B_2^-, \]
\[ \delta B_1 = \delta B^\pm, \]
\[ \delta B_2 = \delta B_2^+ + \delta B_2^-, \]
\[ \delta B^\pm = \mp \sqrt{\mu_0 \rho} \delta u^\pm, \]
where the index $+$ (−) indicates forward (backward) propagating waves.\(^1\)

The reflection and transmission coefficients are, respectively:\(^2\)
\[ \frac{\delta B^-}{\delta B^\pm} = \frac{(M_{A1x} \pm \cos \theta_{B1})(r^{1/2} \mp 1)}{2(M_{A1x} r^{-1/2} - \cos \theta_{B1})}, \quad (B.6) \]
and
\[ \frac{\delta B^+}{\delta B^\pm} = \frac{(M_{A1x} \pm \cos \theta_{B1})(r^{1/2} \pm 1)}{2(M_{A1x} r^{-1/2} + \cos \theta_{B1})}, \quad (B.7) \]

Combining Eqs. (B.6), (B.7), and (B.5), together with (B.2) and (B.3), yields:
\[ [P_w]_1^2 = \left\{ r^2 \left( \frac{M_{A1x}^2 - \cos^2 \theta_{B1}}{M_{A1x}^2 - r \cos^2 \theta_{B1}} \right)^2 - 1 \right\} \frac{(\delta B)^2}{2\mu_0}, \quad (B.8) \]
and
\[ [F_w]_1^2 = \frac{u_{1x} M_{A1x}^2 (r - 1) (2M_{A1x}^2 - (1+r) \cos^2 \theta_{B1})}{(M_{A1x}^2 - r \cos^2 \theta_{B1})} \frac{(\delta B)^2}{2\mu_0}. \quad (B.9) \]

From Eqs. (B.1b), (B.1e) it follows (see also Eq. (2.38b)):
\[ B_{2z} = \frac{(M_{A1x}^2 - \cos^2 \theta_{B1})}{(M_{A1x}^2 - r \cos^2 \theta_{B1})} r B_{1z}. \quad (B.10) \]

Employing this, and by solving Eq. (B.1b) for $u_{2z}$, Eq. (B.1c) can be brought to the form:
\[
\left( \frac{\gamma}{\gamma - 1} \right) p_{q1} u_{1x} + \frac{1}{2} \rho_1 u_{1x}^2 \left( 1 - \frac{1}{r^2} \right) + u_{1x} \frac{B_{1z}^2}{\mu_0} \left[ 1 - r \left( \frac{M_{A1x}^2 - \cos^2 \theta_{B1}}{M_{A1x}^2 - r \cos^2 \theta_{B1}} \right)^2 \right] = \\
\left( \frac{\gamma}{\gamma - 1} \right) p_{q2} \frac{u_{1x}}{r} + \frac{B_{1z}^2}{32 \pi^2 \rho_1 u_{1x}^2} \times \left\{ 1 - 2 r \left( \frac{M_{A1x}^2 - \cos^2 \theta_{B1}}{M_{A1x}^2 - r \cos^2 \theta_{B1}} \right) \right\} + \\
+ r^2 \left( \frac{M_{A1x}^2 - \cos^2 \theta_{B1}}{M_{A1x}^2 - r \cos^2 \theta_{B1}} \right)^2 - 2 M_{A1x}^2 \frac{M_{A1x}^2 - \cos^2 \theta_{B1}}{(M_{A1x}^2 - r \cos^2 \theta_{B1})^2} r (r - 1) \right\} + [F_w]_1^2. \quad (B.11) \]

---

\(^1\)In the shock frame, due to the superalfvénic velocity of the fluid, both waves are advected in the direction of the fluid velocity.

\(^2\)In this Appendix, we drop the index $sub$ for the compression ratio $r = u_{1x}/u_{2x} = \rho_2/\rho_1$. 

By solving the $x$-component of Eq. (B.1b) for $\rho u_{1x}^2$ and substituting it into Eq. (B.11), after some algebra, the following equation can be derived:

\[
[(\gamma + 1) - (\gamma - 1)r] \frac{p_2}{p_1} = (\gamma + 1)r - (\gamma - 1) + (\gamma - 1) \left[ \frac{M_{41x}^4 (r - 1)^3}{(M_{41x}^2 - r \cos^2 \theta_{B1})^2} \right] \frac{p_{B1}}{p_1} +
+ (\gamma - 1)(r + 1) \left[ \frac{P_w}{p_1} \right]^2 - 2 (\gamma - 1) \frac{r \left[ F_w \right]^2}{p_1 u_{1x}},
\]

where $p_{B1} = B_{1x}^2/2\mu_0$. Finally, with the aid of Eqs. (B.2) and (B.3), Eq. (B.12) can be brought to the form:

\[
\frac{p_2}{p_1} = \frac{1}{[(\gamma + 1) - (\gamma - 1)r]} \left[ (\gamma + 1)r - (\gamma - 1) \frac{M_{41x}^4 (r - 1)^3}{(M_{41x}^2 - r \cos^2 \theta_{B1})^2} \frac{(p_{B1} + p_{w1})}{p_1} \right].
\]
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