NUMERICAL MODELING OF PLASMA STRUCTURES AND TURBULENCE TRANSPORT IN THE SOLAR WIND

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Abstract

The thesis focuses on the modeling of the inner-heliospheric solar wind with its embedded magnetic field by numerically solving the equations of magnetohydrodynamics (MHD). The main numerical tool used throughout this work is the state-of-the-art MHD code Cronos, which is extended from its basic setup to adequately describe the supersonic solar wind. First, solar rotation effects are implemented in both an inertial and a co-rotating reference frame, as well as in a conservative formulation for the latter. This setup is used to investigate the formation and evolution of co-rotating interaction regions (CIRs), which can be a dominant agent shaping the inner-heliospheric environment. For a direct comparison with spacecraft data, it is necessary to employ observation-based inner boundary conditions, for which a potential field model for the solar corona in conjunction with the empirically Wang-Sheeley-Arge model is employed. It is demonstrated that this setup can reproduce measured solar wind conditions, and a focus is on Carrington Rotations 2059-2061, during which stable and long-lasting CIRs were observed.

These results provide the essential quantities for subsequent investigations of the influence of CIRs on energetic particle propagation by means of a stochastic differential equation (SDE) approach. The transport coefficients needed in these latter models also depend on the turbulent component of the heliospheric magnetic field, so that for providing such the MHD model is extended to solve a set of equations for the transport of low-frequency turbulence alongside the Reynolds-averaged MHD equations. The resulting model is used to investigate the evolution of turbulence in the supersonic solar wind, and is furthermore applied to the propagation of a coronal mass ejection (CME) scenario. It is found that, on the one hand, turbulence does not act back strongly on the large-scale quantities, but, on the other hand, that CMEs are strong drivers of turbulence. Therefore, such a model is not essential for studies focusing on large-scale CME quantities only, but it does allow for self-consistently computed transport coefficients for future energetic particle propagation studies.

The implementation of all these extensions has been respectively validated by comparing with analytical models or previous numerical studies, which is an important part of working with numerical codes and, thus, of this thesis.

Another line of work is the application of the solar findings to other stars, their stellar winds and resulting astrospheres. For hot stars, these huge cavities are found to modulate the Galactic Cosmic Ray flux, which is an effect that could be responsible for tiny-scale anisotropies in corresponding all-sky maps.

The results presented in this work can be utilized for subsequent studies on numerous topics, such as energetic particle propagation, space-weather effects, or a coupling to outer-heliospheric models.
Zusammenfassung


Die Implementierung all dieser Erweiterungen wird jeweils validiert durch detaillierte Vergleiche mit analytischen Modellen oder bestehenden numerischen Ergebnissen, was einen wichtigen Teil von Studien mittels numerischer Methoden, und somit dieser Arbeit, darstellt.

Ein weiteres Arbeitsfeld ist die Anwendung der bezüglich unserer Heliosphäre gewonnenen Erkenntnisse auf andere Sterne und deren Astrosphären. Es wird gezeigt, dass letztere bei heißen Sternen so groß sind, dass sie galaktische kosmische Strahlung modulieren und somit für kleinskalige Anisotropien in entsprechenden Messdaten verantwortlich sein könnten.

Die Ergebnisse dieser Arbeit können vielseitig weiter verwendet werden, unter anderem für Studien zum Transport energetischer Teilchen, Weltraumwetter oder als Startpunkt für Simulationen der äußeren Heliosphäre.
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Chapter 1

Introduction

This chapter starts with a general overview of the heliospheric environment (Section 1.1), before outlining principal simplifications for modeling purposes and introducing the main numerical code used in this work in Section 1.2. The further outline of the thesis – being based on four publications, and putting them into perspective regarding their significance for solar and heliospheric research – is given in Section 1.3.

1.1 General overview

This section gives a general overview of the protagonists in this thesis: the Sun with its magnetic field (Section 1.1.1), emanating and shaping the turbulent solar wind (Section 1.1.2) that blows a bubble into the interstellar medium to form the heliosphere shielding the Earth from Galactic Cosmic Rays (Section 1.1.3). The hierarchy of the overview is to start from the center of the Sun and advance further and further outwards to the outer boundary of the heliosphere, while eventually the application of the solar findings to other – and thus even more distant – stars and their astrospheres (Section 1.1.4) is outlined.

1.1.1 The Sun

Before embarking on describing the different distinguishing parts of the Sun, a summary of its large-scale features is given (see, e.g., Stix, 2004; Priest, 2014). The Sun is a main-sequence star of spectral type G2 V and is about 4.9 billion years of age. Although it is a rather ordinary star, Earth’s proximity with fairly intelligent lifeforms inhabiting it makes it possibly a unique one. Studying the Sun is of great importance as it has profound influence on our climate, and since it is the main driver for space weather (e.g., Baker, 1998) it is crucial to understand the Sun and the solar wind to circumvent dangers to space-borne and earthbound technology, on which mankind increasingly depends. Furthermore, the insights into stellar physics
gained from studying our close-by star can be transferred to other, more distant stars.

The Sun consists mainly of hydrogen (92%) and helium (8%) with low abundances of heavier elements (0.1%) so that the mean mass density $\rho_\odot = 1.4 \times 10^3 \text{ kg/m}^3$, while the total mass of $M_\odot = 1.99 \times 10^{30} \text{ kg}$ constitutes 99.86% of the mass in the solar system. On a grand scale the Sun is in hydrostatic equilibrium, where the gravitational pull is balanced by the radiation pressure amounting to a luminosity of $L_\odot = 3.86 \times 10^{26} \text{ W}$. The radius of the Sun is defined as $R_\odot = 6.955 \times 10^8 \text{ m}$, and the mean heliocentric distance of the Earth is one Astronomical Unit (1 AU = $1.5 \times 10^{11} \text{ m} \approx 215 R_\odot$). The outer layers of the Sun exhibit differential rotation with respective synodic (as seen from Earth) rotation periods ranging from 26.24 days at the equator up to about 36 days toward the poles (Snodgrass and Ulrich, 1990). The mass-loss rate due to the emitted solar wind is $|\dot{M}_\odot| = 10^9 \text{ kg/s}$.

The solar interior

The interior of the Sun and especially its inner core are inaccessible to direct observations due to the extremely high opacity, although the relatively new field of helioseismology (see, e.g., the review of Kosovichev, 2011) allows for indirect conclusions about the inner structure of the Sun by measuring oscillations on the Sun’s visible surface, the photosphere. However, as the Sun constantly emits energy in the form of radiation, the question as to how the energy is generated inside the Sun has puzzled mankind for a long time. It was not until the early 20th century – after establishing quantum mechanics – that it was recognized by Eddington (1926) that thermonuclear fusion held the answer, whereas earlier ideas like gravitational contraction, which put the Sun’s lifetime at a few million years only, could be discarded. The core’s extreme density ($\rho_c \approx 1.5 \times 10^5 \text{ kg/m}^3$) and temperature ($T_c \approx 1.5 \times 10^7 \text{ K}$) are sufficient to drive fusion processes like the proton-proton chain or the CNO cycle, in which four protons are fused into one helium nucleus, and the mass difference between input and output is converted into energy according to Einstein’s $E = mc^2$. A byproduct of these processes are extremely weakly interacting neutrinos, whose detection on Earth (Davis et al., 1968) is another confirmation of the theory that the Sun’s energy originates from fusion.

The transport of this energy within the solar interior is two-fold (see Figure 1.1). First, above the core from about $0.25R_\odot$ outwards, radiation is the dominant transport process: photons, initially with energies corresponding to gamma rays, are constantly absorbed and re-emitted, leading to a random walk inside the Sun that takes about two hundred thousand years (Mitalas and Sills, 1992) until they leave the Sun mainly as visible light. Second, above some $0.7R_\odot$ convective instability sets in due to a very large temperature gradient (see Schwarzschild, 1992). Consequently, blobs of hot plasma rise, expand and cool so that they eventually descend
1.1. GENERAL OVERVIEW

Figure 1.1: Schematic illustration of the solar interior and the lower atmospheric layers (taken from Priest, 2014).

again. The convection zone exhibits a number of complex motions such as differential rotation, meridional flow and 5-minute oscillations, while at the photosphere, convection is manifested in the so-called granulation. Granules occur at different scales (meso- and supergranulation), but a common feature are the bright centers containing upwelling hot plasma and dim edges of descending cool plasma (see left panel of Figure 1.2).

The transition region between the radiative interior and the convection zone is called tachocline (Spiegel and Zahn, 1992), which is a region of strong shear that is thought to be largely responsible for the generation of the solar magnetic field by means of a dynamo process. Magnetic flux emerges through the photosphere on a variety of scales, which can be pictured as a carpet of magnetic loops closing at different heights (see right panel of Figure 1.2). The most prominent feature caused by the magnetic field in the photosphere are sunspots, which appear darker than their surroundings as the magnetic field inhibits convection so that cooled plasma is prevented from descending quickly (Figure 1.2 (left)). Sunspots have radii ranging from a few kilometers up to 15000 km, which make the largest ones visible to the
CHAPTER 1. INTRODUCTION

The Sun’s lower atmosphere

In contrast to the solar interior, the solar atmosphere is the part of the Sun that photons can directly escape from. Most of the solar radiation originates from the photosphere, which radiates like a black body at a temperature of about 6000K. Contrary to the expectation that the temperature should further decline with radial distance, there is actually an increase in temperature in the chromosphere with a sharp peak in the temperature gradient at the so-called transition region giving rise to coronal temperatures of several million degrees (Figure 1.3, with temperature still increasing beyond the heights shown here). The respectively labeled coronal heating problem remains unsolved, although the most likely candidates for the heating mechanisms are either or both damping and dissipation of waves originating from the turbulent motions in the convection zone (e.g., Carlsson et al., 2007), or magnetic reconnection (e.g., Parker, 1972; Cargill and Klimchuk, 2004).

There is a vast number of magnetic structures in the solar atmosphere, which are often organized in networks. A detailed description would go beyond this brief overview (but see, e.g., Priest, 2014). The most common features in the chromosphere are spiculae of heated, accelerated and uprising, as well as cooled, descending plasma. The extension of the chromosphere is roughly 2.5 Mm, the transition region
is rather narrow (a few 100 km), and the corona’s outer boundary is usually defined by the Alfvénic critical surface at about $r_A \approx 15 - 20R_\odot$. At this surface the solar wind speed equals the Alfvén speed ($v_{sw}(r_A) = v_A(r_A)$), so that no information can travel back to the corona. Two distinct topologies are typical for the coronal magnetic field, namely regions of closed loops on top of active regions, and open field lines in so-called coronal holes above unipolar regions. During solar minimum conditions the global magnetic field is approximately that of a dipole due to the strong unipolar fields of respectively opposing polarity in both polar regions, and large coronal holes occupy the higher latitudes, while closed loops are restricted to the equatorial regions (left panel of Figure 1.4). The influence of the solar wind (see Section 1.1.2)) on the magnetic field becomes more dominant with increasing radial distance and effects an opening of the field at mid-latitudes as well, usually at about $2.5R_\odot$ (Altschuler and Newkirk, 1969), and a radial magnetic field at all latitudes is present beyond the Alfvénic critical surface. During the solar cycle the large polar coronal holes become ever less pronounced towards solar maximum and eventually the predominant polarity of the northern and southern hemisphere changes sign. A magnetic- or Hale-cycle therefore takes about 22 years. In the more active phases around solar maximum the coronal field exhibits a more complex structure, where one can find coronal holes and closed loops at all latitudes (right panel of Figure 1.4).
1.1.2 The solar wind

Large-scale structure

The history of the solar wind is a rather modern one, having found its way into science only in the second half of the 20th century, although it had been proposed already in the 19th century by Sun-observing pioneers such as Carrington and Birkeeland that solar activity was responsible for geomagnetic effects such as the aurora. In the 1950s, Biermann (1951) proposed a corpuscular emission from the Sun to explain the gaseous straight tails of comets. Meanwhile, Chapman and Zirin (1957) argued that – due to the high coronal temperatures already known from X-ray observations – the coronal plasma should expand at least beyond Earth’s orbit. The latter authors, however, assumed a static configuration.

By first demonstrating that such a static solution results in finite – and thus unrealistic – pressure at infinite distance, the modern basic idea of the solar wind as a dynamic, supersonic flow was postulated by Parker (1958). The driving force accelerating the solar wind in his isothermal and hydrodynamic model is the thermal pressure of the hot corona, resulting in terminal solar wind speeds in a range from about 400 to 800 km/s (depending on temperature, see left panel of Figure 1.5). The magnetic field is ”frozen” into (i.e., it is passively advected with) the solar wind, while the footpoints of the field lines remain anchored at the rotating Sun resulting in an Archimedean spiral pattern (see right panel of Figure 1.5).

Parker’s idea met some resistance at first, but when the first measurements (e.g. with the Mariner 2 spacecraft, Snyder and Neugebauer, 1963) confirmed a supersonic flow it became broadly accepted and solar wind measurements made during the space age have confirmed the general picture. The solar wind consists mainly of protons and electrons, with low abundances of alpha particles. Typical values of solar wind
1.1. GENERAL OVERVIEW

Average observed solar wind properties at 1 AU in the ecliptic plane (Priest, 2014).

<table>
<thead>
<tr>
<th>Property</th>
<th>Average value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed</td>
<td>400 km/s</td>
</tr>
<tr>
<td>Number density</td>
<td>6.5 cm$^{-3}$</td>
</tr>
<tr>
<td>Proton temperature</td>
<td>50000 K</td>
</tr>
<tr>
<td>Magnetic field</td>
<td>6 nT</td>
</tr>
</tbody>
</table>

For a long time in-situ observations were restricted to the ecliptic plane. It was only after 1990 when the Ulysses spacecraft was brought into a high-latitude orbit after a swing-by maneuver at Jupiter that the three-dimensional picture of the solar wind topology was revealed. During Ulysses’ 19-year mission it covered almost two solar cycles, and the data taken by Ulysses are nicely summarized in plots such as the one presented in Figure 1.6, which show the following pattern: near activity minimum the solar wind is highly structured, with remarkably steady, fast, hot and tenuous streams (about 750 km/s) towards the poles, while the region within about ±20° of the solar equatorial plane is occupied by variable, slow, dense and cooler streams (about 400 km/s). This pattern was measured during the first (1992-1998; left panel of Figure 1.6) and third (2004-2009; not shown) orbits of the mission. In contrast, there is no discernible global structure during the maximum of solar activity, when fast as well as slow streams can be found at any given latitude. Naturally, this raises the question as to where the different types of solar wind originate from.
in the solar corona and how they are accelerated. As the plasma in the corona has to follow the magnetic field lines, only open field lines allow for an escape. The fast solar wind is clearly associated with the large coronal holes, but the origin of the slow solar wind is still unclear and under debate (see, e.g., Shergelashvili and Fichtner, 2012). Candidates are high-latitude coronal-hole/streamer boundaries for solar minimum, and small coronal holes and active regions for solar maximum. Being related to the coronal heating problem, the acceleration processes for the different types of solar wind are also still subject to ongoing research. One of the prevailing ideas is that the dissipation of Alfvén waves in the corona is the main driver to accelerate the solar wind, where the wave energy is mainly dumped below/above the Alfvénic critical surface for the slow/fast wind (Cranmer and van Ballegooijen, 2005; Cranmer et al., 2007).

Figure 1.6: Solar wind velocity profiles near solar minimum (left) and maximum (right) as measured by the Ulysses spacecraft (taken from Meyer-Vernet, 2007). The white arrows indicate time progressing in an anti-clockwise fashion.

During solar minimum, the coronal magnetic field consists of two oppositely directed large polar coronal holes, which are separated by a so-called helmet streamer, which is a closed magnetic arcade located below the heliospheric current sheet (HCS) that extends into the heliosphere. Because of slight asymmetries and the tilt of the rotation axis of the Sun with respect to the ecliptic plane, in which the planets perform their orbits, there is a typical structure of alternating heliospheric magnetic field (HMF) directions measured at Earth during one rotation around the Sun (see e.g., Schwenn and Marsch, 1990). A crossing of the HCS or neutral line is called a sector boundary, while the recurring phases of alternating polarities are known as sector structure. The situation can be visualized as a flying ballerina skirt or like the brim of a sombrero hat as depicted in Figure 1.7 (left). As the band of slow solar
wind aligns roughly with this wavy current sheet, there are also respective recurrent streams of fast wind extending to ecliptical regions, which are azimuthally embedded into otherwise slow solar wind. Due to solar rotation, these streams become radially aligned so that the fast wind runs into the slow one ahead – leading to a compression region – and outruns the trailing one, resulting in a rarefaction region (see right panel of Figure 1.7). The embedded frozen-in magnetic field prevents the fast wind from overtaking and strong enhancements in plasma and magnetic field density at the compression region develop, which generate pairs of waves traveling forward and backward with respect to the stream interface that separates fast and slow wind. As the critical/characteristic speeds decrease with radial distance, these waves steepen into a forward-reverse shock pair, which usually occurs at about 2 AU (Balogh et al., 1999). These kind of structures as a whole are known as co-rotating interaction regions (CIRs), which have important effects on the propagation of energetic particles because of their associated shocks and turbulence properties. Particularly during the descending and ascending phases in the solar cycle, CIRs can be long-lasting recurrent structures over several solar rotations, constituting the main driver shaping the heliospheric environment.

Figure 1.7: Left: Sketch of the wavy heliospheric current sheet (taken from Sakurai, 1985). Right: Sketch of a co-rotating interaction region (taken from Hundhausen, 1972).

Towards solar maximum the HCS becomes increasingly tilted until a polarity reversal occurs and it becomes flatter again with decreasing solar activity. The topology of the coronal magnetic field and the associated solar wind is not only rather complex during high solar activity with fast and slow streams at arbitrary latitudes, but there are also a number of impulsive events such as flares that are often associated with coronal mass ejections (CMEs) and distort the above outlined picture of otherwise rather steady configurations during a solar rotation. Both flares and CMEs are
caused by reconnection events in the solar corona, but there are many more flares than CMEs (e.g., Priest, 2014). Although there are still many open questions, it is believed that if there is an overlying magnetic arch above the reconnection site, there is usually just a flare, whereas a CME occurs when the reconnection site detaches and releases huge amounts of matter. In a flare the released magnetic energy leads to both the emission of short-wavelength radiation and the acceleration of solar energetic particles (SEPs) up to a significant fraction of the speed of the light (∼0.8c), so that there is only little time to make arrangements for the protection of e.g. astronauts from this radiation. In case of a CME, magnetic energy is also channeled into the acceleration of the ejected mass, which can reach velocities of a few thousand km/s and the propagation time to Earth can be as short as a day or two. CMEs often drive a shock that can also accelerate SEPs.

Figure 1.8: Artistic sketch of a CME set loose at the Sun and propagating towards Earth with its geomagnetic field. [www.land-of-kain.de/docs/spaceweather/nasa_spaceweather_small.jpg].

The geomagnetic field of the Earth is usually able to deflect the solar wind around the Earth’s magnetosphere, but CMEs can strongly distort this protective shield and particles can reach Earth especially from above the poles (see Figure 1.8). In the atmosphere these particles ionize oxygen and nitrogen atoms, leading to the beautiful phenomenon of the aurora, but in some cases particles can also reach the Earth’s
surface (ground level events) and cause shortcuts and other damage in electrical systems. As an ever increasingly technology-dependent society, it is of vital importance to us to be able to understand and predict these kind of events. Respective efforts are made by scientists over the world and are channeled in institutions such as the Space Weather Prediction Center (SWPC, http://www.swpc.noaa.gov/) and the Coordinated Community Modeling Center (CCMC, http://ccmc.gsfc.nasa.gov/).

**Turbulence in the solar wind**

Fluctuations that are super-imposed onto the large-scale magnetic field, solar wind velocity and density, have already been seen in the very first solar wind measurements, and respective studies (e.g., Coleman, 1968; Belcher and Davis, 1971) showed that the solar wind has to be considered as an inherently turbulent plasma. Turbulence is not only generated in the corona from where fluctuations are convected into interplanetary space, but also in-situ by the plasma itself at density gradients throughout the heliosphere, as well as on transients with their associated shocks such as CIRs and CMEs and by the isotropization of newly born pickup ions (see next section).

Turbulence has several important effects (see the review by Miesch et al., 2015). For example, the associated turbulent energy decays with time and radial distance and heats the solar wind plasma particularly in the outer heliosphere (as measured by Voyager 2, Gazis et al., 1994)) due to the increased pickup ion production. Furthermore, turbulence is a catalyst for reconnection (e.g. Yokoi et al., 2013). Another important factor is the influence of turbulence on the propagation of energetic particles: the turbulent magnetic field guides their transport, where the particles not only gyrate about and follow the mean magnetic field lines but are also able to perform a perpendicular diffusion towards neighboring field lines due to the turbulent fluctuations. Respective models for the transport of energetic particles in the heliosphere have – for a long time – been coupled to the solar wind dynamics by parameterizing all relevant processes in terms of the large-scale background quantities, in particular for the treatment of spatial diffusion (see the review of Potgieter, 2013). Only recently have models been developed that formulate the diffusion coefficients explicitly based on the small-scale fluctuations (ab-initio models, e.g., Engelbrecht and Burger, 2013), which has been made possible by new improvements in analyzing turbulence in solar wind measurements (e.g. Horbury and Osman, 2008; Horbury et al., 2012) on the one hand, and respective modeling on the other hand, as described next (for an overview see Zank, 2014).

Models of transport of incompressible low-frequency turbulence in the solar wind describe the evolution of respective integral quantities such as the total turbulent energy density – comprising magnetic and kinetic components – as well as the energy difference between the two and the ratio between inward and outward propagating
modes with respect to the mean magnetic field, which is the so-called cross-helicity. The nonlinear cascade of the fluctuations and the eventual dissipation into heat at the smallest scales is modeled in terms of correlation lengths also subject to respective evolution equations. Such models date back some thirty years (Tu et al., 1984; Zhou and Matthaeus, 1990), which have been followed by first systematic studies of the radial evolution of turbulence quantities in the highly supersonic solar wind (Zank et al., 1996), while the recent decade brought numerous improvements. Amongst those are the inclusion of out-of-ecliptic latitudes (Breech et al., 2008) and the extension to full time-dependence and three spatial dimension, as well as a more self-consistent treatment of the background solar wind by simultaneously solving turbulence transport and large-scale MHD equations (Usmanov et al., 2011). Further directions involve multi-fluid approaches for a better treatment of pick-up ions (Usmanov et al., 2012) and electrons (Usmanov et al., 2014), as well as considering not only one but two, mutually interacting, incompressible turbulence components, namely quasi-two-dimensional turbulent and wave-like fluctuations (Oughton et al., 2011).

These models successfully compare to spacecraft measurements, which show that turbulence decays with time and radial distance, but that it is also generated in-situ at interplanetary disturbances (stream shear) and by pick-up ion isotropization in the outer heliosphere, the latter being responsible for the increased temperature there. The turbulence generation also leads to an eventual equilibrium between inward and outward propagating modes, so that the cross-helicity becomes zero.

A common limitation of the above models is the restriction to conditions where the Alfvén speed is significantly lower than that of the solar wind, which is a valid assumption beyond about 0.3 AU only. The turbulence below this radial distance and its consequences for the dynamics of the solar wind have been studied on the basis of the somewhat simplified transport equations for the wave power spectrum and the wave pressure (e.g., Tu and Marsch, 1995; Shergelashvili and Fichtner, 2012). A generalization of the more involved turbulence transport models as described above – therein removing the Alfvén speed limitation – was recently presented by Zank et al. (2012), see also Dosch et al. (2013). Beyond the validity of their equations in the sub-Alfvénic parts of the heliosphere, the model also involves evolution equations for the energy difference (previously often assumed to be constant) and for separate correlation lengths for the inward and outward propagating modes. The model was solved numerically by Adhikari et al. (2015), which showed that the energy difference between kinetic and magnetic fluctuations does not approach a constant non-zero value as assumed in previous models, but that an equilibrium state is reached in the outer heliosphere instead. However, this numerical model introduced several simplifications that need to be addressed.
1.1.3 The heliosphere

The heliosphere is formed as a consequence of the interaction between the solar wind and the interstellar medium (ISM), through which the Sun moves on its 200 million year lasting orbit around the Galactic center with a speed of 240 km/s, while the relative speed between the Sun and the ISM is only about 25 km/s. From the point of view of the Sun this looks like an inflow of interstellar plasma from the so-called nose region, which leads to a number of interesting structures in the heliosphere (see Figure 1.9):

Figure 1.9: Overview of the heliospheric environment: The solar wind emanating from the Sun (at center) blows a "bubble", the heliosphere, into the interstellar medium. Typical structures are the termination shock and the heliopause (see text). The trajectories of mankind’s most distant spacecraft, Voyager 1 and 2, are also indicated. [www.nasa.gov/vision/universe/solarsystem/voyager_agu.html].

Both the ISM and the solar wind plasma have embedded magnetic fields and are unable to permeate the other under idealized conditions. The boundary between the two plasmas is the bullet-shaped heliopause (HP), a tangential discontinuity at which the solar wind pressure equals the one of the ISM. The radially out-flowing solar wind adapts to this obstacle by first transiting to a heated, sub-sonic state at the termination shock (TS), and in the region between the TS and the HP – the inner heliosheath – the flow is bent towards the heliospheric tail. Similarly, the
ISM flow is also decelerated, resulting in a bow wave or bow shock, depending on whether the ISM speed is supersonic or not, which is still under debate (see Scherer and Fichtner, 2014). While the solar wind plasma can be considered as fully ionized due to the high coronal temperatures, the ISM plasma is a mixture of ions and electrons, as well as neutral atoms (i.e. gas, 99%), but also dust (1%, Boulanger et al., 2000)).

As the interstellar plasma slows down in the outer heliosheath’s nose region and thereby becomes denser, the cross section for charge exchange processes, in which an electron from a neutral atom "jumps" to an ion, increases strongly. This leads to the formation of the so-called hydrogen wall, which is an accumulation of neutral hydrogen that can be observed in the Lyman-\(\alpha\) absorption line (Wood et al., 2000). The majority of neutral atoms, however, can penetrate the heliopause and will eventually (at least beyond about 8 AU) be ionized by photo-ionization, electron impact or charge-exchange with solar wind particles (see, e.g., Scherer et al., 2014), so that they become so-called pickup ions, because they are then assimilated in and convected with the solar wind flow. During this process, in which the initially ring-distributed pickup ions isotropize, Alfvén waves are generated that contribute to the turbulence spectrum in the outer heliosphere, eventually heating the latter. Furthermore, pickup ions are considered as seed population for the generation of anomalous cosmic rays accelerated at the TS (the term "anomalous" stems from the different composition – higher abundances of heavier elements – of these cosmic rays as compared to Galactic Cosmic Rays (GCRs) or SEPs, which are mainly protons, Cummings et al., 1995). If pickup ions are generated in a charge exchange process the former solar wind ion becomes an energetic neutral atom (ENA) and can flow unimpeded by the magnetic field. These atoms are measured by the IBEX spacecraft orbiting Earth and mapping the whole sky (McComas et al., 2014). An unpredicted phenomenon that was found is the so-called IBEX ribbon of enhanced ENA flux that aligns with the plane where the interstellar magnetic field is perpendicular to the heliocentric radius vector. While an undisputed theory has not yet been found to explain the ribbon (see the review of McComas et al., 2011), the IBEX mission provides insights into outer-heliospheric processes and structures by global remote observations, as opposed to the few in-situ spacecraft measurements described next.

Mankind’s most distant spacecraft – Voyager 1 and 2 (V1, V2) – are both headed towards the upwind region of the heliosphere, but offset from the ecliptic by about 30° towards north and south, respectively. V1 crossed the TS in 2004 at 94 AU, whereas V2 crossed it at 84 AU three years later. V1 is the first and of yet only spacecraft that has also left the heliosphere in crossing the heliopause in 2012 at about 122 AU, when particles of solar origin became absent while the GCR intensity went up. The crossing came with some unexpected findings: first, the inner-heliosheath thickness was expected to be much larger – hinting at energy losses there reducing the pressure (Izmodenov et al., 2014), while it was argued by Fisk and Gloeckler (2014) that
the heliopause has not been reached yet after all. Second, the magnetic field did not change much after V1 crossed the heliopause, where it was expected to change from a Parker spiral field of solar origin to the one of the ISM that drapes around the heliopause (see Röken et al., 2015, for a recent model, visualizations and further references). This mystery is still under investigation, but there are ideas that, for example, involve heliopause instabilities or reconnection, yielding a rather turbulent transition (Grygorczuk et al., 2014; Opher and Drake, 2013). V2 is expected to cross the heliopause soon, which will hopefully shed some light on the unresolved issues as this spacecraft – unlike V1 – still benefits from a working plasma instrument. Both V1 and V2 have enough power left to operate until about 2020, which will most likely, however, not be enough time to reach the bow wave/shock expected at about 230 AU. The heliospheric tail is largely uncharted and no current space-probe is scheduled to investigate. Its extent is probably a few thousand AU, and most models predict a single tail that can ”store” several solar cycles with their respective polarity changes (e.g., Pogorelov et al., 2014). However, it was recently proposed by Opher et al. (2015) (reviving an idea by Yu, 1974) that there is a split tail caused by the twisted HMF that channels two separate jets.

It should be stressed though that the distances to the heliospheric structures as given above are very likely to be time- and direction-dependent: on the one hand the solar wind conditions change during the solar cycle and transient structures such as CMEs and CIRs merge and interact with increasing radial distance to form global merged interaction regions (GMIRs) with enhanced pressure, which probably make the TS constantly move back and forth around a mean heliospheric distance of about 90 AU (le Roux and Fichtner, 1999). On the other hand the ISM is also not homogeneous (e.g. de Avillez et al., 2015) and changes the overall size of the heliosphere, albeit on much longer time-scales. Under extreme conditions it is possible that during the Sun’s passage through a hot and dense interstellar cloud the TS distance can shrink down to be within the planetary orbits (Scherer et al., 2008). The heliosphere also acts as a shield from highly energetic GCRs, whose influence on the Earth’s climate is still under debate and probably not negligible, so that during the Sun’s orbit around the galactic center there have been phases of more intense impacts of GCRs on Earth (Scherer et al., 2006; Kopp et al., 2014).

The sources of GCRs are believed to be energetic phenomena such as jets driven by black holes or supernovae remnants (e.g., Büsching et al., 2005), which can accelerate particles to very high energies. The exact origin of such a particle that might eventually end up in a detector near Earth cannot be pinpointed because the transport of GCRs is mainly along the poorly known (inter-)galactic magnetic field. Meanwhile, the modulation of the cosmic ray spectrum in the heliosphere (and possible other astrospheres) and the resulting cosmic ray flux at Earth are more directly accessible due to an increasingly better understanding of the heliospheric structures.
1.1.4 Stellar winds and astrospheres

It was realized already in the late middle ages by Tycho Brahe that stars are not perfect, ever constant celestial objects, but suffer from mass loss (although at that time it was not the stellar wind that was observed, but most likely the more spectacular novae), and it was much later also established that respective line profiles in the continuum of stars could be explained by expanding stellar atmospheres (Beals, 1929) long before the confirmation of the existence of the solar wind. The term stellar wind, however, was again coined by Parker (1960). Recent observational advancements (e.g. Hubble space telescope, or the Wide-field Infrared Survey Explorer (WISE) mission) allowed for all-sky surveys measuring dust emission (mostly infrared, e.g., Groenewegen et al., 2011, see Figure 1.10) or the Lyman-α line (Linsky and Wood, 2014) associated with bow shocks around other stars, thus indicating the existence of respective astrospheres. Therefore, many findings about the solar wind and our heliosphere can be transferred to other stars and their astrospheres.

However, the interstellar environment around those stars is most likely different from our local environment, and the processes driving a stellar wind can be very different from the coronal solar wind (see Lamers and Cassinelli (1999) for an overview). For example, hot (O/B-) stars are associated with radiation or line driven winds by the absorption in spectral lines. These stars posses a completely radiative interior, so that the strength or even the existence of their magnetic fields is highly debated (although some examples have recently been found (Hubrig et al., 2015)). Line
driven winds can have terminal velocities of several thousand km/s leading to huge astrospheres with extents of several parsecs. Surprisingly, such high-velocity winds are also found to be generated by the much cooler M-dwarf stars, where the interior energy transfer is completely convective and are, therefore, magnetically very active. It can be speculated that a considerable amount of the mass loss is probably attributable to flares and CMEs.

The astrospheres around hot stars are of interest, because they represent huge cavities in the ISM that modulate the cosmic ray flux through them and might therefore be responsible for tiny-scale anisotropies in respective all-sky maps of the GCR flux (Scherer et al., 2015). For cool stars that are relatively close-by, it is even possible to infer their photospheric magnetic field distribution (Donati et al., 2008), which allows to apply solar and heliospheric numerical models to such stellar winds as performed by, e.g., Vidotto et al. (2011, 2015); Vidotto (2014). A particular focus lies on M-dwarfs with orbiting exoplanets, and the possible interaction between these stellar winds with planetary magnetospheres (e.g., Ip et al., 2004; Preusse et al., 2007), which should be considered as one of the important factors for habitability. As discussed for the heliosphere above, the size of a respective astrosphere and its capability to shield planets from cosmic rays may also be important, so that global astrospheric models for these cases are also planned.

1.2 Model formulation and numerical setup

1.2.1 Principal simplifications

From a modeling point of view, it is customary and necessary to sub-divide the heliospheric environment because of the very different physical processes and associated length and time scales involved in one region or the other. Roughly speaking, these regions can be thought of as spherical shells of increasing radial distance from the center of the Sun as outlined in the preceding sections, so that – for an outward flow of information – a particular model of one region usually relies on the region below and determines the following one. In particular, this thesis is primarily concerned with the formation of the solar wind in the Sun’s lower atmosphere and its continued dynamical behavior in the supersonic part of the heliosphere, i.e. within the TS.

Following the above reasoning, such a model naturally depends on processes in the solar interior. It is, however, simpler to use the directly accessible observational data from the solar photosphere as a starting point. For large-scale models the knowledge of the photospheric magnetic field suffices to determine the coronal magnetic field, which shapes the emanating solar wind filling the heliosphere. Important processes in the super-Alfvénic heliosphere above the corona primarily involve the interaction between differently fast streams, which leads to interesting structures such as evolving shocks, which have important implications for, e.g., the transport of energetic
particles in the heliosphere, or planetary magnetospheres. With increasing distance from the Sun, the initially rather inhomogeneous solar wind perturbed by CIRs and CMEs – which eventually smear out in GMIRs – becomes relatively homogeneous. Such (time-dependent) conditions can then be used as input to outer-heliospheric models (as done in, e.g., Pogorelov et al., 2014), which is particularly important for a better understanding of the Voyager 1 measurements.

The above mentioned necessity for subdividing the heliosphere is also found in contemporary modeling of the formation of the solar wind: typically one distinguishes the sub-Alfvénic corona and the super-Alfvénic part beyond the so-called heliobase (Zhao and Hoeksema, 2010) at about $20R_\odot$. There are two common approaches to compute the large-scale coronal magnetic field, namely (i) full three-dimensional (3D) MHD models and (ii) potential field models (see Chapters 2 and 3 for details). While the full MHD models are principally better suited to address all the involved physics self-consistently, they have the drawback of being quite complex and requiring large computer resources. Particularly this last issue has made potential field models a popular approach to describe the large-scale coronal magnetic field, which has also been shown to be remarkably similar in both MHD and potential field models (Riley et al., 2006). Both approaches can be applied to observational data of the photospheric magnetic field (i.e. magnetograms) for usage as inner boundary conditions, and both eventually provide the global coronal magnetic field. However, the drawback of the potential field models is that they do not self-consistently compute the resulting solar wind speeds. Instead, empirical models have to be used like the so-called Wang-Sheeley-Arge (WSA; Arge and Pizzo, 2000) model, which uses the coronal magnetic field topology to determine solar wind speeds, i.e. fast wind from coronal holes and slow wind from their boundaries as outlined in Section 1.1.2. Thus, both MHD and empirically based models of the corona provide the resulting magnetic field and solar wind speeds at the heliobase, which can be further utilized in subsequent MHD simulations to investigate the interaction of different solar wind streams. Compared to coronal MHD simulations, these inner-heliospheric MHD simulations are not requiring as much spatial and time resolution, and are more simple to formulate, because the solar wind is super-Alfvénic here and information cannot travel backwards – an issue that otherwise complicates boundary conditions considerably.

Large-scale heliospheric models are usually based on a fluid treatment of the plasma, so that the latter is described by the MHD equations. These equations are only valid under certain conditions (see, e.g., Priest, 2014), which are not well fulfilled everywhere in the heliosphere (such as the assumptions of distribution functions being close to Maxwellian despite the non-collisionality in the solar wind). There are still several reasons to pursue modeling approaches based on MHD: first, alternative descriptions either based on non-Maxwellian distribution functions (meso-scale) or on particle trajectories themselves (micro-scale) are too fine-scaled for a numerical modeling of the large-scale heliospheric structures due to computational limitations.
Such approaches (e.g. particle in cell (PIC) simulations) are instead applied to much smaller computational domains (e.g., Kunz et al., 2014). Second, the fluid picture is still a reasonable good approximation as many respective studies (see, e.g., the review by Zank, 1999) were successful in recreating solar wind properties as compared to spacecraft data. Consequently, this approach is also taken in this thesis by using the state-of-the-art MHD code CRONOS, which is described in more detail in the following section.

### 1.2.2 The CRONOS code

The equations of MHD can be solved analytically for only a few simplified cases so that a numerical approach has to be taken. This section gives a descriptive overview of the CRONOS code that is used in this work. The code was developed by R. Kissmann (based on Grauer et al., 1998; Kleimann et al., 2009), and was used in recent years primarily by his current working group at the University of Innsbruck as well as by his former group in Bochum. Studies focused on astrophysical [ISM turbulence (Kissmann et al., 2008), accretion disks (Kissmann et al., 2011), colliding wind binaries (Reitberger et al., 2014b,a), and astrospheres (Scherer et al., 2015)] as well as heliospherical scenarios [CMEs (Kleimann et al., 2009), magnetic clouds (Dalakishvili et al., 2011), background solar wind (Wiengarten et al., 2013, 2014), and turbulence in the solar wind (Wiengarten et al., 2015)]. The following text summarizes the main features of CRONOS without going into details on numerical issues, but see Appendix C of Wiengarten et al. (2015) and references therein.

In its basic setup the code solves the equations of ideal MHD, given here in normalized form:

\[
\begin{align*}
\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) &= 0 \quad (1.1) \\
\partial_t (\rho \mathbf{u}) + \nabla \cdot [\rho \mathbf{uu} + (p + \|\mathbf{B}\|^2/2) \mathbb{1} - \mathbf{B}\mathbf{B}] &= 0 \quad (1.2) \\
\partial_t e + \nabla \cdot [(e + p + \|\mathbf{B}\|^2/2) \mathbf{u} - (\mathbf{u} \cdot \mathbf{B})\mathbf{B}] &= 0 \quad (1.3) \\
\partial_t \mathbf{B} + \nabla \times \mathbf{E} &= 0 \quad (1.4)
\end{align*}
\]

where \(\rho\) is the mass density, \(\mathbf{u}\) is the velocity of a fluid element, \(\mathbf{B}\) and \(\mathbf{E}\) describe the electromagnetic fields, \(e\) is the total energy density, and \(p\) is the scalar gas pressure. Furthermore, \(\mathbb{1}\) denotes the unit tensor, and the dyadic product is used. So far the system is under-determined, and requires the closure relations

\[
\begin{align*}
\epsilon &= \frac{\rho}{2} \left( \frac{\|\mathbf{u}\|^2}{2} + \frac{\|\mathbf{B}\|^2}{2} \right) + \begin{cases} 
p/(\gamma - 1) : & \gamma \neq 1 \\
0 : & \gamma = 1
\end{cases} \quad (1.5) \\
\mathbf{E} + \mathbf{u} \times \mathbf{B} &= 0 \quad (1.6) \\
\nabla \cdot \mathbf{B} &= 0 \quad (1.7)
\end{align*}
\]

to complete the set of equations. Equation (1.5) for the total energy density \(\epsilon\) distinguishes between adiabatic (\(\gamma \neq 1\)) and isothermal (\(\gamma = 1\)), where in the latter
case Equation (1.3) becomes redundant and does not enter the computations.

The **Cronos** code is written in C++. It has been designed in a user-friendly fashion such that the part in which the user adopts an own specific physical model is strictly separated from the part implementing the algorithms of the underlying numerical schemes, i.e. the code is modularized. This also allows for extensions of the basic equations of ideal MHD, such as additional source or flux terms, as well as the incorporation of equations for additional quantities to be solved along with the original ones.

**Cronos** employs the semi-discrete finite-volume scheme CWENO (Kurganov and Levy, 2000) and integrates the equations forward in time by means of the Runge-Kutta method of adaptable accuracy. The initial time step has to be chosen small enough, so that the Courant-Friedrichs-Lewy condition (CFL; Courant et al., 1928) is fulfilled. Afterwards, adaptive time-stepping is applied such that a subsequent time step is chosen to be the largest possible one fulfilling CFL. The solenoidality condition of the magnetic field (1.7) is ensured by a constrained transport scheme.

The coordinate systems supported by **Cronos** are currently Cartesian, cylindrical, and spherical, where the latter have recently been extended to cover the coordinate singularities (e.g. the polar axis in spherical coordinates) as well. As part of this thesis, non-linearly spaced grids have also been implemented (see Appendix A), but the general description here concentrates on linearly spaced grids for simplicity. The simulation is carried out on a three-dimensional grid, which in C++ is saved in an array whose (integer) indices $i, j, k$ run from 0 to $(N_x, y, z - 1)$. Thus, the grid comprises $N_x \cdot N_y \cdot N_z$ cells where $N_{x,y,z}$ stands for the number of cells for the corresponding dimension. To construct a grid, the user first specifies the desired range for each dimension, either by fixing the first and last cell center locations or the first cells left and last cells right face coordinate. Here, the first possibility is described, so that, considering only the $x$ direction, $x_s$ and $x_e$ denote the start and end cells’ centers, and the length of the interval $x_t$ becomes $x_t = x_e - x_s$. For a linearly spaced grid the cell size $\Delta x$ is then given by

$$\Delta x = \frac{x_t}{N_x - 1}$$  \hspace{1cm} (1.8)

and, accordingly, the coordinate of a cell center can be calculated via

$$r_{i,j,k} = \begin{pmatrix} x_s + i\Delta x \\ y_s + j\Delta y \\ z_s + k\Delta z \end{pmatrix}.$$  \hspace{1cm} (1.9)

The grid can be thought of as being composed of rectangular cells with the grid points at the center. In **Cronos** the fluid variables ($\rho, v_x, v_y, v_z, e, p$) are computed at the cells’ centers so that the corresponding arrays, in which they are stored,
have the same indices as the array storing the grid points. For the magnetic field a constrained transport scheme (Brackbill and Barnes, 1980) is used to ensure conservation of magnetic divergence to machine precision. To compute the flux going in and out of the cells, the magnetic field components at the corresponding orthogonal surfaces of each cell are needed. These would need semi-integer indices, which is not possible in C++. Therefore, the arrays storing magnetic field components are offset from those storing the cell center coordinates by one half, which has to be kept in mind. For example, when computing the absolute magnetic field strength $|\mathbf{B}|$ at a cell center, averaging the components of $\mathbf{B}$ from the corresponding adjacent cell surfaces is required, as can be seen from the layout of the grid shown in Figure 1.11.

Figure 1.11: Sketch of the grid layout: grid points are cell-centered (integer indices) and store fluid variables (abbreviated as $Q$), while magnetic field components are stored at the corresponding adjacent cell surfaces (semi-integer indices in the corresponding direction, integer indices for the others). The concept of ghost cells is also demonstrated as they can be considered as an extension at the simulation box’ faces with negative indices (or indices beyond $N$ at the outer boundary); $y$ indices were chosen arbitrarily.

Cronos makes use of so-called ghost cells (also depicted in Figure 1.11), which are an extension of the actual grid at its boundaries. They are used to implement boundary conditions that can be defined for all six boundaries (two boundaries for each of the three dimensions). Here, variables are not calculated according to the set of equations and instead are given values according to the applied boundary condition. Pre-implemented options for boundary conditions are Periodic, Extrapolation, Outflow, and Reflecting, which are self-explanatory. Additionally, the user has the opportunity to implement own boundary conditions where necessary. If coordinate singularities are detected, the preset boundary conditions are ignored and a respective scheme is applied automatically (see Appendix A).

At the beginning of a simulation the MHD variables have to be initialized (i.e. they are given values according to the model being simulated). This also covers the ghost
cells, so that the initialization process goes hand in hand with the implementation of boundary conditions, especially if a boundary condition is such that it holds on to the initialized values. Special care must be taken when initializing the magnetic field, which has to be done in a divergence-free manner as otherwise the constraint transport algorithm maintains non-zero divergences. A comfortable way of achieving this is to use the vector potential $A$, which by definition gives

$$\nabla \cdot B = \nabla \cdot (\nabla \times A) = 0.$$  \hspace{1cm} (1.10)

In case a vector potential is unavailable for complicated magnetic fields, other methods must be devised, such as the one developed in this thesis (see Section 2.5.2).

The integration proceeds up to a predefined point in time at which the simulation ends. Setting this point requires some experience and depends on the physical model: if a steady-state is sought from time-independent inner boundary-conditions and outward flow of information, the simulation should end by the time a converged solution has been found. This has to be done manually, but can be estimated by the propagation time of the slowest plasma parcels to the outer boundary. In other cases – investigating time-dependent phenomena – this consideration can be more complex.

It is possible to let the code run in parallel using MPI (Message Parsing Interpreter) on stand-alone computers using multiple cores, but also on several computers linked by a network connection. Output is saved in the HDF5 (Hierarchical Data Format; http://www.hdfgroup.org/HDF5/) format, which can be written to individual files by each core (and have to be reassembled into a single file afterward), but also in a parallel fashion into a single file. Output can be set to be done at fixed intervals in time and should be limited to actual needs (output can amount to several Gigabytes): in simulations converging towards steady-state the initial and final state may suffice, but output is also important for debugging when errors are encountered. It is also possible to create movies of a simulation, which requires a lot of time steps with output.

For analysis and visualization, the files can later be read using plotting tools such as SectorPlot written by J. Kleimann in IDL (interactive data language\footnote{http://www.ittvis.com/language/en-us/productsservices/idl.aspx}). It allows the user to choose quantities to be visualized from different output time steps of a selected project. Besides several other options, the user has to select a (2D) cross section to be plotted since 3D visualizations are difficult to handle and are not implemented here. Alternative tools for visualizing results also in (pseudo-) 3D are Visit\footnote{https://wci.llnl.gov/simulation/computer-codes/visit/} and Paraview\footnote{http://www.paraview.org}.
1.3 Outline of the thesis

This section puts the work described in this thesis in perspective with respect to the previously outlined interplay of the protagonists in the heliosphere. Details are postponed to the subsequent chapters.

The building blocks of the present thesis are four accepted publications (three as first author) in peer-reviewed astrophysical journals, as well as some recent work, which will be published in the near future. For each of these there is a separate chapter, respectively starting with a summarizing introduction, followed by a copy of the actual publication – sometimes appended with additional details – and concluded with follow-up thoughts and developments leading to the subsequent chapters.

Chapter 2 is centered around my initial first-author publication *MHD simulation of the inner-heliospheric magnetic field* (Wiengarten et al., 2013), where I pursue the goal to implement observations-based inner boundary conditions to drive 3D simulations of the inner heliosphere (0.1 to 1 AU) in the CRONOS framework. This required several extensions to the code such as introducing the effects of solar rotation and solving the full energy equation (instead of previously adopted isothermal models (Kleimann et al., 2009; Wiengarten, 2011)). The respective implementations were validated by reproducing the analytic models of Parker (1958) and Weber and Davis (1967).

These latter models have been quite successful in describing general features of the solar wind and the HMF, but are too simple for reproducing more complex conditions (e.g. wavy current sheets, CIRs) as measured by spacecraft. To that end, in a collaboration with colleagues from the Max Planck Institute for Solar System Research (MPS) in Katlenburg-Lindau (now in Göttingen), maps of the radial magnetic field at the heliobase for solar minimum and maximum conditions served as inner boundary conditions for my subsequent MHD simulations. These maps are the result of a coupled solar surface flux transport (SFT) and a coronal potential field model as described in Jiang et al. (2010). The common approach in potential field models is to use magnetogram data as inner boundary conditions, which has the drawback that the data is composed of measurements taken during one solar rotation, so that especially the far side of the Sun is described by somewhat outdated data. SFT models aim to model the photospheric motions and evolution of sunspots to allow for a better treatment of the far side of the Sun. Moreover, by using sunspot group data, which is available for longer times than modern magnetograms, the model can recreate conditions from before the space age. The subsequent utilization of these results as input to MHD simulations therefore provided a novel possibility to model the accompanying solar wind conditions.

As the CRONOS code is usually operated with analytic prescriptions for initial and inner boundary conditions, it was necessary to extend the code by devising routines to read-in and interpolate the input data on arbitrary grids, as well as to find a method for a divergence-free initialization of the magnetic field. Furthermore, inner
boundary conditions for the remaining MHD quantities had to be set, which follow from the coronal magnetic field topology (fast wind from coronal holes, slow wind from their boundaries (Wang and Sheeley, 1990)), where I adopted an empirical model of Detman et al. (2011), based on the WSA model (Arge and Pizzo, 2000; Arge et al., 2003).

MHD simulations were performed for typical solar minimum and maximum conditions, and the results I obtained appeared reasonable at the time as they were roughly compared to spacecraft data and agreed with the general topologies expected for the respective phases in the solar cycle. A subsequent detailed comparison with spacecraft data after publication revealed that the input data used so far were insufficient, so that a different approach for the coronal modeling became necessary and was subsequently taken as described next.

The work described in Chapter 3 was done in the framework of a joint project with the University of Kiel and the North-West University, Campus Potchefstroom, South Africa, on the influence of CIRs on the propagation of energetic particles, where the respective CIR disturbed background solar wind resulting from my MHD simulations is used as input to a respective stochastic differential equation (SDE) model for the transport of energetic particles in the heliosphere. My MHD modeling is described in Cosmic Ray transport in heliospheric magnetic structures. I. Modeling background solar wind using the Cronos magnetohydrodynamic code (Wiengarten et al., 2014), while the subsequent SDE modeling paper is in preparation, but see Kopp et al. (2012) for a detailed description of the idea behind the SDE modeling as well as the respectively developed code.

Once again, a test case for validating the ability of the CRONOS code to correctly compute CIR structures was performed by reproducing the numerical results of Pizzo (1982). After successful validation, a time period in the ascending phase of solar cycle 23 (August 2007) – during which a stable CIR configuration was present – was chosen for a subsequent detailed comparison with spacecraft measurements in the ecliptic at 1 AU (Stereo-A/B; see Kaiser, 2005) and out-of-ecliptic (Ulysses).

The required potential field modeling of the solar corona providing the boundary conditions for my simulations had to be performed in a different fashion as compared to my previous work, because the input data used there were found to be incorrect. The employed WSA model for deriving the resulting solar wind speeds is tuned to the usage of GONG (Global Oscillation Network Group) magnetograms in coupled potential field source surface (PFSS) (Altschuler and Newkirk, 1969) and Schatten current sheet models (Schatten, 1971), so that these were adopted. Instead of using the common spherical harmonics approach to solve the Laplace equation in these models, a finite difference approach was taken and for the first time coupled to the WSA formalism. For the analysis of the resulting coronal field topology a field line tracing algorithm was devised, which is also required to derive the resulting solar wind speeds. The results showed good agreement with spacecraft data allowing to expect insights for energetic particle propagation from the ongoing SDE modeling.
1.3. OUTLINE OF THE THESIS

For the latter, transport coefficients are employed that actually depend not only on the large-scale MHD quantities, but also on the fluctuations of the magnetic field. These cannot be resolved in large-scale MHD simulations, but there are models describing the evolution of integral turbulence quantities such as the total turbulent energy density and the ratio between inward and outward propagating modes. In order to eventually be able to provide these quantities for an improved SDE modeling, a turbulence transport model was implemented alongside the large-scale MHD equations in the CRONOS framework, which is the topic of Chapter 4 based on my publication Implementing turbulence transport in the CRONOS framework and application to the propagation of CMEs (Wiengarten et al., 2015). I started again by validating the implementation by comparing with previous work of Usmanov et al. (2011), during which some discrepancies were found that could be traced back to errors made by these authors (A. Usmanov, priv. comm). A corrected model was used, which was further extended by removing the constraint of being only applicable in regions of highly super-Alfvénic solar wind ($U \gg V_A$), while I had the goal to have a model that can eventually be coupled with my previous WSA driven MHD simulations that start in regions where $U \geq V_A$. This was achieved by simplifying a more general model of turbulence transport by Zank et al. (2012).

The resulting model was then applied for the first time to the propagation of CMEs, and – although there is little observational data – the obtained results for the turbulence levels are in general agreement with estimates provided by Subramanian et al. (2009). Furthermore, it is found that, on the one hand, turbulence does not act back strongly on the large-scale quantities, but, on the other hand, that the CME is a strong driver of turbulence. Therefore, such a model is not required for studies focusing on large-scale CME quantities only, but it does provide another interesting scenario for a related energetic particle propagation study.

Chapter 5 describes the subsequent implementation of the complete model of Zank et al. (2012), which thus far had been solved neither in 3D nor self-consistently coupled with the MHD equations. A simplified implementation in the ecliptic plane only and neglecting some of the involved terms was done by Adhikari et al. (2015), whose results were used for validation purposes. Afterward, the full model is solved, which gives some yet not fully understood results. Consequently, this work is unpublished as of yet, but ongoing.

Another line of work in our team is the modeling of the large-scale heliosphere and astrospheres, i.e. the interaction between the solar/stellar wind and the interstellar medium. An analytic model for the interstellar magnetic field in the vicinity of the heliopause was recently presented by Röken et al. (2015), in which it was also compared to numerical results obtained with the CRONOS code by J. Kleimann. This numerical setup was altered by K. Scherer and myself for the application to the astrosphere of the O-star λ Cephei. Due to the large terminal velocities of its stellar wind, the associated astrosphere is a cavity of several parsecs in diameter and is thus able to modulate high-energy cosmic rays that pass through it, which
could be responsible for tiny-scale anisotropies in all-sky maps of the cosmic ray flux as measured, e.g., by IceCube. This is the topic of Chapter 6 based on the paper *Cosmic rays in astrospheres* (Scherer et al., 2015).
Chapter 2

MHD simulation of the inner-heliospheric magnetic field

2.1 Overview

On a large scale the unperturbed HMF inside the termination shock is remark-
ably well described by the Archimedean spiral pattern frozen-into the solar wind
as proposed first by Parker (1958). Close to the Sun, where the magnetic field is
energetically dominant as compared to the kinetic energy density of the solar wind,
the latter follows the magnetic field anchored on the rotating Sun, leading to a
transfer of angular momentum to the solar wind, which has slowed the Sun’s solar
rotation over its lifetime (Weber and Davis, 1967). The photospheric motion of
these anchored footpoints motivated yet another analytic prescription of the result-
ning HMF (Fisk, 1996), which in this model also has a latitudinal component (see
Figure 2.1). Several adaptions have been proposed by, e.g., Jokipii and Kota (1989);
Smith and Bieber (1991); Schwadron (2002); Burger and Hitge (2004); Burger et al.
(2008); Schwadron et al. (2008) that have been compared by Wiengarten (2009) and
Scherer et al. (2010).

These analytic models can account for the large-scale behavior of the HMF par-
ticularly during solar quiet times. However, for a more quantitative and realistic
modeling MHD simulations have to be performed. It is customary to distinguish
the sub-Alfvénic corona from the super-Alfvénic part beyond the so-called heliobase
(Zhao and Hoeksema, 2010) at about $20R_\odot$, with two common approaches to com-
pute the coronal magnetic field:
on the one hand, modern computers have made it possible to use fully 3D MHD
codes to model the corona, thereby directly taking into account the effect of the evolv-
ing solar wind (e.g., Usmanov and Goldstein, 2003; Cohen et al., 2007; Feng
et al., 2010; Riley et al., 2011; van der Holst et al., 2014, and many more). These
models account for more realistic physics, but require enormous amounts of com-
puting power and are of considerable complexity as they have to address the coronal
heating problem and respective acceleration of the solar wind, as well as the tran-
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Figure 2.1: Field lines in the Parker (left) and Fisk model (right). (Taken from Sternal et al., 2007).

Position from sub- to super-Alfvénic conditions, which leads to a severe complication of boundary conditions as information can travel back towards the inner boundary (Nakagawa, 1981).

On the other hand, potential field models for the coronal magnetic field (Altschuler and Newkirk, 1969; Schatten et al., 1969) have been used for decades already, as they are computationally cheap and were shown to yield remarkably similar results to respective MHD models (Riley et al., 2006). Such potential field models assume the corona to be current-free ($\nabla \times \mathbf{B} = \mathbf{J} = 0$)\(^1\) that together with $\nabla \cdot \mathbf{B} = 0$ allows to compute the coronal magnetic field by solving the Laplace equation for a scalar potential $\Delta \Psi = 0$. While the imposed inner boundary condition is a magnetogram, the outer boundary condition is to force the field to become radial at the so-called source surface (typically at $2.5R_\odot$), which is to mimic the effect of the solar wind eventually dragging the magnetic field. An example for a PFSS solution within the source surface radius as presented in Altschuler and Newkirk (1969) is shown in Figure 2.2 for solar minimum conditions in 1966. More elaborate potential field models have also been proposed, e.g. to realize thin and sharp current sheets (Schatten, 1971) or for a better treatment of the opening of field lines by introducing an intermediate cusp surface (Bogdan and Low, 1986). Another more elaborate approach can also be taken via force-free models assuming $\mathbf{B} \parallel \mathbf{J}$ (see, e.g., the review by Wiegelmann et al., 2014).

The resulting solar wind speeds that are not inherently taken into account in potential field models can, however, be deduced from the coronal magnetic field topology: as found by Wang and Sheeley (1990), there is an inverse relationship between the

\(^1\)again in normalized notation
2.1. OVERVIEW

Figure 2.2: Example of a PFSS solution for the coronal magnetic field within the source surface at $2.5R_\odot$ (taken from Altschuler and Newkirk, 1969).

topology-characterizing flux tube expansion factor and the respective solar wind speed at the heliobase – which basically quantifies the association of fast wind with coronal holes and slow wind with coronal hole boundaries. This finding motivated the WSA model (Arge and Pizzo, 2000; Arge et al., 2003) as a space weather forecasting tool, estimating the solar wind speed at Earth either by means of simple kinematic propagation (e.g., the HAF model Akasofu et al., 1983) or by MHD simulations (e.g. Odstrčil et al., 2004). Respective frameworks have transitioned to operation at the space weather prediction center (SWPC) and the coordinated community modeling center (CCMC).

In my following initial first-author publication *MHD simulation of the inner-heliospheric magnetic field* (Wiengarten et al., 2013, in the following abbreviated as W13) I extended the work done in my Master’s thesis (Wiengarten, 2011). A first step was the numerical reproduction of known analytic formulations for the HMF by Parker and Weber & Davis, for which the Cronos code had to be extended to account for solar rotation effects (Section 2 in W13), which was realized in two frames of reference: co-rotating with the Sun, and an inertial observer frame. The Weber &
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Davis test case is illustrated in Section 3 of W13, and a more thorough description of its analytic formulation in its original form and the previously unpublished form in the co-rotating frame of reference are discussed in more detail in an addendum found in Section 2.5.1.

For a more realistic modeling of the solar wind as compared to these analytic models, the computationally easier way of a potential field description of the coronal magnetic field was pursued, the results of which serve as input to my MHD simulations of the inner heliosphere. The potential field modeling was performed by our collaborators from the MPS, and the respective work is described in Jiang et al. (2010) and Section 4.1 of W13. The common approach in potential field models is to use magnetograms of the observed photospheric magnetic field as inner boundary conditions. This has the disadvantage that the solar disk cannot be completely observed from Earth at any given time. Instead, data is accumulated during one solar rotation, so that changes especially at the far side of the Sun during a rotation remain neglected. This can be circumvented by surface flux transport (SFT) models, which take into account the photospheric motions and evolution of magnetic flux. In Jiang et al. (2010) such a model was fed with sunspot group data, which are also available for longer times in the past in contrast to magnetograms, which allows for estimates of the heliospheric open magnetic flux before the space age. The resulting modeled "magnetogram" was then used in a potential field approach (current sheet source surface (CSSS) model) yielding the radial magnetic field at a source surface at 10 solar radii. Respective maps were provided for typical solar minimum and maximum conditions for utilization as inner boundary conditions in my MHD simulations.

The code also requires boundary conditions for the remaining plasma quantities, for which I used a set of empirical formulas as in Detman et al. (2006, 2011) based on the WSA approach. The radial velocity formula relies on the finding of Wang and Sheeley (1990) that it is inversely proportional to the flux-tube expansion factor (EF), which relates field strengths at the source surface with the one at the photosphere as connected by a field line. A large expansion is found for flux tubes originating at coronal hole boundaries (resulting in slow solar wind speed), while small expansion is found within coronal holes. Therefore, another quantity that can be used to set the resulting solar wind speed is the so-called footpoint distance (FPD) to the nearest coronal hole boundary. Both EF and FPD were found to give better results if used in conjunction than used alone (Arge et al., 2003). The required quantities needed to compute them, which are the footpoint locations of open field lines in the photosphere and their mapping via these field lines to the source surface, were also provided along with the radial magnetic field. I developed an algorithm to identify the position of the coronal hole boundaries and to compute the DFP, so that all the inner boundary conditions could be set. Another complication, however, arises from the necessity to initialize the magnetic field in the whole computational domain in a divergence-free manner. This cannot be done with
analytic prescriptions for this arbitrary read-in magnetic field, but instead another algorithm was constructed to achieve this (for details see Section 2.5.2).

The obtained results at Earth’s orbit for the solar minimum case were crudely compared to spacecraft data from that time, proving the existence of a modeled high-speed feature in the ecliptic at that time. Meanwhile, the typical structure of high-speed polar flows and low speeds in the ecliptic was also recreated. Therefore, my results were considered to be suitable for further usage in outer heliospheric models that put the inner boundary at a few AU and investigate the interaction with the ISM. A more detailed analysis of the results and comparison with spacecraft data for several more sets of input data from our collaborators at the MPS revealed later on that these data used in this study were inaccurate (see Section 2.3). This forced me to model the input data (i.e. the coronal magnetic field) by myself, which was the starting point for the work described in Chapter 3.
2.2 Wiengarten et al. (2013)

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MHD simulation of the inner-heliospheric magnetic field

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[1] Maps of the radial magnetic field at a heliocentric distance of 10 solar radii are used as boundary conditions in the MHD code CRONOS to simulate a three-dimensional inner-heliospheric solar wind emanating from the rotating Sun out to 1 AU. The input data for the magnetic field are the result of solar surface flux transport modeling using observational data of sunspot groups coupled with a current-sheet source surface model. Among several advancements, this allows for higher angular resolution than that of comparable observational data from synoptic magnetograms. The required initial conditions for the other MHD quantities are obtained following an empirical approach using an inverse relation between flux tube expansion and radial solar wind speed. The computations are performed for representative solar minimum and maximum conditions, and the corresponding state of the solar wind up to the Earth’s orbit is obtained. After a successful comparison of the latter with observational data, they can be used to drive outer-heliospheric models.


1. Introduction

[2] Since Parker’s explanation of the expansion of the solar atmosphere as the solar wind [Parker, 1958], its basic, long-term average features have been validated by direct in situ as well as indirect remote measurements. At a radial distance of a few solar radii, i.e., at the so-called source surface, the heliospheric magnetic field (HMF) is essentially directed radially and “frozen in” into the radially expanding solar wind plasma. Because the magnetic field remains, due to an anchoring of the field line footpoints in the solar atmosphere, influenced by the solar rotation, the field lines form three-dimensional Archimedean or so-called Parker spirals [Parker, 1958] if, in a first approximation, the Sun is considered as a rigid rotator.

[3] For shorter periods, a more complex magnetic field structure was suggested by Fisk [1996], who took into account both the motion of magnetic footpoints on the solar surface and the existence of a nonvanishing latitudinal field component. He was able to derive analytical expressions that generalize the Parker field correspondingly. Subsequent analytical investigations [Zurbuchen et al., 1997; Kobyliński, 2001; Schwadron, 2002; Schwadron et al., 2008] have quantified the complex structure of this so-called Fisk-field and its deviations from the Parker field, and numerical simulations [Lionello et al., 2006] have revealed that the original choice of parameters by Fisk [1996] represented an extreme, which has recently been confirmed via a study of the consequences of the Fisk-field for cosmic ray modulation [Sternal et al., 2011].

[4] Several authors have suggested modifications of both fields [Jokipii and Kota, 1989; Smith and Bieber, 1991; Schwadron, 2002; Burger and Hütte, 2004; Burger et al., 2008; Schwadron et al., 2008], which have been quantitatively compared in a study by Scherer et al. [2010]. Although very useful for many purposes, these analytical representations of the HMF cannot be used to reproduce actual measurements in sufficient detail at any given time in the solar activity cycle.

[5] For solar activity minima they are often too crude to catch small-scale HMF structures and for the HMF during maximum solar activity none of these analytical representations is valid. The field expressions suggested by Zurbuchen et al. [2004] for use during solar maximum are a simple modification of a representation for solar minimum [Zurbuchen et al., 1997] obtained by assuming a rather unlikely so-called Fisk angle [see Sternal et al., 2011].

[6] While, physically, the HMF originates in the Sun, it is conceptually customary to distinguish for modeling purposes between the coronal magnetic field—filling the region from the solar surface out to a spherical “heliobase” [Zhao and Hoeksema, 2010] at several (tens of) solar radii—and the HMF beyond. This concept is used in many modeling attempts, which can be divided in two groups, potential field reconstructions and MHD models [see Riley et al., 2006]. The latter approach is computationally more expensive but can account for more physics, direct time dependence and self-consistency. Examples for such
MHD modeling of the coronal magnetic field are Usmanov and Goldstein [2003], who computed a (tilted) axisymmetric solution for solar minimum conditions with the assumption of a constant polytropic index, Cohen et al. [2007], who extended this to a varying polytropic index and solar maximum conditions, or Lionello et al. [2009] and Riley et al. [2011], who employed phenomenological heating functions that are unrelated to the magnetic field direction. In more recent MHD models Nakamizo et al. [2009] and Feng et al. [2012] improved heating and momentum source functions have been used and the two-region setup has been dropped by exploiting advanced numerical grids providing high resolution close to the Sun as well as avoiding both coordinate-related singularities and extreme cell size differences. For the construction of the heating functions these models are, however, implicitly using results from potential field reconstructions as, e.g., described in Feng et al. [2010]. Although in general MHD treatments should be preferred, all models published so far still have severe limitations like those indicated for the mentioned examples.

Not only computationally advantageous, but also with respect to their ability to resolve structures beyond those that can be handled by current MHD models [Riley et al., 2006], are potential field models. These pure potential field source surface (PFSS) models, initially developed by Altschuler and Newkirk [1969] and Schatten et al. [1969], were significantly refined by recognizing that the observed photospheric field should first be corrected for line-of-sight projection and then matched to the radial component of the potential field [Wang and Sheeley, 1992], by explicitly taking into account additional sheet currents [Zhao and Hoeksema, 1995] resulting in the so-called current sheet source surface (CSSS) model, and by connecting such approaches to the solar wind expansion [Arge and Pizzo, 2000], which resulted in the so-called Wang-Sheeley-Arge model, which is also used for the two-region setup [Pizzo et al., 2011].

In the new model presented in this paper, we follow a similar approach, i.e., we consider a two-region model distinguishing between a coronal magnetic field region and that of the HMF, which are separated by the heliobase as described above. In difference and improvement of earlier approaches, however, the input data for the magnetic field are the result of solar surface flux transport (SFT) modeling [Jiang et al., 2010] using observational data of sunspot groups coupled with the CSSS model by Zhao and Hoeksema [1995]. This approach allows for higher resolution than that of comparable observational data from synoptic magnetograms. The heliobase conditions for the other MHD quantities are obtained following the empirical approach by Detman et al. [2006, 2011], who employed the Wang-Sheeley-Arge approach.

Besides the need for high-resolution models of the three-dimensional magnetized solar wind for studies of coronal mass ejections (CMEs) [see, e.g., the recent review by Kleimann [2012]], magnetic clouds [see, e.g., Dalalikshvili et al., 2011, and references therein], or corotating interaction regions [see, e.g., Gosling and Pizzo, 1999], there is the need for improved boundary conditions at 1 AU for large-scale heliospheric models [see, e.g., Pogorelov et al., 2009]. Our new model is of particular interest in the context of long-term modeling of the heliosphere, because with the employed method based on sunspot data the heliobase conditions can be reconstructed backward in time for more than three centuries [Jiang et al., 2011a, 2011b].

### 2. The Model

In its basic setup, CRONOS solves the equations of ideal MHD in a one-fluid model, this being a justifiable approach for the solar wind plasma [e.g., van der Holst et al., 2005]. In its normalized form (see Table 1) the set of equations to be solved reads

\[
\begin{align*}
\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) &= 0 \quad (1) \\
\partial_t (\rho \mathbf{v}) + \nabla \cdot \left( \rho \mathbf{v} \mathbf{v} + \left( p + |\mathbf{B}|^2 / 2 \right) \mathbf{I} - \mathbf{B} \mathbf{B} \right) &= \mathbf{f} \quad (2) \\
\partial_t e + \nabla \cdot \left( e + p + |\mathbf{B}|^2 / 2 \right) \mathbf{v} - (\mathbf{v} \cdot \mathbf{B}) \mathbf{B} &= \mathbf{v} \cdot \mathbf{f} \quad (3) \\
\partial_t \mathbf{B} + \nabla \times \mathbf{E} &= 0, \quad (4)
\end{align*}
\]

where \( \rho \) is the mass density, \( \mathbf{v} \) is the velocity of a fluid element, \( \mathbf{B} \) and \( \mathbf{E} \) describe the electromagnetic field, \( e \) is the total energy density, and \( p \) is the scalar thermal pressure. \( \mathbf{f} \) is the sum of the gravitational force density \( \mathbf{f}_g = -\rho GM_\odot r^2 \hat{r} \), and additional force terms that may enter. Furthermore, \( I \) denotes the unit tensor, and the dyadic product is used. So far the system is underdetermined, and to complete the set of equations we use the closure relations

\[
\begin{align*}
e &= \rho [\mathbf{v} \cdot \mathbf{v}]^2 / 2 + \left( |\mathbf{B}|^2 / 2 \right) + \frac{p}{\gamma - 1} \quad (5) \\
\mathbf{E} + \mathbf{v} \times \mathbf{B} &= 0 \quad (6) \\
\nabla \mathbf{B} &= 0, \quad (7)
\end{align*}
\]

where \( \gamma \) is the adiabatic exponent.

While in the isothermal case (\( \gamma = 1 \)) the last term in (5) is dropped and equation (3) becomes redundant and needs not enter the calculations, a temporally varying temperature requires using the full set of equations with \( \gamma \neq 1 \). We follow Pomoell et al. [2011] in setting \( \gamma = 1.05 \) to accelerate the solar wind. To model shock structures correctly, it would be necessary to work with adiabatic exponents as actually present in the solar wind, which are higher. To accomplish this, further following the approach

### Table 1. Summary of Normalized Quantities and Normalization Constants

<table>
<thead>
<tr>
<th>Physical Quantity</th>
<th>Normalization Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length ( L )</td>
<td>( L_0 )</td>
</tr>
<tr>
<td>Number density ( n )</td>
<td>( n_0 )</td>
</tr>
<tr>
<td>Magn. induction ( B )</td>
<td>( B_0 )</td>
</tr>
<tr>
<td>Mass density ( \rho )</td>
<td>( \rho_0 = n_0 \rho_0 )</td>
</tr>
<tr>
<td>Mass ( m )</td>
<td>( m_0 = m_0 n_0^2 )</td>
</tr>
<tr>
<td>Velocity ( v )</td>
<td>( v_0 = \frac{v}{L_0} )</td>
</tr>
<tr>
<td>Acceleration ( g )</td>
<td>( g_0 = \frac{g}{L_0} )</td>
</tr>
<tr>
<td>Time ( t )</td>
<td>( t_0 = L_0 v_0 )</td>
</tr>
<tr>
<td>Energy density ( e )</td>
<td>( e_0 = m_0 v_0^2 )</td>
</tr>
<tr>
<td>Current density ( J )</td>
<td>( J_0 = \sqrt{2 \rho_0} )</td>
</tr>
<tr>
<td>Gas pressure ( p )</td>
<td>( p_0 = \frac{p}{\rho_0} )</td>
</tr>
<tr>
<td>Temperature ( cs )</td>
<td>( T_0 = \frac{T}{\rho_0} )</td>
</tr>
</tbody>
</table>
of Pomoell et al. [2011], we would take the so far obtained solution as solar wind background input for a new simulation with introduced shocks. However, the model presented here does not involve shock structures. Nevertheless, extending our model in this direction can be a subject for future work. We use spherical coordinates \((r, \theta, \phi)\) with the origin at the center of the Sun. Thus, \(r\) is the heliocentric radial distance, \(\theta \in [0, \pi]\) is the polar angle (with the north pole corresponding to \(\theta = 0\)) and \(\phi \in [0, 2\pi]\) is the azimuthal angle. The reference point for \(\phi\) as follows: For the test cases (see section 3) azimuthal symmetry is used so that results are the same for all \(\phi\), and it is not necessary to define a reference point. The observationally based data in section 4 are given in Carrington longitudes and the position of the Earth serves as a reference point. It depends on the time at which the data were taken. This will be described in section 4.1 after explaining how the data were obtained.

[12] Neglecting differential rotation, solar rotation can be described via an angular frequency

\[ \Omega = 14.71^\circ / d \]  

(8)

according to Snodgrass and Ulrich [1990], which corresponds to the sidereal rotation period of 24.47 days. Accordingly, the Sun’s rotation axis’ tilt of about 7.25° relative to the axis of the Earth’s orbit is also not taken into account.

[13] Implementing solar rotation into the model can be done in both the solar wind plasma rest-frame and the frame corotating with the Sun. The first choice introduces azimuthal components of \(B\) and \(v\) by applying respective boundary conditions while solving the original set of equations (1)–(7). The latter choice cannot be implemented by boundary conditions only, but requires the introduction of fictitious force terms that occur in rotating (and thus noninertial) frames of reference, namely the Coriolis force, the centrifugal force, and the Euler force

\[ f_{cor} = -2 \Omega \times \mathbf{v} - \rho \mathbf{v} \times (\mathbf{\Omega} \times \mathbf{r}) - \rho \frac{\partial \mathbf{\Omega}}{\partial t} \times \mathbf{r} \]  

(9)

[14] In the chosen spherical coordinate system the angular velocity is directed along the \(z\) axis of the corresponding Cartesian coordinate system, coinciding with the axis of rotation of the Sun: \(\mathbf{\Omega} = \Omega \mathbf{e}_z\). Solar rotation is assumed constant in time (\(\Omega \neq \Omega(t)\)) so that the Euler force term vanishes. With the Cartesian unit vector transformed to the spherical system, this finally gives

\[ f_{cor} = \rho \left[ (2 \Omega \sin \theta \dot{\phi} + r \Omega^2 \sin^2 \theta) \mathbf{e}_r ight. \\
+ (2 \Omega \cos \theta \dot{\phi} + r \Omega^2 \sin \theta \cos \phi) \mathbf{e}_\phi \\
\left. - (2 \Omega \cos \theta \dot{\phi} + \sin \theta \dot{\phi}) \right] \mathbf{e}_z \]  

(10)

3. Model Validation: Weber and Davis Model

3.1. Analytical Formulation

[15] Mandatory tests have been performed to check the correct implementation of our model. First, Parker’s solar wind model was reconstructed, using a respective isothermal model. It could be shown that implementations in both frames of reference produced correct results of the typical radial velocity profile, and magnetic field lines bent to spirals resulting from solar rotation were obtained. A more thorough comparison with analytical results, however, can be made with the more complex Weber and Davis model [Weber and Davis, 1967, hereafter WD]; Parker’s assumption of frozen-in field lines is not valid close to the Sun because there the kinetic energy density is smaller than the magnetic energy density. Consequently, it can be assumed that the plasma flow follows the magnetic field lines instead well inside the Alfvénic radius \(r_A\). This corotation should weaken when approaching \(r_A\), and for the limiting case \(r \gg r_A\) Parker’s model \((v_r \propto r^{-1})\) should be a good approximation. Assuming an azimuthal component of the flow velocity and solving a steady state model with axial symmetry in the equatorial plane, the final equations of WD for the azimuthal components of velocity and magnetic induction in the solar wind plasma frame of reference read

\[ v_r(r) = \frac{\Omega_W D}{1 - v_r/(r_A)} \]  

(11)

\[ B_r(r) = -\frac{B_r}{\Omega_W D^2} \frac{1 - (r/r_A)^2}{v_r/(r_A)} \]  

(12)

where \(v(r_A)\) and \(M_A\) denote the radial velocity at the Alfvénic critical point and the radial Alfvén Mach number, respectively. Furthermore, \(B_r = B_0 r^2\) as follows from the solenoidality condition. It is important to note that here, \(\Omega_W D\) is, according to WD, the “angular velocity of the roots of the lines of force in the Sun”, whose value is not easily accessible. It can be shown [Barker and Marlborough, 1982; MacGregor and Pizzo, 1983] that \(\Omega_W D\) is related to the observed angular velocity of the photosphere \(\Omega\) (as in equation (8)) via

\[ \Omega_W D = (1 + f) \Omega \]  

(13)

with

\[ f = \frac{v_{\theta,0}}{v_{\phi,0}} \]  

(14)

where the quantities with zero-subscript indicate the respective values at the solar photosphere that are easily accessible in a simulation starting at \(r = R_\odot\).

[16] This derivation can be adopted for the corotating frame of reference as well, taking the initial value for the azimuthal velocity \(v_{\phi,0}(r_\odot) = 0\), and extending the equation of motion by the fictitious force terms (in the ecliptic plane). The final result is

\[ v_{\phi}(r) = \frac{1}{M_r^2 - 1} \left[ v_{\phi}(r_\odot) - \left( \frac{B_r}{B_0} \right) \left( 1 - M_r^2 \frac{B_r(r)}{B_r(r_\odot)} \right) \right. \\
\left. - M_r^2 \Omega_D \left( 1 - \frac{r_A^2}{r^2} \right) \right] \]  

(15)

and

\[ B_r(r) = \frac{(R_\odot/r) v_{\phi}(r_\odot) + v_r(r) B_0}{v_r(r)} \]  

(16)

3.2. Numerical Simulations

[17] The analytic results shown above can be compared to the numerical results obtained from respective simulations in
the corotating and the rest frame. In both cases the simulation box is restricted to extend from the Sun to ten solar radii and the number of grid points in radial direction is chosen to be \(N_r = 400\), yielding a cell size of \(\Delta r = 9R_\odot / 400 \approx 0.02R_\odot\). Because the WD solution is valid for the ecliptic plane only, \(\vartheta\) is restricted to the interval \([0.4\pi, 0.6\pi]\) and a resolution of \(N_\vartheta = 41\), using an odd number, gives a cell centered at \(\vartheta = \pi/2\) and a cell size of \(\Delta \vartheta \approx 0.005\pi\). The complete \(\varphi\) interval can be covered with a single layer of cells due to the symmetry.

For the implementation of boundary conditions, CRONOS makes use of so-called ghost cells that are extensions of the actual grid at its boundaries. \(\vartheta\) boundaries are set to “reflecting”, which basically ensures conservation of both mass and magnetic flux, but influences the adjacent cells. This is compensated by a modest resolution so that there is no effect on the equatorial cells. Periodic boundary conditions are used for \(\varphi\). The outer radial boundary condition is set to “outflow” and is self-explanatory. The inner radial boundary condition depends on the respective quantity and either fixes it at \(r = R_\odot\) or extrapolates inward into the boundaries ghost cells; for the initial number density, \(n(r) = n_0(R_\odot / r)^2\) is fixed. Radial velocity is initially set to \(v_\varphi(r) = C \cdot r\) with an arbitrary constant \(C = 0.2\) so that the steady state equation of continuity is fulfilled. For this flux conserving inward extrapolation is applied. The radial magnetic field is initialized as \(B_\varphi(r) = B_0(r) / r^2\). This is in accordance with the solenoidality condition because latitudinal components are set to zero (\(B_\vartheta = 0, v_\vartheta = 0\)) and the azimuthal initialization (see below) yields \(B_\varphi \neq B_0(\varphi)\).

The azimuthal components of \(B\) and \(v\) depend on the frame of reference. For the rest frame, \(v_\varphi(r) = \Omega r\), while in the corotating frame, \(v_\varphi,\text{cor}(r) = 0\) initially, both being fixed at the inner boundary. The azimuthal magnetic field component is actually not initialized (i.e., set to zero), but the computed values at the innermost cells during runtime is extrapolated into the inner boundaries ghost cells according to

\[
B_\varphi(r \leq R_\odot) = \left[B_\varphi(R_\odot + \Delta r) / B_\varphi(R_\odot + \Delta r)\right] B_\varphi(r) .
\]

This can be done for both reference frames because the magnetic field is invariant under the respective transformation.

### 3.3. Comparison

Figure 1 shows the results for the azimuthal components for the rest frame and the corotating frame: In the rest frame (Figure 1a) \(v_\varphi\) exhibits the expected behavior as for \(R_\odot < r < 1.5R_\odot\) a decreasing corotation is found. In the region near the Alfvénic critical radius at \(r \approx 2.2R_\odot\) the influence of the magnetic field is still evident: there is not yet an \(1/r\) behavior as it develops for even larger \(r\) in Parker’s model. The WD solution (dashed line) matches the code’s solution except near the Alfvénic point, which numerically cannot be exactly resolved due to a singularity that, analytically, is a removable one. For the corotating frame of reference (Figure 1b) the code also reproduces the analytic solution. The corotating behavior of the plasma near the solar surface is only slightly recognizable because the \(y\)-axis scale is 10 times coarser.

The azimuthal magnetic field (Figure 1c) is also very similar to that of the WD solution, and for \(r > 4R_\odot\) they overlap. The discrepancy for smaller \(r\) can be explained by the inner boundary condition that extrapolates the ratio between azimuthal and radial magnetic field component into the boundary. This gives higher absolute values in the boundary because \(B_\varphi\) has an \(1/r^2\) behavior while for \(B_\varphi\) it is an \(1/r\) behavior. These higher absolute values are taken into the simulation box but their influence vanishes as \(r\) increases. Consequently, a refinement of the boundary condition is not essential to get correct results for larger \(r\).

### 4. Observationally Based Inner Boundary Condition

After successfully reproducing analytic results, we now use observationally based input data, i.e., magnetic field distributions at 10 solar radii, which are the result of a solar surface flux transport model coupled with an extrapolation of the heliospheric field that uses observational data of sunspot groups [Jiang et al., 2010]. Although this is the key input to our code, it is however necessary to provide the code with initial conditions for all MHD variables. For this purpose the approach by Detman et al. [2006, 2011] is followed, which uses the empirical inverse relation between flux tube expansion factor and solar wind speed to determine the latter.

### 4.1. Radial Magnetic Field

As input data for our modeling, maps of the radial magnetic field at 10 solar radii will be used. Their complete derivation is described in Jiang et al. [2010] and Schüssler and Baumann [2006], but because it is the key input to the model presented here, in the following it is summarized how the input data was generated. The idea is to use sunspot group records as input to a solar SFT model yielding the magnetic flux at the solar surface, which is then extrapolated to 10 solar radii by means of the so-called CSSS model. The United States Air Force (USAF)/NOAA sunspot group records date back to 1976 and provide the basis of magnetic flux input, because sunspots are associated with emerging bipolar magnetic regions (BMRs). This allows for a model of the whole photosphere, whereas in observations, the back of the Sun cannot be seen. Along with flux cancellation and transport by surface flows the SFT model describes the formation of the magnetic flux distribution at the solar surface, which then is subject to latitudinal differential rotation, meridional flow, and turbulent diffusion due to granulation and supergranulation, so that all the relevant physical processes are implemented. Additionally, computation parameters for the magnetic flux are calibrated to match observed values.

In a next step the HMF has to be determined. The most widely used approach to achieve this is the PFSS model [Schatten et al., 1969; Alschuler and Newkirk, 1969], which solves Laplace’s equation between the photosphere and the so-called source surface at \(r = R_\odot\), at which the field is forced to be radial. Ulysses data, however, motivated an extension of the PFSS model to explicitly take into account the heliospheric current sheet (HCS), yielding the CSSS model [Zhao and Hoeksema, 1995; Zhao et al., 2002]. As well as adding horizontal volume currents, the CSSS
Figure 1. (a) The azimuthal velocity (rest frame) exhibits corotation up to the Alfvénic critical point and afterward decreases as $1/r$. It matches the analytic reference solution except at the Alfvénic critical point that, analytically, is a removable singularity, which cannot be resolved here. (b) Azimuthal velocity (corotating frame) where corotation cannot be seen as clearly as for the rest frame because the scale is 10 times coarser. (c) The azimuthal magnetic field matches the analytic solution only for $r > 4R_\odot$ because of the inner radial boundary condition (see text).
model includes the effect of sheet currents by introducing another spherical surface, the so-called cusp surface at $r = R_{ss} = 1.55 R_\odot < R_\odot = 10 R_\odot$, within which the field contains only horizontal volume currents with a characteristic length scale of $0.2 R_\odot$. This corresponds to $a = 0.2$ in the model of Bogdan and Low [1986]. Between the cusp surface and the source surface the field is configured by current sheets so that all field lines passing through the cusp surface reach the source surface. The field lines are assumed to be radial at the source surface. In our case the source surface is located at $R_{ss} = 10 R_\odot$ and the results of the coupled SFT/CSSS model will be used as input to the model described here. [27] The question as to why the photospheric magnetic field distributions are not used to run our MHD model, therefore starting at the Sun, can be answered as follows: First, an MHD code requires high spatial resolution near the Sun, so that even on massively parallel architectures it is time consuming. Additionally, such efforts are known to encounter difficult boundary condition related problems, because the inner radial boundary lies within the Alfvénic critical radius [Nakagawa, 1981a, 1981b]. Second, second surface models are easy to implement and require modest computer resources. The MHD approach as well as the source surface models are both simplifications of reality. Even if MHD models incorporate more physics, they cannot claim to cover everything. Furthermore, comparisons between the MHD and PFSS models have been performed by Riley et al. [2006] and their “results endorse the PFSS approach, under the right conditions and with appropriate caveats […].” Given that they clearly acknowledge the significance of the various refinements of the PFSS model (e.g., current sheets, non-spherical source surface), one should consider their finding as support not only for the usefulness of PFSS models but rather of static extrapolation models in general. Here, the input data have been derived using the augmented CSSS model, as well as a sophisticated SFT model so that it can be assumed that for the general survey presented here the magnetic field distributions at ten solar radii are a very good input. [28] One of the main advantages of the CSSS model is that, as discussed in Schüssler and Baumann [2006], it yields an unsigned field strength at and beyond the source surface, which is only very weakly latitude-dependent. The PFSS model, by contrast has a strong latitudinal variability, which is in conflict with the Ulysses spacecraft observations. This difference in the latitudinal distribution directly affects the expansion of field lines from the photosphere to the source surface, which is important in our modeling of the plasma properties of the inner heliosphere. Hence, for our purposes the CSSS model is preferred to that of the PFSS model. [29] In comparison with synoptic magnetograms often used as input data to models such as ours, our input data has some advantages because it allows for higher angular resolution and the whole photosphere can be modeled whereas in observations only part of the Sun is visible. [30] Even though a whole time series as output of these models exists, we will not make use of all of them in this case study, but reserve it for future work. Instead, the focus lies on two maps at different times in the solar cycle, i.e., one at solar minimum (1987.2) and one at solar maximum (2000.5). The respective radial magnetic field maps are shown in Figure 2. All figures are the same (apart from color scaling) as in Figures 4a–4b and 4e–4f of Jiang et al. [2010]. At solar minimum (left panel) the Sun is relatively quiet, and, accordingly, the solar surface (top row) displays few to no sunspots and thus BMRs, while the overall structure is dipole-like. At the source surface (bottom row) the HCS is rather flat and the magnetic field reflects the dipole-like structure of the coronal magnetic field becoming radial at $R_{ss}$. However, the overall magnetic field strength is rather homogeneous. The latter is also true at solar maximum, but the HCS shows strong excursions to high latitudes, and even additional current sheets may occur. This is due to the large number of BMRs at the solar surface that are more prominent than the dipole structure. [31] The maps cover the full longitudinal and latitudinal intervals except for the poles (i.e., $\vartheta \in [1^\circ, 179^\circ]$) and have a resolution of $1^\circ \times 1^\circ$. The latitudinal coordinate was described in section 2. For the longitudinal coordinate Carrington longitudes are used that, together with a given time at which the data (which is a snapshot) was taken, define a reference system. It is however instructive to demonstrate how the position of the Earth can be found from the given time of the snapshot: The Carrington rotation system of reference is based on the synodic solar rotation rate as viewed from the Earth, giving the time required for one rotation $T_{\text{Carr}} = 27.2753$ days. At the beginning of a Carrington rotation the position of the Earth is at $360^\circ$ with values decreasing to $0^\circ$ toward the next rotation. The dates at which a new rotation commences can be found in respective tables (e.g., http://alpo-astronomy.org/solar/rotn_nos.html). Taking the example of the data set from $t_{\text{map}} = 1987.2$, the respective Carrington rotation number is 1786 commencing at $T_{\text{Carr}} = 1987.15727$. The difference in time can be used to calculate the longitude of the Earth according to

$$\varphi_{\text{Earth}} = 360^\circ - 360^\circ \frac{t_{\text{map}} - t_{\text{Carr}}}{T_{\text{Carr}}}$$

which puts the position of the Earth at respective values $\varphi_{1987.2} = 154^\circ$ and $\varphi_{2000.5} = 114^\circ$ (with Carrington rotation 1964 commencing at 2000.44899).

4.2. Remaining MHD Quantities

[32] The simulation requires initial values for the full set of the MHD variables, while so far only the radial magnetic field component is known from the previously described data set. One possible approach to derive the remaining quantities from the radial magnetic field data at the inner radial grid boundary is described in Detman et al. [2006, 2011] and shall be briefly summarized: As input data a sequence of photospheric magnetic maps composed of daily magnetograms is used. A source surface current sheet model is used to extrapolate the HMF, which is then fed into an MHD code with an inner radial grid boundary at $R_{gb} = 0.1 AU = 21.5 R_\odot$. It is not possible to start the MHD simulations at the source surface most of the time. Instead, the Alfvénic critical point must be located outside the grid, which ensures that the plasma flow speed is higher than any characteristic plasma speed (specifically the fast mode wave speed), so that there cannot be any flow of information back into the boundary. The lower radial grid boundary is thus set to 0.1 AU, where this condition is met. It is then required to develop an interface to translate the input
data from the source surface model to the lower radial grid boundary, which gives maps of all the necessary MHD variables there. This can only be achieved by empirical formulas, because it has to mimic the main plasma physics in the corona, which is not incorporated in source surface models. The resulting set of equations contains a number of adjustable parameters that can be tuned to give best fits to observational data at Earth. This is an ongoing process and will go hand in hand with advancements in other areas to further augment these kinds of models. The following set of equations is taken from Detman et al. [2006], but has been adapted. An augmented formula for the radial velocity is taken from Detman et al. [2011], which additionally uses the footpoint distance \( d_{FP} \) to the nearest coronal hole boundary because using both footpoint distance and expansion factor \( f_s \) gives better results than either one alone [Arge et al., 2003], which was found to be true for the data used here as well. Furthermore, the azimuthal velocity is transformed to the corotating reference frame. The following set of equations is to be understood as to give initial values at the inner radial grid boundary at \( R_{gb} \), while initialization at larger radii will be addressed subsequently:

\[
\begin{align*}
\rho &= \frac{F_{mass}}{v_r} \\
T_p &= \frac{p_{tot} - B^2/2}{\rho} \\
B_r &= b_{scale}B_{ss} \\
v_{\phi} &= \Omega R_s \sin(\theta) - \Omega R_{gb} \sin(\theta) \\
B_r &= \left( B_r/v_r \right) v_{\phi} \\
v_r &= v_{\min} + \frac{V_{del}}{V_{exp}} + \frac{d_{FP}}{V_{exp}^2 - \frac{B}{\rho}} \\
\end{align*}
\]
Before describing the parameters in and the implementation of these formulas, it should be mentioned that there are differences between this model and Detman et al. [2006, 2011]. Most importantly, their extrapolation scheme puts the source surface at smaller radial distances, and the extrapolation method is not the same as the one that generated the input data used here. Thus, their parameter tuning might not be optimal for our purpose, but repeating this process for the data used here would go beyond the scope of this work.

Equation (19) is based on the empirical inverse correlation between flux tube expansion factor $f_\text{ES}$ (hereafter EF) and radial solar wind speed $v_r$, observed near the Earth reported for potential field models as described in Wang and Sheeley [1990] and Wang et al. [1997]. Additionally, $d_{FP}$ is the footpoint distance to the nearest coronal hole boundary. The remaining unknowns are tuning parameters. The formula for the expansion factor reads

$$f_\text{ES} = \left(\frac{R}{R_\odot}\right)^2 B(R_\odot, \vartheta_0, \varphi_0) / B(R, \vartheta, \varphi),$$

(27)

where $B(R_\odot, \vartheta_0, \varphi_0)$ and $B(R_s, \vartheta, \varphi)$ are the magnetic field strengths at a point in the photosphere and (following a magnetic field line) at the source surface at $R_\odot$. In order to know how points on the two respective magnetic field maps are connected, it is necessary to find a mapping $(\vartheta, \varphi)$ to $(\vartheta_0, \varphi_0)$. The resulting footpoint locations are shown in Figure 3 as black/red dots. During solar minimum (Figure 3a) field lines originate from polar regions, but in this case there also exist excursions extending toward the equator. At solar maximum (Figure 3b) there is no discernible structure to be made out; field lines originate from coronal holes that can be located anywhere on the solar surface. To test whether these results are realistic, they can be compared to their observational counterparts, which are coronal holes inferred from National Solar Observatory He maps. This is shown for the case of solar maximum in Figure 3; model data are shown in red dots, observational data in black contours. There is some discrepancy, because the model is based on very different data (sunspot areas) and is a snapshot, while the observed synoptic map is pasted together from 27 days of data (because the whole solar surface cannot be seen from Earth at a time). Additionally, the observational technique misses very thin structures. Keeping this in mind the match between the data sets seems reasonable.

The location of the gridpoints of the map of magnetic field strength at the solar surface do not necessarily coincide with the derived footpoint locations and interpolation is applied, allowing to compute the magnetic field strength at the footpoints of the open field lines $B(R_\odot, \vartheta, \varphi)$ and from this the expansion factor $f_\text{ES}$ at every grid point on the source surface. The footpoint locations also allow to compute $d_{FP}$ for every corresponding grid point on the source surface by finding the nearest point that can be designated as part of a coronal hole boundary (yellow dots in Figure 3). Tuning parameters have been adopted from the original paper ($v_{\text{min}} = 154$ km/s, $v_{\text{red}} = 300$ km/s, $V_{\text{exp}} = 0.3$, $x = 7.4$ km/s, and $\beta = 3.5$). The resulting initial radial velocities at the inner radial grid boundary are shown in the respective top left panels of Figures 5 and 6 for both minimum and maximum conditions.

Typical solar minimum conditions are rather well known (high-speed streams in polar regions and low-speed streams in the ecliptic) and this general structure is reconstructed here. An interesting feature of high-speed wind in the equatorial region is also found, and a comparison with OMNIweb http://omniweb.gsfc.nasa.gov/ data at the time in question does indeed show large equatorial speeds at the Earth at the time in question (see Figure 4 showing wind speeds of up to 700 km/s), which supports the assumption that this feature is real. For solar maximum there is neither a typical structure nor a sufficient amount of out-of-ecliptic measurements to compare with. There are however attempts to describe solar maximum conditions [Zurbuchen et al., 2004], but a comparison is still difficult, because the background field is constantly distorted by the large number (≈5/day) of CMEs (as is also pointed out in Zurbuchen et al. [2004]). We therefore omit a detailed comparison for solar maximum because CMEs are not incorporated in this model as of yet.

Equation (20) uses the value of the radial velocity and in its original form assumes constant mass flux $F_{\text{mass}}$, thus yielding an inverse relation between mass density $\rho$ and radial velocity $v_r$. We calculated $F_{\text{mass},0}$ by taking values of $\rho v_r$ at the Earth at 1 AU and applying an $r^2$ scaling to get values at 0.1 AU. For this, 27 day averages of both quantities at the time in question are taken from the OMNIweb interface. The adopted values can be found in Table 2.

We introduced an improvement to be in agreement with Ulysses data [McComas et al., 2000], which showed for solar minimum conditions that the mass flux associated with high-speed streams is about half the one of low-speed streams. This is implemented by having the mass flux depend on the radial velocity by introducing a transition function $f(v)$ [see Scherer et al., 2010] defined as

$$f(v) = \frac{1}{2} (\tanh(5(v - v_1)) - \tanh(5(v_2 - v_1)))$$

(28)

gives a sharp, but steady transition at $v_1$ with $\Delta = 20$. The value of $v_1$ is chosen such that the transition from high to low speed occurs at $v = \pm 35$° for our solar minimum data, which yields $v_1 = 1.5 v_0$. Mass flux can then be calculated via

$$F_{\text{mass}} = (0.5 + 0.5 f(v)) F_{\text{mass},0}.$$  

(29)

Results are shown in Figures 5 and 6b.

Equation (21) is the pressure balance between gas pressure and magnetic pressure solved for proton temperature (which is the only temperature in this one-fluid model). The tunable parameter $p_{\text{tot}}$ is the total pressure, but its optimal values derived by Detman et al. [2006] change over the solar cycle, so that a rough tuning has been performed on our part to get realistic results and we chose $p_{\text{tot,min}} = 3.8 p_0$ and $p_{\text{tot,max}} = 4.2 p_0$ for solar minimum and maximum, respectively.

The radial magnetic field strength has to be scaled from source surface values $B_{B}(R_\odot)$ to values at the lower radial grid boundary at $R_{\text{BB}}$. The scale factor simply mimics the usual $r^{-2}$ behavior, so that $B_{\text{scale}} = (R_\odot/R_{\text{BB}})^2$. This is a very simple approach, which is not optimal everywhere, because an inhomogeneous azimuthal magnetic field component yields deviations from the $r^{-2}$ behavior for the radial magnetic field because of the solenoidality condition. However, at small
radial distances, such deviations should not be too serious since azimuthal components are small. Equations (23) and (24) set the $\vartheta$ components of both the velocity and the magnetic field equal to zero. We found that both $v_\vartheta$ and $B_\vartheta$ remain negligible throughout the computational volume, so that these approximations are affirmed.

As was demonstrated in the WD test case, the Parker spiral can be realized in two frames of reference (i.e., one corotating with the Sun and the other at rest with respect to the Sun’s rotation), both of which have been found to give equivalent results. Equations (25) and (26) model the Parker spiral in the corotating frame, whereas in Detman et al. [2006] the rest frame is implemented. The equation for the azimuthal velocity mimics the behavior of the low corona rotating approximately like a rigid body, thus using the solar rotation frequency $\Omega$ multiplied with the radius of corotation, which Detman et al. [2006] put at $R_{\vartheta} = 1.5R_\odot$. This approach is questionable in view of the behavior of the azimuthal velocity derived by Weber and Davis [1967] shown in Figure 1, because from the radius of corotation outward an approximate $r^{-1}$ behavior is evident that would yield considerably smaller values at $R_{gb}$. Correction for this with a respective scale factor has been applied here, so that $R_{\vartheta} = 1.5R_\odot(R_{gb}/R_\odot)$. This has been done in the recent update in Detman et al. [2011] also, as $R_{\vartheta}$ is now described

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{foot.png}
\caption{Location of footpoints of open magnetic field lines in the photosphere (black/red crosses) for (a) minimum and (b) maximum conditions. In Figure 3a yellow dots indicate coronal hole boundaries and cyan dots indicate field lines with the smallest expansion factors and thus result in the highest velocities. In Figure 3b a comparison with coronal holes inferred from National Solar Observatory He maps (black contours) is superimposed. The indicated polarities were also found to be in good agreement with our data.}
\end{figure}
as “a length scale which determines the azimuthal velocity,” but no specific value is given to compare with. This is still a rather crude estimate because the radius of corotation depends on the magnetic field strength near the Sun and simple 1/r scaling does not exactly reproduce the azimuthal velocity solution that should be similar to the WD solution. However, for this simple empirical model it shall suffice.

The equation for the azimuthal magnetic field (26) is the result of the induction equation in the rotating steady state corona in corotating spherical coordinates. This is a different approach than the one used for the test cases (see equation (17)), which became necessary for the following reason: in the Weber-Davis model the azimuthal magnetic field is homogeneous and can be extrapolated into the inner boundaries ghost cells from the values obtained from the innermost computed cells. The observationally based input for the magnetic field used here, however, is inherently inhomogeneous and makes extrapolation a challenging task, because of the staggered mesh implemented in CRONOS. Occasionally, this even gave rise to instabilities. To avoid this, we chose to fix the azimuthal magnetic field components according to Equation (26). In view of the inherently empirical nature of the whole set of equations to determine the remaining MHD quantities, this approach seems justifiable.

4.3. Radial Initialization

The values of the MHD quantities at the lower radial boundary derived above will now also serve to find initial values for the rest of the numerical domain. Here, radial velocity along with mass density is to fulfill the stationary equation of continuity, which is achieved by having \( v_r \propto r \) and \( \rho \propto r^{-3} \). Azimuthal velocity in the corotating frame of reference is basically proportional to radial distance \( (v_\varphi \propto r) \). For adiabatic expansion the radial dependence of temperature should approximately behave like \( T \propto r^{-\frac{4}{\gamma}} \) where \( \gamma \) is the number of degrees of freedom, related to the polytropic index via \( f = 2/\gamma - 1 \). In our case of \( \gamma = 1.05 \) this gives \( f = 40 \).

The magnetic field has to be initialized in a divergence-free manner, so that for later times the code retains a divergence-free field due to the constrained transport algorithm. This has been achieved by going through every cell layer radially, and solving the solenoidality condition to find the next cell’s magnetic field components. A detailed description of this algorithm would require a discussion of the grid layout and the operation of the code, and is therefore omitted here (but see Kissmann et al. [2009] and Kissmann and Pomoell [2012]).

4.4. Boundary Conditions and Grid Layout

Boundary conditions are chosen similarly to those used for the test cases, i.e., reflecting \( \vartheta \) boundaries, periodic boundary conditions for \( \varphi \), and an outflow condition at the outer radial boundary. At the inner radial boundary specific conditions are applied for each on quantity.

The radial velocity and mass density were kept fixed at the inner radial boundary. Additionally, the ghost cells are assigned values derived from extrapolation according to the governing power law in the first computed cell. Magnetic field components and \( v_\varphi \) remain fixed to their initial values as well, but no extrapolation for the ghost cells is applied. The azimuthal velocity \( v_\varphi \) is expected to be dominated by the transformation term to the corotating frame of reference, giving \( v_\varphi \approx -r \Omega \sin(\vartheta) \). Thus, a radial extrapolation for the inner radial ghost cells is applied according to

\[
v_{\varphi,i} = \frac{r_i}{r_0} v_{\varphi,0},
\]

where \( i \) indicates the negative index of the ghost cells, while the first cell in the computational domain carries the index 0.

For the observationally based input data the following grid layout has been chosen. For the latitudinal coordinate the ghost cells at each boundary should not coincide with or go beyond the poles because in the current setup coordinate singularities have to be excluded, but this can be treated in the near future as well. Here, we are not primarily concerned with the polar regions.

Furthermore, using the highest possible angular resolutions \((1^\circ \times 1^\circ)\) with an adequate radial resolution was found to require too long to converge. Instead we took half the possible angular resolution and a comparison with full resolution simulations yielded no significant differences. This gives \( \Delta \vartheta_{\text{grid}} \in [8^\circ, 172^\circ] \) and a cell size of \( \Delta r = 2^\circ \) gives 172 cells. Similarly, for the longitudinal coordinate \( \varphi_{\text{grid}} \in [0^\circ, 360^\circ] \), requiring 180 cells. The radial length of the simulation box is determined by Earth’s orbital distance \((215R_\odot)\) and the lower radial grid boundary \((21.5R_\odot)\), where we chose a radial cell size of \(1.5R_\odot\).

5. Simulation Results

5.1. Global Magnetic Field Structure

To get an impression of the results, pseudo three-dimensional visualizations of the respective data sets are
shown in Figure 7. The inner radial grid boundary can be extrapolated from the set of data by performing a spherical clip at the respective radius (giving the sphere in the center). After applying $1/r^2$ scaling, the color bar is for the radial magnetic field strength $B_r$ and is in accordance with the input data as was shown in Figure 2. The current sheet is the $B_r = 0$ contour through the computational grid. It can be seen that, at solar minimum, the current sheet is slightly wavy as expected from the input data, and it is subject to solar rotation as well, which can be seen by the bent wavy features. Magnetic field lines are colored black and are not uniformly distributed. The spiral structure can be made out as well by the bent field lines. For solar maximum conditions the current sheet’s structure is rather extreme, with steep gradients in excursions toward the poles.

Figure 5. Initial values at the inner radial grid boundary (left panels) and results at the outer radial grid boundary for the converged state (right panels) for solar minimum. The shown quantities are (top to bottom) radial velocity, mass density, radial, and azimuthal magnetic field. For the normalizations see Table 1.
5.2. Plasma Structure at 1 AU

The results at the outer radial grid boundary for radial velocity, mass density, and magnetic field components are shown on the right-hand sides of Figures 5 and 6, respectively. Comparing with the initial data, it can be seen that the results are strongly dependent on the input data, i.e., the input determines the results. Initial features can still be observed at the outer radial boundary but appear smoother. The effect of solar rotation is also visible as features shift in longitude. At solar minimum, for velocity and mass density it can be observed that the transit from slow to fast speed is sharper than it was initially due to the differently strong acceleration. In equatorial regions we get speeds of about 400 km/s and the high-speed feature is at 700 km/s in accordance with the observational data taken from the OMNIweb (Figure 4). At polar regions, speeds of about 650 km/s are found. Because there is no observational data

Figure 6. Same as Figure 5 for solar maximum conditions.
for polar regions from that time it cannot be judged whether this value agrees with the conditions present at that time. Mass density is inversely correlated with radial velocity and the obtained values at Earth’s orbit again agree with the observational data. The features of the magnetic field input are also preserved but the current sheet slightly broadens, which may be due to the finite spatial resolution. An interesting feature that is not present initially occurs at the location of the high-speed feature where we find an enhancement of the magnetic field strength. This is associated with the compression of the magnetic field when fast solar wind runs into slow one ahead, also known as corotating interaction regions.

At solar maximum there is no typical global structure in wind speed features to compare with so that with the limited number of observational data it is difficult to determine the quality of our results. It can, however, be stated (two top-right panels of Figure 6) that the obtained values for wind speed and mass density are again in the right order compared to the observational data. The initial magnetic field is largely preserved but is again modulated by features in the wind speed.

5.3. Three-Dimensional Velocity Structure

The radial velocity profiles at solar minimum are shown in Figure 8 in a meridional (\( \phi = 0 \)) and an equatorial (\( \phi = \pi/2 \)) slice through the computational grid. The meridional slice illustrates the dependence on latitude and Figure 9 shows a line plot accompanying the meridional slice, in which the radial velocity curves for different latitudes can be seen. The top curves correspond to high-speed polar regions and the bottom ones to equatorial regions. The red-dashed line is the Parker solution for a temperature
T = 0.49T_0 = 1.4 \cdot 10^6 \text{K} corresponding to the initial temperatures at polar regions, and shows that our results are close to it. The drop in some of the curves is due to slow wind features shifting to this longitude at larger radial distances, which is an effect of solar rotation. These effects are also visible in Figure 8b. At close inspection it can also be seen that the shift in longitude between the start surface and the outer radial grid boundary due to solar rotation depends on the radial velocity. This corresponds to the so-called Parker angle, which is the ratio between azimuthal and radial components. At the Earth it is usually at about 45° for radial velocities of about 400 km/s, which is also the case here near the ecliptic and we, too, find the corresponding shift in longitude to be at about 45°. We compared the winding angle (i.e., the ratio between the magnetic field components) with the Parker prediction and found good agreement for all latitudes except at the current sheet, which is understandable, because the Parker prediction does not involve dipolar fields.

6. Conclusions and Outlook

[55] In this work we successfully used observationally based input data of the radial magnetic flux to drive an inner heliospheric MHD simulation to calculate solar wind quantities at radial distances up to 1 AU. Testing the code has been done by a comparison to the simplified analytical models by Parker [1958] and Weber and Davis [1967]. It could be demonstrated that the code successfully reproduced the analytic results.

[56] The input data for the radial magnetic flux and its derivation are described in Jiang et al. [2010], which amongst several advancements allows for higher angular resolution than that of comparable observational data from synoptic magnetograms. While here the focus lay on two representative sets of data, those being one set at solar minimum and one at solar maximum, data are available for a whole time series going back to 1976. The possibility to run the code for more sets of data is present, including the opportunity to combine them to drive a time-dependent simulation.

[57] The MHD code requires input data for all plasma quantities, and it is necessary to use empirical formulas to derive them. The respective set of equations was taken from Detman et al. [2006, 2011], who work on a very similar goal, i.e., space weather forecasting, for which they use input data similar to those used here. These kinds of interfaces are constantly augmented as testing goes on. In this respect, this work can be understood to be part of this process with the difference of using more sophisticated input data and applying the empirical formulas developed and tuned for a specific code to the one used here.

[58] The results give values for solar wind quantities at 1 AU that can be used as input for outer-heliospheric large-scale models [e.g., Ferreira et al., 2007; Scherer et al., 2008], as background solar wind for coronal mass ejection simulations [e.g., Kleimann et al., 2009] or to model solar wind plasma structures [e.g., Dalakishvili et al., 2011, and references therein] such as corotating interaction regions.

[59] Acknowledgments. Financial support for the project FI 706/8-2 (within the Research Unit 1048) and for the project FI 706/14-1 funded by the Deutsche Forschungsgemeinschaft (DFG) is acknowledged.

References


2.3 Errata

Some minor mistakes were introduced by the publisher during the production process:

- Equation (26) should read \[ B_\phi = \frac{B_r}{v_r} \phi \].

- On page 36, paragraph [38]: reference to the boundary conditions for number density should be "Panel (c) of Figures 5 and 6".

2.4 Further development

As mentioned in the introduction of this chapter, a more detailed subsequent evaluation of the results presented in W13 by comparing with multi-spacecraft observations revealed that they are inaccurate. The first possibility I considered was that the empirical interface used to derive the boundary conditions – in particular for the solar wind speeds – would need additional tuning since the approach of Detman et al. (2011) uses a different potential field model and source surface location. Although such a tuning would probably indeed have been necessary, a more severe problem turned out to be the location of the current-sheet in the radial magnetic field maps, because these maps were used as direct input in the boundary conditions and could therefore not be tuned. Although there are always slight differences in the location of the current-sheet depending on the magnetogram source and the potential field model used, the differences found for the input data used thus far were rather severe, as demonstrated in Figure 2.3. The Figure shows the resulting radial magnetic field from the SFT/CSSS model of Jiang et al. (2010) at ten solar radii around 2007.5 (a), 2007.87 (c), 2008.24 (e) in the left panels compared to GONG maps\(^2\) of footpoints of open field lines (red/green dots), as well as projections of the highest closed coronal field lines (blue), and the indicated neutral line position (black) at the respective times (right panels). Although these figures are in a different format (Hammer projections on the left) and show different quantities, they do allow for a comparison of the neutral line/current-sheet position. While the tilts in the current-sheet in the left panels vary only slightly over the course of more than half a year, this is not the case in the right panels, and there is only a resemblance found between the bottom two panels. A discussion of this finding with our colleagues from the MPS yielded that their model did not properly take into account newly emerging active regions near the equator. This issue was addressed in Jiang et al. (2014), but for my work I chose to take a different approach as described in the next chapter.

\(^2\)obtainable from http://gong.nso.edu/
CHAPTER 2. MHD SIMULATION OF THE INNER-HELIOSPHERIC MAGNETIC FIELD

Figure 2.3: Resulting radial magnetic field strength from the SFT/CSSS model of Jiang et al. (2010) at ten solar radii around 2007.5 (a), 2007.87 (c), 2008.24 (e) on the left. In the right panels GONG maps of footpoints of open field lines (red/green dots), as well as projections of the highest closed coronal field lines (blue), and the indicated neutral line position (black) at the respective times is shown for comparison.
2.5 Addenda

2.5.1 Weber-Davis model in the inertial and co-rotating reference frame

Parker’s assumption of magnetic field lines following the plasma flow is not valid close to the Sun since there the kinetic energy density is smaller than the magnetic energy density. Consequently, one can assume that the plasma flow follows the magnetic field lines well inside the Alfvénic radius \( r \ll r_A \). This co-rotation should weaken when approaching \( r_A \), and for the limiting case \( r \gg r_A \) Parker’s model should be a good approximation.

This was calculated by Weber and Davis (1967, hereafter WD) who assumed an azimuthal component of the flow velocity and solved a steady-state model with axial symmetry (no \( \varphi \)-dependence) in the equatorial plane. An extension for arbitrary latitudes was given by Sakurai (1985), but as it is solved numerically a comparison would go beyond the scope of a test case as intended here (but see, e.g., Preusse et al., 2005). Therefore the test case is restricted to the equatorial plane.

In the WD model the components of the magnetic field and the flow velocity have azimuthal components so that

\[
B = B_r(r)\hat{e}_r + B_\varphi(r)\hat{e}_\varphi
\]

\[
v = v_r(r)\hat{e}_r + v_\varphi(r)\hat{e}_\varphi.
\]

The solenoidality of \( B \) (1.7) gives \((R_\odot \equiv \text{solar radius})\)

\[
B_r(r) = B_0 \frac{R_\odot^2}{r^2}
\]

and the equation of continuity (1.1) yields

\[
 r^2 \rho v_r = \text{const.}
\]

In the considered steady state the induction equation (1.4) reads

\[
\partial_t (r(v_r B_\varphi - v_\varphi B_r)) = 0
\]

\[
\Rightarrow r(v_r B_\varphi - v_\varphi B_r) = \text{const.}
\]

WD determine this constant by noting that in a perfectly conducting fluid \( v \) is parallel to \( B \) in a frame that rotates with the Sun, yielding

\[
v_r B_\varphi - v_\varphi B_r = -\Omega_{WD} R_\odot^2 B_0 / r
\]

where \( \Omega_{WD} \) is the angular velocity of the roots of the lines of force in the Sun (a detailed derivation is given in MacGregor and Pizzo (1983)). In their paper WD omitted any subscript on \( \Omega_{WD} \) so that one is tempted to consider it to be the photospheric solar rotation frequency. This in turn makes the original results of WD

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seemingly unphysical and, consequently, Barker and Marlborough (1982, hereafter BM) took a different approach to determine the constant in Equation (2.3) by taking values at the solar surface $B_\varphi(R_{\odot}) = B_{0,\varphi}$, $B_r(R_{\odot}) = B_{0,r}$, $v_\varphi(R_{\odot}) = v_{0,\varphi} = \Omega R_{\odot}$ and $v_r(R_{\odot}) = v_{0,r}$, yielding

$$v_r B_\varphi - v_\varphi B_r = -\Omega R_{\odot}^2 B_0 / r \cdot (1 + f)$$

(2.5)

where

$$f = \frac{v_{0,r}|B_{0,\varphi}|}{v_{0,\varphi}B_{0,r}}$$

(2.6)

and $\Omega$ (without subscript) denotes the solar rotation frequency.

Later, MacGregor and Pizzo (1983) compared the approaches of WD and BM concluding that they just differ by the definition of the angular velocity $\Omega$ (as is obvious here from comparing Equations (2.4) and (2.5)), yielding

$$\Omega_{WD} = (1 + f)\Omega$$

(2.7)

which does not change the involved physics.

Nevertheless, for comparing WD with the numerical results it is better to deal with the known value of the photospheric solar rotation frequency as was used by BM instead of the poorly known value for the angular velocity of the roots of the lines of force in the Sun, which are located within the Sun. Additionally, the values at the solar radius used by BM are also easily accessible for the numerical results.

The following steps are again taken from WD who continue to solve (2.4) for $B_\varphi$:

$$B_\varphi(r) = \frac{v_\varphi(r) - r\Omega_{WD}}{v_r(r)} B_r(r) .$$

(2.8)

To derive the azimuthal component of the flow velocity, the $\varphi$-component of the equation of motion (1.2)

$$\rho \frac{v_r}{r} \partial_r(r v_\varphi) = \frac{B_r}{\mu_0} \partial_r(r B_\varphi)$$

(2.9)

is considered, and after multiplication by $r^3$

$$\left[ \rho v_r r^2 \right] \partial_r(r v_\varphi) = \left[ \frac{B_r r^2}{\mu_0} \right] \partial_r(r B_\varphi)$$

(2.10)

is obtained, which allows to identify the terms in square brackets as constants (see Equations (2.1) and (2.2)). Integration yields

$$r v_\varphi - \frac{B_r}{\mu_0 \rho v_r} r B_\varphi = \text{const.} \equiv L ,$$

(2.11)

which corresponds to the total angular momentum carried away from the Sun per unit mass loss. Furthermore, the radial Alfvén Mach number

$$M_A \equiv \frac{v_r}{B_r/(\mu_0 \rho)^{1/2}}$$

(2.12)
can be introduced so that substituting Equations (2.8) and (2.12) into Equation (2.11) and solving for \( v_\varphi \) gives
\[
v_\varphi(r) = \Omega_{WD}r \frac{M_A^2L/(\Omega_{WD}r^2) - 1}{M_A^2 - 1}.
\]
(2.13)

Here, \( M_A \) is a steadily rising function of \( r \), reaching unity at the Alfvén critical radius \( r_A \), at which the denominator in Equation (2.13) vanishes. In order to keep \( v_\varphi \) finite at \( r_A \), the numerator must vanish as well, so that \( L = \Omega_{WD}r_A^2 \). From Equations (2.1), (2.2), and (2.12) it can be deduced that
\[
\frac{M_A^2}{v_r r^2} = \frac{1}{v_A(r_A)r_A^2}
\]
(2.14)
is a constant (evaluated at \( r_A \)), finally allowing to find
\[
v_\varphi(r) = \Omega_{WD}r \frac{1 - v_r/v_A(r_A)}{1 - M_A^2}
\]
(2.15)
and when substituted into Equation (2.8)
\[
B_\varphi(r) = -B_r \frac{\Omega_{WD}r}{v_A(r_A)} \frac{1 - (r/r_A)^2}{1 - M_A^2}
\]
(2.16)
from which the BM solution can easily be obtained by inserting Equation (2.7).

The asymptotic behavior is qualitatively derived as follows: the radial velocity becomes almost a constant for large \( r \), and with the equation of continuity follows \( M_A \propto r \) so that \( B_\varphi \), as well as \( v_\varphi \), vary as \( 1/r \) according to Parker’s prediction.

Following BM’s approach (i.e. using initial values at the solar surface), the above derivation can be adopted for the co-rotating frame of reference as well. The initial value for the azimuthal velocity \( v_\varphi(R_{\odot}) = 0 \) has to be used here, and the equation of motion is extended by the fictitious force term (in the ecliptic plane), such that
\[
\rho \frac{v_r}{r} \partial_r (rv_\varphi) = \frac{B_r}{\mu_0 r} \partial_r (rB_\varphi) + 2\rho \Omega v_r r^2
\]
(2.17)
instead of Equation (2.9). This, after following the above steps, eventually yields
\[
v_\varphi(r) = \frac{1}{M_A^2 - 1} \left[ v_{0,r} \frac{R_{\odot} B_{0,\varphi}}{r B_r(r)} \left( 1 - M_A^2 \frac{B_r(r)}{B_r(r_A)} \right) - M_A^2 \Omega r \left( 1 - \frac{r_A^2}{r^2} \right) \right]
\]
(2.18)
and
\[
B_\varphi(r) = \frac{(R_{\odot}/r)v_{0,r} B_{0,\varphi} + v_r(r)B_r(r)}{v_r(r)}.
\]
(2.19)

Here, for the latter \( v_\varphi \) has to be substituted, which was not done here to avoid lengthy expressions.

The final equations for the inertial (2.15 & 2.16) as well as for the co-rotating frame of reference (2.18 & 2.19) are used to validate the numerical realizations of these reference frames in the preceding publication.
2.5.2 Divergence-free initialization for arbitrary input data

It is crucial to initialize the magnetic field in a divergence-free manner in CRONOS with its constrained transport scheme, because it maintains the respective initial values of $\nabla \cdot \mathbf{B}$. For simple HMFs such as a Parker spiral with a flat current-sheet, this can be easily achieved, as such fields can also be described in terms of vector potentials, whose curl automatically fulfills the solenoidality condition (see Equation (1.10)). For arbitrary inner boundary conditions for the radial magnetic field as used here, additional care must be taken as there are no analytic descriptions available, and the situation is further complicated by the staggered-grid layout (see Section 1.2.2) employed in CRONOS, where the magnetic field components are not cell-centered but centered on respective cell-faces.

Starting from an arbitrary radial magnetic field distribution at the previous radial cell-face of the inner radial grid boundary $B_r(r_0 - \Delta r/2, \vartheta, \varphi)$, an estimate for the azimuthal magnetic field component of the first cell layer is calculated via

$$B_\varphi(r_0, \vartheta, \varphi \pm \Delta \varphi/2) = \frac{B_{r \text{avg}}}{v_{r \text{avg}}} v_{\varphi \text{avg}}.$$

Due to the offset locations of these quantities (see Figure 1.11), respective averaging is required at the location of $B_\varphi$. While $v_{r,\varphi}$ are known throughout the computational domain from respective simple radial initializations (see Section 4.3 in W13), which do not have to fulfill such severe restrictions as the magnetic field, the next cell’s radial magnetic field is actually not known at this point. This is estimated initially by a $r^{-2}$ dependence, which can be augmented by repeated execution of the following algorithm. A further necessary, but valid approximation that has to be made is that the $\vartheta$-components vanish, which is in agreement with open and radial field lines resulting at the outer boundary of potential field models of the solar corona.

The idea for a divergence-free radial initialization is to go through all cell layers in order of increasing radial position and adapting $B_r$ such that solenoidality holds in the subsequent cells. This can be achieved by solving the discretized solenoidality condition for the radial magnetic field $B_r(r_{i+1/2,j,k})$ in the next cell (notation according to Equation (1.9)), while the previous one $B_r(r_{i-1/2,j,k})$, as well as the azimuthal magnetic fields $B_\varphi(r_{i,j,k-1/2})$ and $B_\varphi(r_{i,j,k+1/2})$ at the respective cell boundaries are known at this point. It has also to be considered that the divergence itself is computed at the cell center at $r_{i,j,k}$.

Starting with the solenoidality condition, where $B_\vartheta$ is already set to zero,

$$0 = \nabla \cdot \mathbf{B} = \frac{1}{r^2} \partial_r (r^2 B_r) + \frac{1}{r \sin(\vartheta)} \partial_\varphi (B_\varphi),$$

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and discretizing with finite differences yields

\[
0 = \frac{1}{r_{i,j,k}^2} \left( \frac{1}{2} \Delta r B_r(r_{i+1/2,j,k}) - \frac{1}{2} \Delta r B_r(r_{i-1/2,j,k}) \right) + \frac{1}{\|r_{i,j,k}\| \sin(\vartheta_j)} B_\varphi(r_{i,j,k+1/2}) - B_\varphi(r_{i,j,k-1/2}) \Delta \varphi ,
\]

so that solving for \( B_r(r_{i+1/2,j,k}) \) finally gives

\[
B_r(r_{i+1/2,j,k}) = \left( \frac{\|r_{i-1/2,j,k}\|}{\|r_{i+1/2,j,k}\|} \right)^2 B_r(r_{i-1/2,j,k}) + \frac{\|r_{i,j,k}\| \Delta r (B_\varphi(r_{i,j,k+1/2}) - B_\varphi(r_{i,j,k-1/2}))}{r_{i-1/2,j,k}^2 \Delta \varphi} .
\]

The steps described above have to be performed for each cell layer. This causes difficulties when running on multiple CPUs: in order to compute the next cell layer, one needs to know the quantities from the previous one, but this is not necessarily the case here as usually each processor has only access to its respective sub-grid. The solution is to devise a global array and have each CPU calculate the initialization on the whole grid and then to assign only the respective sub-grid values to the single CPUs. It has been made sure that the solenoidality condition is satisfied to the degree of machine precision.

The following code fragment depicts the actual implementation in the User class:

```cpp
void OBS::div-free-init (Data &gdata, int ibeg[3], int iend[3])
{
  /*
   The globally declared array containing the initial fields looks like
   REAL global[3][3][rad_cells+7][190][370];
   with dimensional sizes due to:
   2 for sets in time between which to average +1 for initial divergence-free-init,
   3 for vr,brad,bradphi, rest due to resolution
   */
   //apply div-free-init to time-interpolated global array if using time
   int p;//p corresponds to first dimension in global array
   if (time_usage == 1){p=2;} else {p=0;}
   //some declarations
   REAL B_r_neu = 0;
   REAL delta_Bphi =0;
   REAL v_phi = 0;
   REAL v_r = 0;
   REAL B_r = 0;
   REAL B_phi = 0;
   // apply solenoidality condition while initializing Bphi:
   // go through whole grid, starting at inner radial grid boundary
   for (int i = -1; i < gdata.global_mx[0]+3; i++){
     // set Bphi first:
```
for (int j = ibeg[1]; j <= gdata.global_mx[1]+3; j++){
    REAL xx = gdata.get_x_global(i,0); //radial coordinate
    REAL theta = gdata.get_y_global(j,0);
    int i_min = i - 1; //previous radial index

    //assume v_phi=0 in inertial frame and transform to co-rotating one
    v_phi = -w*xx*sin(theta);

    //averaged quantities at location of Bphi are required to compute it
    if (k==gdata.global_mx[2]+3){ //periodic treatment at outer phi boundary
        v_r = (global[p][0][i+3][j+3][k+3] + global[p][0][i+3][j+3][ibeg[2]+7+3])/2;
        B_r = (global[p][1][i+3][j+3][k+3] + global[p][1][i_min+3][j+3][k+3]
            + global[p][1][i+3][j+3][ibeg[2]+7+3] + global[p][1][i_min+3][j+3][ibeg[2]+7+3])/4;
    }
    else{
        v_r = (global[p][0][i+3][j+3][k+3] + global[p][0][i+3][j+3][k+1+3])/2;
        B_r = (global[p][1][i+3][j+3][k+3] + global[p][1][i_min+3][j+3][k+3]
            + global[p][1][i+3][j+3][k+1+3] + global[p][1][i_min+3][j+3][k+1+3])/4;
    }

    //B_phi follows from the vanishing electric field (E = v x B) in the co-rotating frame
    //and neglected theta-components
    B_phi = B_r/v_r * v_phi;
    global[p][2][i+3][j+3][k+3] = B_phi; //store bphi in global array
}

// set Br accordingly:
for (int j = ibeg[1]; j <= gdata.global_mx[1]+3; j++){
    for (int k = ibeg[2]; k <= gdata.global_mx[2]+3; k++){
        REAL r_i = gdata.get_x_global(i,1); //radial distance at current Br-position
        REAL r_ip = gdata.get_x_global(i-1,1); //radial distance of previous Br-position
        REAL B_rp = global[p][1][i-1+3][j+3][k+3]; //value of previous Br
        REAL dr = gdata.getCen_dx_global(0,i); //radial cell size
        REAL dphi = gdata.getCen_dx_global(2,k);//azimuthal cell size
        REAL theta = gdata.get_y_global(j,0); //theta coordinate
        if (k==ibeg[2]) //periodic treatment at lower azimuthal boundary
            delta_Bphi = -global[p][2][i+3][j+3][gdata.global_mx[2]+3-7+3]
                + global[p][2][i+3][j+3][k+3];
        else
            delta_Bphi = -global[p][2][i+3][j+3][k-1+3]
                + global[p][2][i+3][j+3][k+3];

        //difference in Bphi at current cell
        REAL r_phi = gdata.get_x_global(i,0); //radial distance at cell center
        B_r_neu = power(r_ip/r_i,2)*B_rp
            - power(r_phi/r_i,2)*dr*delta_Bphi/(r_phi*sin(theta)*dphi);
        //solenoidality condition solved for next Br
        global[p][1][i+3][j+3][k+3] = B_r_neu; // store in global array
    }
}

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Chapter 3

Modeling background solar wind

3.1 Overview

The work described in this chapter based on the publication Cosmic Ray transport in heliospheric magnetic structures. I. Modeling background solar wind using the Cronos magnetohydrodynamic code (Wiengarten et al., 2014, W14) was done in the framework of a joint project with the Universities of Kiel and Potchefstroom, South Africa. The project focused on the influence of CIRs on the propagation of energetic particles, where the respective CIR disturbed background solar wind modeled in my MHD simulations is used as input to a respective SDE model for the transport of energetic particles in the heliosphere.

The idea behind this work is that the transport of charged energetic particles such as GCRs or Jovian electrons is largely governed by the properties of the plasma that these particles traverse. Due to the large amount of simultaneous in-situ measurements of the heliospheric plasma environment as well as of energetic particles, the heliosphere can be considered as a natural laboratory to investigate these transport processes. Meanwhile, the transport in the Galaxy is also important, but modeling suffers from the very small number of measurements there and at the sites of acceleration to high energies such as supernovae remnants. Of particular importance for the heliospheric modulation is the influence of transient structures such as CIRs and CMEs (with a focus on CIRs in this case) on the energetic particle propagation, because these structures are associated with magnetic field and turbulence enhancements, as well as shocks that can serve as diffusion barriers (see Figure 3.1), but also as accelerators of low-energy particles. A fully three-dimensional and possibly also time-dependent description of the heliospheric plasma is necessary for an adequate energetic particle modeling. Although simple analytical prescriptions such as the Parker (1958) model (undisturbed solar wind) or the Giacalone et al. (2002) model (CIR-disturbed wind) are useful starting points for such investigations, a much more coherent approach is to use MHD models that can self-consistently account for stream interactions and the formation of shocks, and which can be driven by observations-based input data. Therefore, the work described in the previous
A first mandatory task is the demonstration of the MHD code’s ability to correctly model CIR structures. This is the topic of Section 3 of W14, where analytic inner boundary conditions of alternating fast and slow streams were prescribed, and the resulting CIR configuration – including pressure enhancements, stream interfaces between fast and slow wind, as well as waves steepening into shocks traveling away from the interface – was successfully compared to previous work of Pizzo (1982). The further evolution of interacting – initially distinct – CIRs to eventually form merged interaction regions with increasing heliocentric distance was also analyzed.

This successful validation allowed for an investigation of these structures in a re-
3.1. OVERVIEW

A more suitable model was required for the coronal magnetic field that drives the WSA model to derive inner boundary conditions for the MHD simulations as described in Section 4 of W14. Since the empirical formulas in the WSA approach are tuned to be applied to the coupled PFSS (Altschuler and Newkirk, 1969) and SCS (Schatten, 1971) models in conjunction with GONG magnetograms, this road was followed by implementing these models in Matlab. The PFSS solution describes the coronal magnetic field out to the source surface at $2.5R_\odot$, where the field is forced to become open and radial. A drawback is that the resulting radial magnetic field distribution at the source surface does not exhibit a thin current sheet as opposed to observations. This is addressed by subsequently involving the SCS model in the region from the source surface out to the inner boundary location of the MHD simulations at 0.1 AU. Both PFSS and SCS usually solve the Laplace equation for a scalar potential $\Delta \Psi = 0$ for the coronal magnetic field by means of spherical harmonics. Such an approach was initially taken by myself as well, but for grid resolutions approaching the magnetograms’ one is faced with numerical artifacts in the reconstructed magnetograms, which is the so-called ringing effect related to Gibb’s phenomenon occurring at sharp or discontinuous reconstructions of periodic signals with Fourier series. This can be avoided by solving the Laplace equation with a finite differences approach, and therefore I used a respective public code (FDIPS$^1$) for the PFSS model henceforth. A respective coupling of such a finite-difference approach to the coronal potential field with the WSA model as used in this work had not been undertaken previously.

The set of empirical formulas based on the WSA approach was slightly adapted in this work, but is otherwise the same as in W13. However, particularly for the resulting solar wind speeds, which rely on the topology of the coronal potential field via the flux tube expansion factor (EF) and the distance to the nearest coronal hole boundary (FPD), it is necessary to perform field line tracings (FLT) in the solutions for the coronal magnetic field. Previously, these data were provided by the collaborators at the MPS, so that I had to perform the FLT by myself now. The basic idea in FLT for a given vector field is simply to take a small step tangentially to the field at a predefined starting point and repeat it from the newly reached point until a predefined boundary is reached. This can be done numerically by simple forward integration schemes, however, the tricky part is the size of the small steps. I implemented a method of taking adaptive step sizes, namely the embedded Runge-Kutta 4/5 algorithm (e.g. as described in Press et al. (2007)), which takes adequately large or small steps depending on the fields topology at the current point. The algorithm in application to the field line tracing in the coronal potential field was validated by comparing with respective data from the GONG web page, and consequently – after computing the EF and FPD as in W13 – the complete set of inner boundary conditions for all MHD quantities could be set.

$^1$http://csem.engin.umich.edu/tools/FDIPS/
While this procedure was principally applicable to any period of time for which GONG magnetograms are available (back to 2006), a time period of descending solar activity (August 2007) was chosen, because of recurrent and stable CIR structures observed at that time. Furthermore, a unique spacecraft constellation was present then with *Ulysses* crossing the equatorial plane during its third fast-latitude scan and the recently launched *Stereo* twin spacecrafts leading and trailing Earth (see Section 1 of W14). MHD simulations during that time (Carrington Rotations 2059-2061) were performed on new computer clusters at our institute comprising of 64 and 48 cores, which put typical run-times at several hours to a week (depending on resolution). The results (Section 5 of W14) were compared to respective spacecraft data provided by our collaborators of the University of Kiel. This required me to perform an interpolation of my results on the numerical grid along the spacecraft trajectories. In order to obtain results as close as possible to the reference data, the tuning parameters in the empirical formulas for the inner boundary conditions were adapted, and the final results (Figures 9–11 in W14) show usually good agreement. Particularly the timing and strength of high-speed streams and resulting CIR structures could be reproduced. Nevertheless, some discrepancies remain and reasons for this are discussed in the conclusions (Section 6 of W15).

For the comparison with spacecraft data, the simulation box was restricted by an outer boundary at 2 AU to save computing time while still including the trajectories of the considered spacecraft with *Ulysses* at approximately 1.3 AU at that time. For further utilization in the SDE modeling, the simulation box has to be extended to at least include Jupiter (at about 5 AU), but ideally to much larger distances. Here, additional simulations have been performed out to 10 AU and the evolution of the CIR structures with heliocentric distance was analyzed in a similar fashion as for the validation case described above.
3.2 Wiengarten et al. (2014)

Cosmic Ray transport in heliospheric magnetic structures. I. Modeling background solar wind using the Cronos magnetohydrodynamic code

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COSMIC RAY TRANSPORT IN HELIOSPHERIC MAGNETIC STRUCTURES. I. MODELING BACKGROUND
SOLAR WIND USING THE CRONOS MAGNETOHYDRODYNAMIC CODE

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ABSTRACT
The transport of energetic particles such as cosmic rays is governed by the properties of the plasma being traversed. While these properties are rather poorly known for galactic and interstellar plasmas due to the lack of in situ measurements, the heliospheric plasma environment has been probed by spacecraft for decades and provides a unique opportunity for testing transport theories. Of particular interest for the three-dimensional (3D) heliospheric transport of energetic particles are structures such as corotating interaction regions, which, due to strongly enhanced magnetic field strengths, turbulence, and associated shocks, can act as diffusion barriers on the one hand, but also as accelerators of low energy CRs on the other hand as well. In a two-fold series of papers, we investigate these effects by modeling inner-heliospheric solar wind conditions with a numerical magnetohydrodynamic (MHD) setup (this paper), which will serve as an input to a transport code employing a stochastic differential equation approach (second paper). In this first paper, we present results from 3D MHD simulations with our code CRONOS: for validation purposes we use analytic boundary conditions and compare with similar work by Pizzo. For a more realistic modeling of solar wind conditions, boundary conditions derived from synoptic magnetograms via the Wang–Sheeley–Arge (WSA) model are utilized, where the potential field modeling is performed with a finite-difference approach in contrast to the traditional spherical harmonics expansion often utilized in the WSA model. Our results are validated by comparing with multi-spacecraft data for ecliptical (STEREO-A/B) and out-of-ecliptic (Ulysses) regions.

Key words: magnetohydrodynamics (MHD) – methods: numerical – shock waves – solar wind – Sun: heliosphere – Sun: magnetic fields

Online-only material: color figures

1. INTRODUCTION
1.1. Cosmic Ray Transport

The understanding and appropriate modeling of the transport of charged energetic particles in turbulent magnetic fields remains one of the long-standing challenges in astrophysics and space physics. The many simultaneous in situ observations of both the heliospheric magnetic field and different energetic particle populations make the heliosphere a natural laboratory for corresponding studies. Of particular interest in this context are galactic cosmic rays (GCRs) and Jovian cosmic ray electrons. While the former traverse the whole three-dimensionally structured heliosphere and allow for studies of its large-scale variations as well as of the evolution of heliospheric turbulence (e.g., Zank et al. 1996; Heber et al. 2006; Potgieter 2013a; Bruno & Carbone 2013), the latter represent a point-like source and are, thus, well suited for analyses of anisotropic spatial diffusion (e.g., Ferreira et al. 2001a, 2001b; Sternal et al. 2011; Strauss et al. 2013).

In order to exploit this natural laboratory in full, it is necessary to reproduce the measurements with simulations that do contain as much as possible of the three-dimensional structure of the plasma background within which the cosmic rays are propagating. Significant progress has been made regarding the modeling of the quiet solar wind (e.g., Potgieter 2013b), but much remains to be done to implement the many features that are structuring the solar wind and the heliospheric magnetic field, into transport models of cosmic rays. Particularly interesting structures are the corotating interaction regions (CIRs) that are formed during the interaction of fast solar wind streams from coronal holes with preceding slow solar wind and usually persist for several solar rotations (e.g., Balogh et al. 1999, and references therein). These structures not only lead to particle acceleration, but also to the modulation of GCR and Jovian electron spectra (Richardson 2004). Indeed Ulysses measurements, as described in, e.g., Marsden (2001), at high heliolatitudes during the first orbit of the spacecraft around the Sun indicated that CIRs represent the major constituent for the three-dimensional heliospheric structure close to solar minimum (e.g., Heber et al. 1999). A major surprise came from the measurements of accelerated energetic particles and GCRs that showed clear periodic signals even above the poles of the Sun where no in situ signals of CIRs were registered by the plasma or magnetic field instrument (Kunow et al. 1995). Electron measurements, however, indicate no variation at these region. It can be speculated that the differences are caused by the fact that both GCRs and locally accelerated particles have an extended source, while MeV electrons in the inner heliosphere originate from a point-like source as mentioned above (Chenette 1980). Thus, there is a different influence of CIRs on GCR and Jovian electron flux variations as investigated recently by Kühl et al. (2013).

If the electron source is a well-localized point-like source in the heliosphere—namely the Jovian magnetosphere—it is mandatory to describe the structure of the plasma stream in the whole inner heliosphere up to several AU and not only at the location of different spacecraft measuring these particles.
A unique constellation of spacecraft to investigate these intensity variation was present in 2007 August, when Ulysses crossed the heliographic equator during its third so-called fast latitude scan. Figure 1 (left) displays the trajectories of Ulysses (blue), STEREO-B (red), and STEREO-A (green) in ecliptic coordinates. The right panel of that figure shows the spacecraft position projected onto the ecliptic plane on September 24. The dotted and colored lines display Parker spirals using a velocity of 400 km s\(^{-1}\).

Figure 2 displays the corresponding solar wind and MeV electron measurements by SWOOPS (Bame et al. 1992) and SWEPAM (McComas et al. 1998) instruments as well as the MeV electron fluxes from the COSPIN/KET and the COSTEP/EPHIN detectors (Müller-Mellin et al. 1995) aboard Ulysses, ACE, and SOHO, respectively, for the period of interest. While a recurrent structure of the electron intensities is present for the whole period shown in Figure 2, the Ulysses measurements only show such variation when the spacecraft is embedded in a CIR region. A first analysis of the EPHIN measurements has been reported by Kühl et al. (2013), who showed that over half a year of measurements the electron flux can be correlated or anti-correlated with the solar wind speed depending on the CIR region. A far more realistic modeling of the heliospheric environment can be obtained with MHD simulations: while physically the heliospheric magnetic field (HMF) originates in the Sun, it is conceptually customary to distinguish for modeling purposes between (1) the coronal magnetic field filling the region from the solar surface out to a spherical so-called heliobase (Zhao and Hoeksema 2010) at several (tens of) solar radii and (2) the HMF beyond. There are two popular modeling approaches for the coronal magnetic field, namely potential field reconstructions and MHD models (see Riley et al. 2006). The latter approach is computationally more challenging but can account for more physics, direct time-dependence and self-consistency. There are numerous examples for such MHD modeling of the coronal magnetic field, including the work of, e.g., Usmanov and Goldstein (2003), Cohen et al. (2007), Lionello et al. (2009), Riley et al. (2011), Feng et al. (2012).

The second popular approach for deriving solar wind conditions utilizes potential field reconstructions of the coronal field that account for the solar wind’s influence by introducing a so-called source surface beyond which the field is required to be purely radial. The basic technique of potential field source surface (PFSS) models, originally introduced by Altschuler & Newkirk (1969) and Schatten et al. (1969), is still widely used and was found to provide a means for predicting solar wind speed at Earth via the so-called fluxtube expansion factor of open coronal field lines (Wang & Sheeley 1990). Another quantity that can be derived from potential field models, the footprint distance of an open field line to the nearest coronal hole boundary, was used by Riley et al. (2001) to empirically quantify the resulting solar wind speeds. Combining such approaches and incorporating the Schatten current sheet (SCS) model (Schatten 1971) to account for thin current sheets resulted in the so-called Wang–Sheeley–Arge (WSA) model (Arge & Pizzo 2000; Arge et al. 2003). A variety of versions of the WSA model predict solar wind speed distributions at different solar distances rather close to the Sun from where the predictions must be propagated further outward. Earlier models used simple kinematic propagation schemes, while nowadays MHD codes are utilized.
since they can account for more physics needed, e.g., for the proper modeling of stream interactions and shock formation. Such combined models are in operation at space weather forecasting facilities such as the Community Coordinated Modeling Center (CCMC) or the Space Weather Prediction Center (SWPC).

The main advantage of the latter empirical models are their significantly reduced computational costs as compared to coronal MHD models. Additionally, the empirical models avoid the problems arising due to sub-Alfvénic solar wind speeds—complicating boundary conditions as perturbations may travel back toward the photosphere—and the issue of coronal heating. Furthermore, it was demonstrated by Riley et al. (2006) that PFSS solutions often closely match those obtained by numerical MHD models.

In the present study, we are mainly interested in the influence of CIRs on the transport of energetic particles from distant sources toward the Earth (galactic cosmic rays, Jovian electrons), such that a detailed coronal model is not mandatory. In this light, we postpone the implementation of a coronal MHD model to future studies and instead use the empirical WSA model as input to MHD simulations in a domain from 0.1 AU to 10 AU and possibly further out. This will provide a realistic heliospheric environment for the Stochastic differential equation (SDE) transport code to study propagation of energetic particles, which will be addressed in the second paper of this series. The paper at hand describes the MHD modeling and is organized as follows.

Section 2 briefly describes the CRONOS MHD code in the specific application to heliospheric modeling. This setup is validated in Section 3 where we compare results for analytically prescribed boundary conditions for CIRs with those originally obtained by Pizzo (1982) for the same setup. Section 4 gives an overview of the WSA model comprising potential field modeling and a set of empirical formulae to derive the inner boundary conditions for the MHD simulations. The acquisition of data from in situ measurements from the STEREO and Ulysses spacecraft and the comparison with our results is addressed in Section 5 before giving our conclusions and an outlook on future tasks.

2. CODE SETUP

The tool of choice for our simulations is the state-of-the-art MHD code CRONOS, which has been used in recent years to model astrophysical (e.g., ISM turbulence, Kissmann et al. 2008; accretion disks, Kissmann et al. 2011) and heliospheric scenarios (Kleimann et al. 2009; Dalakishvili et al. 2011; Wiengarten et al. 2013). Amongst its main features the code employs a semi-discrete finite-volume scheme with Runge–Kutta (RK) time integration and adaptive time-stepping, allowing for different approximate Riemann solvers. The solenoidality of the magnetic field is ensured via constrained transport, provided the magnetic field is initialized divergence-free. Supported geometries are Cartesian, cylindrical, and spherical (including coordinate singularities) with the option for non-equidistant grids. Here, we use spherical coordinates \((r, \vartheta, \varphi)\) with the origin being located at the center of the Sun. Thus, \(r\) is the heliocentric radial distance, \(\vartheta \in [0, \pi]\) is the polar angle (with the north pole corresponding to \(\vartheta = 0\)) and \(\varphi \in [0, 2\pi]\) is the azimuthal angle. \(\varphi\) corresponds to Carrington longitude in this paper, except for the test case in Section 3, where a reference longitude is arbitrary. The code runs in parallel (MPI) and supports the HDF5 output data format.

In its basic setup, the code solves the full, time-dependent, normalized equations of ideal MHD

\[
\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0
\]

(1)
\[ \partial_t (\rho v) + \nabla \cdot [\rho vv + (p + |B|^2/2) I - BB] = f \]  
\[ \partial_t e + \nabla \cdot [(e + p + |B|^2/2) v - (\mathbf{v} \cdot \mathbf{B}) B] = \mathbf{v} \cdot \mathbf{f} \]  
\[ \partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0 \]

where \( \rho \) is the mass density, \( \mathbf{v} \) is the fluid velocity, \( \mathbf{B} \) and \( \mathbf{E} \) describe the electromagnetic field, \( e \) is the total energy density, and \( p \) is the scalar thermal pressure.

Additional force densities \( \mathbf{f} \) can be introduced by the user. In our setup these are the gravitational force density \( \mathbf{f}_g = -\rho G M_\odot / r^2 \mathbf{e}_r \) and, since it is convenient to perform calculations in a frame of reference corotating with the Sun, the fictitious forces \( \mathbf{f}_{\text{cor}} = -2 \rho \mathbf{\Omega} \times \mathbf{v} - \rho \mathbf{\Omega} \times ( \mathbf{\Omega} \times \mathbf{r}) \), where \( \mathbf{\Omega} = \mathbf{\Omega}_c \).

Since we know of no consistent way to connect the Sun’s observed differential surface rotation from the photosphere to the lower radial boundary of our computational domain, we are forced to neglect this effect and, therefore, choose a constant solar angular rotation speed \( \Omega = 14:71 \text{ day}^{-1} \) (Snodgrass & Ulrich 1990). Furthermore, \( I \) denotes the unit tensor, and the dyadic product is used in Equation (2).

Amongst the closure relations
\[ e = \frac{\rho |v|^2}{2} + \frac{|B|^2}{2} + \frac{p}{\gamma - 1} \]  
\[ \mathbf{E} + \mathbf{v} \times \mathbf{B} = 0 \]  
\[ \nabla \cdot \mathbf{B} = 0, \]

an adiabatic equation of state is used with an adiabatic exponent \( \gamma = 1.5 \), which is the same value as used in the heliospheric part of the ENLIL setup (Odstrcil et al. 2004).

## 3. MODEL VALIDATION

As mentioned in the Introduction, the modeled heliospheric background will be used as an input for a SDE transport code in order to investigate the propagation of energetic particles in a forthcoming study. During solar quiet times, CIRs are the most prominent agents that can have significant influence on the transport coefficients as they act as diffusion barriers due to the associated magnetic field enhancements. We, therefore, first demonstrate the capability of our setup to model these structures. Further detailed model validation for the application of the CRONOS code to inner-heliospheric scenarios were performed by Wiengarten et al. (2013).

There are no exact analytic expressions for the plasma quantities in CIR associated structures, although there exist simplified models (e.g., Giacalone et al. 2002, see also Vogt 2013), but the expressions given therein perform a heuristic fit to data and lack a description of the CIR associated shocks. Therefore, to validate our model we instead compare with results obtained with previous numerical simulations, namely the pioneering work by Pizzo (1982) who investigated a variety of different steady-state scenarios, one of which will be summarized and compared with here. The inner radial grid boundary is chosen to be located at \( r_0 = 0.3 \text{ AU} \), well beyond the critical surfaces, so that the solar wind speed is super-magnetosonic everywhere. Therefore, perturbations cannot travel toward the Sun and constant (corotating) boundary conditions can be chosen. A circular region patch of fast, tenuous and hot wind centered at the equator is embedded into the ambient slow, dense and cool wind, providing the basic ingredients for a CIR (see Figure 3 to get a first expression). The inner radial boundary conditions are shown in an equatorial slice in Figure 4(a) and are ascribed as follows. The formula used to specify radial velocity at the inner boundary in our setup reads \( v(r_0, \theta, \phi) = v_0(1 + a) \) with \( v_0 = 300 \text{ km s}^{-1} \) and \( a \in [0, 1] \), so that the ambient slow velocity is \( 300 \text{ km s}^{-1} \) and the fast wind is at \( 600 \text{ km s}^{-1} \). Specifically,
\[ a = \sum_{m=1}^{M} 0.5 \left[ \tanh(A(\xi_m + A \Delta \xi)) - \tanh(A(\xi_m - A \Delta \xi)) - \tanh(A \xi_m) \right] \]

where \( \xi_m = \sqrt{(\theta - \theta_0)^2 + (\phi - \phi_m)^2} \) is the angular distance from the center of the high-speed stream at \( (\theta_0, \phi_m, \Delta \xi) \) is its angular extent, and \( A \) controls the steepness of the transition from slow to fast wind. This approach was necessary since there is no explicit formula given by Pizzo (1982), but instead the initial configuration shown (their Figure 5) was digitalized (http://digitizer.sourceforge.net/) and fitted with parameters for the above formula resulting in \( A = 30, \Delta \xi = 13^\circ, \theta_0 = \pi/2, \phi_{m,0} = (2n - 1)\pi/M \). The upper index \( M \) in the sum of Equation (8) is set to \( M = 6 \) in accordance with the Pizzo setup, which refers to the fact that there are actually six high-speed streams in the whole \( 2\pi \) interval, giving a periodicity of \( 60^\circ \), so that \( \phi_m \) gives the longitudinal center of the respective high-speed stream. Other values for \( M \) could be chosen to investigate the interaction of different CIRs depending on their longitudinal separation.

Density is inversely correlated to velocity via \( n(r_0, \theta, \phi) = n_0(1 + a)^{-1.5} \) with \( n_0 = 120 \text{ cm}^{-3} \) so that with a prescribed constant pressure, temperature is inversely proportional to \( n \) with a value \( T_0 = 0.16 \text{ MK} \) for the ambient wind. For the magnetic field strength, Pizzo (1982) assumes a constant value of \( B_0 = 45 \text{ nT} \). In our setup we prescribe a constant \( B_{r,0} \) and calculate \( B_{\phi,0} = -B_{r,0} v_{r,0}/v_{\phi,0} \) so there is a small deviation from a constant \( B_{r,0} \) since \( v_{\phi,0} \) varies as described above. Furthermore, we assume a small value for the azimuthal velocity component \( u_{\phi,0} = \Omega R_\odot / r_0 \sin(\theta) \) in the inertial frame with a radius of corotation \( R_c = 1.5 R_\odot \), as follows from the Weber–Davis model (Weber & Davis 1967) also considered in our previous work (Wiengarten et al. 2013). The azimuthal velocity in the corotating frame then is \( v_{\phi,0} = u_{\phi,0} - \Omega R_\odot \sin(\theta) \). The longitudinal periodicity, giving a total of six high-speed streams in the whole \( 2\pi \) interval, allows for a rather high angular resolution (\( \Delta \phi = \Delta \theta = 0.25^\circ \)): the computational costs are kept low by performing the calculations for just one embedded structure and applying periodic boundary conditions in the azimuthal direction, so that the azimuthal extent of the simulation box \( \phi \in [0, 2\pi/6] \). For the results presented below, the simulation results have been copied and appended to cover the whole \( 2\pi \) interval. The polar regions are not significant here and are excluded to avoid small time-steps, thus \( \phi \in [0.2\pi, 0.9\pi] \). In the radial direction the simulation box extends to \( 10 \text{ AU} \), with the radial cell size set to \( 1 \text{ AU} \) on a linear grid. Computations are performed until a steady state is reached. A 2D visualization is shown in an equatorial slice (for
Figure 3. Visualization of the modeling test case in an equatorial slice: color coding refers to radial velocity, magnetic fieldlines are shown in white. (A color version of this figure is available in the online journal.)

the whole longitudinal interval, restricted to 1 AU) in Figure 3 with the color coding according to radial velocity. The density distribution of the magnetic field lines indicates the formation of compression and rarefaction regions. Quantitative results at 1 AU are shown in Figure 4(b) in the same manner as the inner boundary conditions, where the results to compare with have been digitized as above from Figure 6 in Pizzo (1982). The agreement between our results and Pizzo’s is very satisfactory, bearing in mind that on the one hand there are slight differences in boundary conditions and on the other hand different codes and numerical schemes were used. In fact, Pizzo solved the steady-state MHD equations, while the full time-dependent set of equations is treated here.

Compression occurs at the leading edge of the high-speed stream at a longitude of \( \phi \approx 187^\circ \) with respective elevations in the pressure associated quantities in the bottom panels. There are two waves propagating away from this interface in opposite directions, one forward (\( \phi \approx 196^\circ \)) and one backward (\( \phi \approx 177^\circ \)), which have already steepened into MHD shocks. This is the result of the initial sharp transition between the streams, causing a high compression. For different initial conditions shocks may evolve only beyond several AU of radial distance or not at all. The flow angle (second panel) shows that the interface is a region of shear, with azimuthal speeds directing away from the interface, which causes the latter to broaden and smear out with increasing distance from the Sun. Further steepening of the forward-reverse shock pair and a broadening of the interaction region occur for larger radial distances.

This is explicitly visible in Figure 5, depicting the evolution and interaction of two adjacent structures out to a radial distance of 9 AU. Here, radial velocity is shown in solid black with a fixed y-axis scaling, while total pressure shows as dashed blue with adaptive y-axis scaling to account for the rapidly decreasing values. The longitudinal interval shown in all panels is extended to 120° and is fixed in the arbitrary range from 110° to 230°. At 2 AU the forward (FS) and reverse (RS) shocks are more pronounced and are indicated via horizontal dashed lines in orange and red, respectively. The stream interface (SI) is identified as local maxima in total pressure, which coincides with the zero-crossing of the flow angle \( \phi \) (not shown here). The SI is indicated as green dashed-dotted vertical line. Note, for the following panels, that it is not the same two CIRs shown in the consecutive panels: due to the Parker angle of 45° AU^{-1}, the structures experience a respective shift in longitude to the right from one panel to the next one, while the periodicity of 60° gives the impression of structures apparently moving to the left. For the SI this gives exactly the difference of 15° to the left per panel, while the shocks propagate away from it. They encounter each other just before 4 AU and a corotating merged interaction region (CMIR) is formed. The shocks move through each other and propagate further at a lower relative speed, due to energy losses in the collision process (Parker 1963, p. 110). This gives rise to another compression region that is more pronounced than the original one at the SI by 5 AU and it continues to be the dominant structure out to 9 AU, while the shocks weaken to pressure waves. This demonstrates the different dynamics: In
Figure 4. Comparison with Pizzo for (left) initial conditions (at 0.3 AU) and (right) 1 AU results in the equatorial plane. Shown quantities are (top to bottom): radial velocity \( v_r \), flow angle in corotating frame \( \phi \) and in inertial frame \( \psi \), proton number density \( n \), temperature \( T \), magnetic field strength \( B \), and total pressure \( p \). CRONOS data are in black-solid, Pizzo data in red-dashed.

(A color version of this figure is available in the online journal.)

the inner heliosphere it is momentum driven by streams, while beyond several AU it is driven by the evolution and interaction of interaction regions and shocks (Burlaga 1995, p. 137).

This rather simple setup will also provide a good first test for the SDE transport modeling, because the relevant structures are regular and fairly easy to identify.

4. UTILIZING OBSERVATIONAL INPUT DATA

Having validated the numerical framework, we now seek to model more realistic solar wind conditions as present during a given period of time. With a focus on CIRs, we chose a time period in late 2007 (Carrington Rotations (CR) 2059 to 2061) when, due to coronal hole excursions to low latitudes, several fast wind streams were present in the otherwise slow ambient solar wind. Because there were no transient events, this time period is also favorable for the present study as the used WSA model does not cover coronal mass ejections. The WSA model relies on the topology of PFSS models of the coronal magnetic field. To simulate the effect that the solar wind has on the magnetic field, which is to drag it out with increasing radial distance, a source surface is introduced (typically at \( R_s = 2.5 R_\odot \)) beyond which the field is assumed to be purely radial. Laplace’s equation is commonly solved by series of spherical harmonics. While this provides a computationally cheap way to describe the large-scale coronal magnetic field, an inherent disadvantage of the spherical harmonics approach is the occurrence of ringing artifacts around sharp features when the order of spherical harmonics approaches the resolution of the magnetogram (Tran 2009). An alternative approach using a finite difference scheme to solve Laplace’s equation was proposed by Toth et al. (2011), and their code FDIPS was made publicly available (http://csem.engin.umich.edu/tools/FDIPS/).

4.1. Potential Field Modeling

PFSS models (Altschuler & Newkirk 1969; Schatten et al. 1969) assume a current-free corona, so that from \( \nabla \times \mathbf{B} = 0 \) the magnetic field can be expressed in terms of a scalar potential \( \mathbf{B} = -\nabla \psi \) that, due to the solenoidality condition \( \nabla \cdot \mathbf{B} = 0 \), has to fulfill Laplace’s equation \( \nabla \cdot (\nabla \psi) = 0 \). To simulate the effect that the solar wind has on the magnetic field, which is to drag it out with increasing radial distance, a source surface is introduced (typically at \( R_s = 2.5 R_\odot \)) beyond which the field is assumed to be purely radial. Laplace’s equation is commonly solved by series of spherical harmonics. While this provides a computationally cheap way to describe the large-scale coronal magnetic field, an inherent disadvantage of the spherical harmonics approach is the occurrence of ringing artifacts around sharp features when the order of spherical harmonics approaches the resolution of the magnetogram (Tran 2009). An alternative approach using a finite difference scheme to solve Laplace’s equation was proposed by Toth et al. (2011), and their code FDIPS was made publicly available (http://csem.engin.umich.edu/tools/FDIPS/).
Figure 5. Evolution and interaction of two adjacent CIR structures in the equatorial plane from 2 AU to 9 AU. Radial velocity is shown in solid black with a fixed y-axis scaling, total pressure in dashed blue with adaptive y-axis scaling. The longitudinal positions of the stream interface (SI, dashed-dotted green), forward shock (FS, dashed orange) and reverse shock (RS, dashed red) are depicted by respective vertical lines. See the text for details. (A color version of this figure is available in the online journal.)

Their approach completely avoids artifacts and the magnetogram is exactly reproduced. The computational costs to obtain the potential field solution are also fairly low on modern computers (i.e., minutes when using the parallelized version on a 16 core machine). We use FDIPS with GONG integral synoptic magnetograms in the Fits-Format and apply a resolution of $[N_r, N_\vartheta, N_\varphi] = [150, 180, 360]$ grid points, so that the angular resolution matches that of the magnetograms. The resulting grid’s radial resolution $\Delta r = 0.01 R_\odot$ agrees with the stepsize in tracing magnetic field lines in the WSA model (C. N. Arge 2014, private communication). The resulting potential field configuration for CR2060 is shown in Figure 6: the reconstructed photospheric magnetogram is shown on the inner sphere (see top panel of Figure 7 for a full map), where the data range is restricted to $\pm 15$ Gauss to better illustrate the small scale structures (active regions in this magnetogram have maximum values up to 500 G). The outer half-sphere represents the source surface. Selected field lines display rather typical solar minimum conditions with open field lines in polar regions (giving rise to the fast polar wind) and closed loops toward the ecliptic plane (resulting in a slow wind there). Excursions of open field lines to lower latitudes give rise to high-speed streams there that will interact with the ambient slow wind to form CIRs.

It has been demonstrated that PFSS solutions often closely match respective MHD results (Riley et al. 2006). One shortcoming of the PFSS models, however, is that they do not produce a thin current-sheet, which can be seen in Figure 7, middle panel, showing a map of the source surface radial magnetic field where the transition between the different polarities is rather broad. This is in contrast to observations that show sharp and thin current sheets at magnetic field polarity reversals. To overcome this problem, the WSA model further utilizes the Schatten current sheet (SCS) model (Schatten 1971) to compute the magnetic
field beyond the source surface: the magnetic field at the source surface is first re-oriented where necessary to point (radially) outward everywhere, and is then used as a boundary condition for another potential field approach from which respective spherical harmonic coefficients are calculated. In contrast to the reconstruction of the highly structured magnetograms, the spherical harmonics approach does not suffer from ringing artifacts in this case, since a small maximal order of 9 is sufficient and applied here. The initial orientation has to be restored in the resulting configuration, which can be achieved by tracing field lines from the outer boundary of the Schatten model at \( R_{\odot} = 0.1 \) AU back to the source surface. The resulting map of the radial magnetic field (Figure 7, bottom panel) at \( R_{\odot} \) is topologically similar to the one at the source surface with smaller maximal tilt angles of the current sheet. The map is used in defining the inner boundary condition in the MHD calculations as described in the next section.

4.2. Empirical Interface

To derive boundary conditions for the remaining plasma quantities at \( R_{\odot} = 0.1 \) AU, a set of empirical formulas is employed, which are largely based on the topology of the coronal potential field configuration. Wang & Sheeley (1990) found an inverse relationship between the flux-tube expansion factor

\[
f_s(\vartheta, \varphi) = \left( \frac{R_{\odot}}{R_i} \right)^2 \cdot \frac{B(R_{\odot}, \vartheta_0, \varphi_0)}{B(R_i, \vartheta, \varphi)}
\]

and the resulting solar wind speed: large expansion factors (low solar wind speeds) are usually associated with field lines that have their photospheric footpoints at coronal hole boundaries (i.e., the boundary between open and closed field lines), while small expansion factors (high solar wind speeds) are associated with those originating from deep within a coronal hole. Therefore, the further away an open field line footpoint is located from a coronal hole boundary the higher is the resulting solar wind speed. This can be expressed in terms of the quantity \( \theta_b \), the footpoint distance to the nearest coronal hole boundary, introduced first by Riley et al. (2001). It was since then found that using both \( f_s \) and \( \theta_b \) in conjunction gives better results than either one alone (Arge et al. 2003). The actual computation of \( f_s \) and \( \theta_b \) requires field lines being traced back to their respective footpoints in the photosphere at \((\vartheta_0, \varphi_0)\). Our algorithm implemented for tracing the field lines employs an adaptive step-size method inherent to embedded RK methods (Press et al. 2007), where in our setup the maximal allowable deviation \( D_{RK} \) from unity ratio taken of 5th order RK and embedded 4th order RK is used to determine the step-size. For the tracing in the PFSS domain below 2.5 \( R_{\odot} \) we used \( D_{RK} = 10^{-3} \) and \( D_{RK} = 10^{-4} \) below 1.1 \( R_{\odot} \), respectively, resulting in stepsizes in the range from 0.1 to 0.01 \( R_{\odot} \), where the lower limit corresponding to the grid’s cellsize. A comparison using \( D_{RK} = 10^{-4} \) everywhere yielded no difference in resulting footpoint locations within 0.01, which is far below the magnetograms resolution. Similarly, for the SCS models domain beyond 2.5 \( R_{\odot} \) step-sizes can go up as high as 0.8 \( R_{\odot} \) for \( D_{RK} = 10^{-3} \). The resulting photospheric footpoint locations are shown in Figure 8(a): The red/green dots indicate footpoints with positive/negative polarity, respectively. Besides the large coronal holes in the polar regions there are excursions
Maps of radial magnetic field strength, top: at the photosphere, middle: at the inner radial MHD grid boundary from SCS model.

(A color version of this figure is available in the online journal.)

to equatorial latitudes, which are the sources of respective high-speed streams there. Also shown are the highest closed fieldlines in blue, which are traced in both directions from just below the source surface \( (r_b = 2.49 \, R_\odot) \) and characterized as closed if the photosphere is reached in both directions. A qualitative comparison can be made with similar plots available on the GONG website,\(^4\) which is shown for CR2060 in panel (b) of Figure 8. Even though there are slight differences in the details, the global topology is very similar to that in panel (a), especially concerning the locations of the equatorial extensions of open fieldline footpoints and regions with fieldlines closing below \( r_b \). Differences may arise due to the different potential field approaches (the plot from the GONG webpage uses spherical harmonics) and the method to calculate the field lines.

The coronal hole boundary can now be defined to be situated where footpoints of open field lines are adjacent to those of closed field lines. This was achieved by binning the respective photospheric map into a \( 1^\circ \times 1^\circ \) grid and then labeling cells based on whether or not they contain open field lines. The coronal hole boundary is defined where an “open cell” has at least three of its eight neighboring cells marked as “closed.” We calculate the distance to the nearest coronal hole boundary (CHB) for each footpoint of an open field line (FP) by taking the distance

\[
d = \arccos(\sin(\theta_{\text{CHB}}) \cos(\varphi_{\text{CHB}}) \sin(\theta_{\text{FP}}) \cos(\varphi_{\text{FP}}) + \sin(\theta_{\text{CHB}}) \sin(\varphi_{\text{CHB}}) \sin(\theta_{\text{FP}}) \sin(\varphi_{\text{FP}}) + \cos(\theta_{\text{CHB}}) \cos(\varphi_{\text{FP}}))
\]

(10)

along a great circle to all cells marked as coronal hole boundary and choosing the smallest value.

The computation of the fluxtube expansion factor \( f_i \) is carried out along with the determination of open footpoints by taking the respective magnetic field values at the source surface and the photosphere as connected by a field line and using Formula (9).

The set of empirical formulae to determine the boundary and initial conditions for the remaining MHD quantities is similar to the one used by Wiengarten et al. (2013), with the following adaptations: the formula for radial velocity now reads

\[
v_r = V_0 + \frac{V_1}{(1 + f_i)^{3/2}} \cdot \left(1 - 0.8 \exp \left(-\left(\frac{\theta}{\phi}\right)^{1/3}\right)\right)^3
\]

(11)

as discussed by McGregor et al. (2011). A number of such formulae can be found in the literature (e.g., Feng et al. 2010; Detman et al. 2011), differing in form as well as in scaling parameters. The parameters have values \( V_0 = 240 \, \text{km s}^{-1}, V_1 = 675 \, \text{km s}^{-1}, \beta = 1.25 \) and \( \phi = 2.8 \) at SWPC while McGregor et al. (2011) found \( V_0 = 200 \, \text{km s}^{-1}, V_1 = 750 \, \text{km s}^{-1}, \beta = 3.6 \) and \( \phi = 3.8 \) by fitting solar wind velocity distributions. We performed a rough tuning to be in better agreement with the spacecraft data and found for our setup more suitable values \( V_0 = 200 \, \text{km s}^{-1}, V_1 = 675 \, \text{km s}^{-1}, \beta = 2.0 \) and \( \phi \in [2.8, 3.2] \), which are comparable to the values listed above. A more thorough tuning would go beyond the scope of this paper, and optimal parameters may vary for different CRs.

Since potential field models systematically underestimate the magnetic flux (Stevens et al. 2012), we apply a correction to the initial magnetic field for better accordance with 1 AU data while keeping the orientation of \( B_{\phi0} \). Specifically, a value of 300 nT is applied for a respective solar wind speed of 625 km s\(^{-1}\) and linearly scaled for other speeds, as is done in the WSA–Enlil model (McGregor et al. 2011). Additional estimates for mass flux and total pressure are obtained from OMNI-web \((http://omniweb.gsfc.nasa.gov/)\) data by taking respective 27-day averaged values. These are then scaled with radial distance to the inner grid boundary and used for defining boundary conditions for density and temperature as described in Wiengarten et al. (2013).

The derived boundary conditions are assumed to remain stationary in the corotating frame during the evolution of a single CR so that the simulations can be advanced in time until a steady state is reached. The simulation box extends to 2 AU in order

\(\begin{align*}
\frac{\theta}{\phi} & = \frac{1}{2} \arccos(\sin(\varphi) \sin(\theta) + \cos(\varphi) \cos(\theta) \cos(\varphi)) \\
\frac{\theta}{\phi} & = \frac{1}{2} \arccos(\sin(\varphi) \sin(\theta) + \cos(\varphi) \cos(\theta) \cos(\varphi)) \\
\frac{\theta}{\phi} & = \frac{1}{2} \arccos(\sin(\varphi) \sin(\theta) + \cos(\varphi) \cos(\theta) \cos(\varphi))
\end{align*}\)

\(\begin{align*}
\frac{\theta}{\phi} & = \frac{1}{2} \arccos(\sin(\varphi) \sin(\theta) + \cos(\varphi) \cos(\theta) \cos(\varphi)) \\
\frac{\theta}{\phi} & = \frac{1}{2} \arccos(\sin(\varphi) \sin(\theta) + \cos(\varphi) \cos(\theta) \cos(\varphi))
\end{align*}\)

http://gong.nso.edu/data/magmap/QR/mqf/200708/mrmqf070828/mrmqf070828t0501c2060_000.gif
to include \textit{Ulysses} at \( r \approx (1.4-1.5) \) AU during the time period considered, and also to study the formation of CIR-associated shocks. The applied resolution is \( \Delta r = 2 \, R_\odot \), \( \Delta \theta = 1^\circ \), \( \Delta \varphi = 1^\circ \), and, since we focus on the validation of the results with spacecraft data, the simulation box is restricted to extend to 2 AU only in the radial direction and to \( \theta \in [0.2\pi, 0.8\pi] \) in latitude. This gives a runtime \( T_{\text{run}} \approx 15 \) hr on a 64 core cluster, while the physical convergence time \( T_{\text{conv}} \approx 300 \) hr, which is estimated from the slowest wind (\( v_r \approx 250 \, \text{km s}^{-1} \)) to propagate to the outer boundary. Taking the simulation to larger radial distances for usage in the SDE code is straightforward, but requires the grid to be coarsened to maintain reasonable required computer resources. The polar regions could be included as well, but this would further restrict the global timestep in the simulations due to small cell sizes as \( \sin(\theta) \rightarrow 0 \) toward the poles.

5. RESULTS—COMPARISON WITH SPACECRAFT DATA

The simulation results of the solar wind speed, density, and temperature as well as of the magnetic field are compared to spacecraft data of both the \textit{Ulysses} and the two \textit{STEREO} spacecraft. \textit{Stereo-A}(head) leads Earth while \textit{STEREO-B}(hind) trails Earth. In detail, the \textit{Ulysses} data are based on measurements from the \textit{Ulysses} SWOOPS (Bame et al. (1992)) and the magnetometer onboard (VHM; Balogh et al. (1992)). For the \textit{STEREO-A/B} twin spacecraft, measurements were taken from the PLASTIC (Galvin et al. 2008) instrument and the spacecraft’s magnetometers (MAG; Acuña et al. 2008).

We first discuss the results for CR 2060 and only briefly address the results for CR 2059 and CR 2061 presented afterward. For a comparison with the spacecraft data the MHD results have been interpolated along respective spacecraft trajectories. Panel (a) in Figure 9 shows the resulting map for the radial velocity at the radial distance of the \textit{STEREO-A} spacecraft (at \( \approx 1 \) AU and separated in longitude from Earth by less than \( 15^\circ \), see \text{http://stereossc.nascom.nasa.gov/where.shtml}). The white line indicates its trajectory as the spacecraft traverses from right to left as indicated by the corresponding day of year (DOY) used as the horizontal axis. A respective map for \textit{STEREO-B} is very similar to panel (a) and is, therefore, omitted. Instead panel (b) shows the equivalent map for the \textit{Ulysses} spacecraft.
spacecraft, which at that time performed a fast-latitude scan and was located at heliocentric distances of $r \approx (1.4–1.5)$ AU. Quantitative comparisons with the in situ measurements are presented in the bottom panels (c)–(e), where the quantities shown are (top to bottom) radial velocity $v$, particle number density $n$, temperature $T$, radial magnetic field $B_r$, and magnetic field magnitude $B$. The spacecraft data (red lines) have been averaged to the $1^\circ$ angular resolution of the simulated data (black lines). A quite good match is found along the orbit of STEREO-B (panel (d)), where the prominent high-speed streams centered around DOYs 239 and 246 are captured in terms of magnitude and stream width, while a third high-speed stream at DOY 250 is somewhat underestimated. Furthermore, the simulation data shows an additional feature at DOY 236, which is not present in the spacecraft data, and can be identified as an excursion of the northern coronal hole in panel (a). A similar behavior is found for STEREO-A. Here we demonstrate the effect of artificially shifting the spacecraft position slightly ($4^\circ$ south in latitude) which results in the dashed blue curve. The comparison seems significantly improved as the additional features prominence is mitigated while the observed stream at DOY 250 is now captured very accurately. This shows that a comparison strictly along a spacecraft trajectory may not always be satisfactory at first glance, but that a thorough inspection of such maps as presented in panels (a) and (b) can help identifying the actually observed ones, which may just be slightly off the trajectory in the simulation (see Section 6 for further discussion). The comparison with Ulysses data for radial velocity is also somewhat dominated by the additional feature around DOY 239, however, apart from that the comparison is quite satisfactory throughout the course of this CR.

The pressure associated quantities $n$, $T$, and $B$ exhibit magnitudes of the correct order with respective strong enhancements in compression regions associated with the forming CIRs at the leading edges of high-speed streams. The magnetic field strength, however, seems to be systematically underestimated and might have to be increased in future simulations.

Another interesting quantity is the radial magnetic field component, through which sector boundaries (i.e., current sheet crossings) can be identified, which is difficult, however, due to rapid fluctuations in the spacecraft data. Still, the average polarity and sector boundaries are captured fairly well, e.g., for STEREO-B, current sheet crossings occur at DOY 243 and 250 in good agreement with the measurements.

Figure 10 shows results for CR 2059 in the same format as Figure 9. Most features are captured relatively well in the STEREO comparisons with the largest deviations occurring at the beginning and end of this CR where the simulation data show...
a high-speed feature not seen in the measurements. A shift in latitude for STEREO-A shows again that a small deviation from the actual trajectory gives better results and proves the presence of respective high-speed features, which are just slightly offset. The comparison with Ulysses data shows excellent agreement.

The results for CR 2061 are shown in Figure 11 which are similar to the ones for CR 2060 along the STEREO trajectories, and satisfactory agreement is found. Ulysses, on its way to northern polar regions, encounters predominantly the fast solar wind coming from the respective northern coronal hole. The simulation data along its trajectory, however, does not show the return to slow-speed wind occurring twice. Again, these are present in the global topology (see panel (b)) but are located too far south so that an 8° shift south in latitude is necessary to produce results more similar to the measurements.

We believe to have found a reasonable agreement with spacecraft data at relatively small heliocentric distances and, therefore, we feel that the results we obtain at greater distances can be trusted to also be a good representation to the local solar wind conditions. An arising problem, however, is the common assumption of stationary boundary conditions during the course of a CR. On the one hand, this is reasonable for propagating solutions out to 1–2 AU only, because the solar wind takes a relatively short time to propagate there (∼4 days AU−1) as compared to the duration of a CR (∼27 days). On the other hand, when extending the simulations to larger radial distances, stationary boundary conditions may become unreasonable if there is a significant change from one CR to the next one, because the propagation time becomes comparable to and eventually even larger than the duration of a CR, so that the heliosphere is filled with solar wind whose composition changes according to the different boundary conditions. This latter effect will have to be considered when we extend the simulation box to larger radial distances, so that time-dependent boundary conditions have to be applied. This will, however, take considerably longer computation time. A simpler approach appears to be possible for CR 2060–2061, because the boundary conditions change rather little and stationary boundary conditions still appear to be a reasonable assumption. A respective simulation was carried out applying constant inner radial boundary conditions of CR 2060 and extending the simulation box in the radial direction to 10 AU with a resolution of [Δr, Δθ, Δϕ] = [2 R⊙, 2°, 2°].

An equatorial slice of the simulation box depicting radial velocity is shown in Figure 12. Three initially distinct high-speed streams can be identified that—with increasing heliocentric distance—begin to interact and form a CMIR with a large angular extent. This is shown in a quantitative manner in Figure 13, which is similar to Figure 5 as it shows radial
velocity (black solid) and total pressure (blue dashed) at the equator at radial distances from 1.5 to 9.5 AU. The horizontal axis uses a longitude, which is Carrington Longitude minus 180° in order to show the evolution and interaction out to 6.5 AU without hitting the longitudinal periodic boundary. Only one of the three initial high-speed streams at 1.5 AU shows a strong compression region at its stream interface (SI1, green dashed-dotted). At 2.5 AU two stream interfaces with respective forward (FS orange, dashed/dotted) and reverse shocks (RS, red dashed/dotted) propagating away from them can be seen. FS1 and RS2 move toward and finally through each other between 3.5 and 4.5 AU and a CMIR is formed, which further interacts with the third initial high-speed stream’s shocks a little beyond 8 AU. The only prominent structure left at 9.5 AU is a large merged interaction region bounded by the forward and reverse shocks (FS1 and RS1) of the initially steepest high-speed feature with a complicated internal structure as a result of the merging process. The influence of such complicated structures on particle transport will be interesting to investigate.

6. SUMMARY AND DISCUSSION

We demonstrated the capability of the MHD code CRONOS to model CIR-associated structures (compression regions, shock pairs) in a test case where we are in agreement with the earlier results by Pizzo (1982). To model more realistic solar wind conditions, we used GONG magnetograms and the FDIPS potential field solution as input to the WSA model to derive inner boundary conditions for our MHD code. To our knowledge this is the first time that the WSA model is used in conjunction with the FDIPS model, which can make use of the full resolution of a given magnetogram without introducing numerical artifacts that can arise in the usual spherical harmonics expansion of the coronal potential field. Our results could be shown to be in reasonable agreement with spacecraft data.

Other studies have looked at CR 2060 using input from the WSA model. In one example, Pahud et al. (2012) validated their findings by comparison with ACE and MESSENGER spacecraft data, though no comparison with Ulysses data was performed to validate out-of-ecliptic results. The agreement of the in-ecliptic results is comparable to the one found here. Ulysses comparisons for this time period were performed by Broiles et al. (2013), but the focus was on single CIR structures instead of investigating the whole CR. Therefore, in performing simulations to reproduce simultaneous multi-spacecraft observations including out-of-ecliptic data and also considering temporally adjacent CRs our modeling extends previous work and provides
There are several reasons for occasional deviations when directly comparing simulation results to spacecraft in situ measurements which can essentially be attributed to the simplifications made in the model. Among others the following reasons can be listed. First, it has been shown that results using input from different solar observatories may differ quite substantially (Pahud et al. 2012; Gressl et al. 2013). Along this track Riley et al. (2013) investigated an ensemble modeling technique taking into account results from different models and observatories, which when combined give a better solution. Second, the empirical formulas used to set the inner radial boundary conditions are not well constrained and need some tuning that may depend on the observatories input data and the phase of the solar cycle. Similarly, the PFSS and SCS models are rather crude estimates of the inner and outer coronal fields, and are also subject to empirical parameters such as the source surface radius, which may not be constant as commonly assumed, but may vary depending on angular position (Riley et al. 2006) and solar cycle (Tran 2009). A tuning of all these parameters could be performed to diminish differences between simulations and in-situ measurements, however, this does not give insight into the underlying physics on the one hand, and is also a very time consuming undertaking on the other hand. Third, since the whole solar surface is not visible from Earth at a given time, synoptic magnetograms always contain non-simultaneous observations. Flux-transport models (e.g., Jiang et al. 2010) may be an effective tool to model the unobserved hemisphere of the Sun and improve magnetograms, however. These are not implemented in our model, but may be subject to future work.

A related problem is the common assumption of stationary boundary conditions during the course of a CR. While this remains reasonable for propagating solutions out to about 1 AU only—because the solar wind’s crossing time is much smaller than the duration of a CR—it becomes necessary to apply time-dependent boundary conditions when extending the simulations to larger radial distances so that the heliosphere is filled with solar wind with composition changes according to the changing coronal conditions.

This latter effect will have to be considered when we extend the simulation box to larger radial distances, so that time-dependent boundary conditions may have to be applied. This will, however, take considerably longer computation time. A simpler approach presented here was taken for CR 2060–2061, because the boundary conditions change rather little and stationary boundary conditions might still be a reasonable assumption. Time-dependent simulations and the inclusion of the poles will be addressed in an upcoming paper, where we will utilize the modeled 3D solar wind structure to investigate the transport of energetic particles, such as Jovian electrons and galactic cosmic rays.
Figure 13. Evolution and interaction of adjacent CIR structures in the equatorial plane from 1.5 AU to 9.5 AU for CR 2060. The format is similar to Figure 5. (A color version of this figure is available in the online journal.)

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3.3 Further development and future directions

The companion paper of W14 describing the utilization of my MHD simulations’ results in the SDE code is currently in preparation. For the respective modeling of the charged energetic particle propagation, it is desirable to have MHD results within the whole heliosphere and the surrounding disturbed ISM. This would require on the one hand an MHD model of the solar corona, and on the other hand the coupling of my setup with global heliospheric models, which are also performed in our group by J. Kleimann and K. Scherer (see Chapter 6).

A coronal MHD model is a challenging task as mentioned before, and for the SDE modeling focusing on the influence of CIRs on GCRs and Jovian electrons, it is not vital to have such a model, as CIRs develop at much greater heliocentric distances only. However, for a study of SEPs such a model would be desirable. A coupling of coronal MHD simulations for rather simple configurations (but, e.g. including a CME) with SEP models is already going on in the framework of a more elaborate future project with W. Dröge at the University of Würzburg. Meanwhile, a coupling with global heliospheric models is principally possible, but on the one hand, the necessary computer resources become huge due to the long propagation times and different required scales, and on the other hand, the SDE modeling beyond the TS in the heliosheaths is more difficult due to the present sub-Alfvénic flows and unknown turbulence evolution there.

Therefore, for the current SDE modeling, MHD simulations within the TS have been the next desired step. As the propagation time of typical solar wind parcels from the Sun to the termination shock is about a year, it is unreasonable to assume stationary inner boundary conditions due to the changes in the coronal field, and a time-dependent approach is necessary. This has been achieved by respective interpolation in time between incrementing data sets for the inner boundary values of adjacent Carrington rotations. To reduce computational costs, the grid has been coarsened with increasing radial distance, and the polar axis’ have been included with one large cell each to avoid small time steps (see Appendix A). Furthermore, it was found that the implementation of solar rotation via the fictitious forces as source terms becomes problematic for large heliocentric distances beyond about 10 AU. Instead, a respective conservative scheme was implemented as described in the next chapter (specifically Section 4.4). Due to the still enormous computational costs even on a new 256 core cluster at our institute, simulations were performed out to 20 AU only, and since there is no principle change in the resulting configuration it is not further presented here.

Another way of improving the subsequent SDE modeling is to include a turbulence model to be solved self-consistently alongside the MHD equations, because in the SDE model transport coefficients are employed that actually depend not only on the large-scale MHD quantities, but particularly the diffusion coefficients depend
on the magnetic fluctuations. A respective implementation of such a turbulence transport model is the topic of the next two chapters.
Chapter 4

Implementing turbulence transport

4.1 Overview

From the early measurements of the solar wind it was already apparent that there are random fluctuations super-imposed onto the large-scale magnetic field, solar wind velocity and density, so that it has to be considered as an inherently turbulent plasma (Coleman, 1968; Belcher and Davis, 1971). While astrophysical plasmas should be considered as turbulent media in general due to the very high Reynolds numbers, the numerous available spacecraft measurements made in the heliosphere make the latter a natural laboratory for respective investigations. It is assumed that sources for turbulence (see, e.g., the review by Zank, 1999) are located not only in the corona from where it is advected into interplanetary space, but that it is also generated in-situ by the turbulence itself at density gradients throughout the heliosphere. In the inner heliosphere (within about 10 AU) the main drivers for turbulence are shear at differently fast solar wind stream interfaces, as well as transients such as CIRs and CMEs with their associated shocks. These, however, weaken with increasing heliocentric distance as these structures become merged interaction regions. In the outer heliosphere isotropization of newly born pickup ions is the main agent for generating fluctuations, during which the initially ring-distributed pickup ions isotropize and generate Alfvén waves, which cascade to ever smaller scales and eventually dissipate and heat the solar wind as measured by the Voyager 2 spacecraft (see Figure 4.1). Thus, the temperature does not behave as expected for an adiabatically expanding and cooling gas, but there is actually even an increase.

Amongst the further important effects of turbulence (see, e.g., the review by Miesch et al. (2015)) are its catalytic impact on reconnection (e.g. Yokoi et al., 2013), which is one explanation for the heating of the solar corona, as well as its relevance for the propagation of energetic particles. Although particles mainly follow the mean magnetic field, the magnetic field fluctuations, which are usually perpendicular to
the mean one, lead to a perpendicular diffusion of energetic particles towards neighboring field lines. In the first attempts to involve these effects in models for the transport of energetic particles in the heliosphere, diffusion parameters have been approximated by expressing the fluctuations in terms of the large-scale fields (see the review of Potgieter, 2013). Some recent so-called \textit{(ab-initio models} (e.g. Engelbrecht and Burger, 2013), however, formulate the diffusion coefficients explicitly based on the small-scale fluctuations, on which new insights have been gained both from improved analysis of solar wind measurements (e.g. Horbury and Osman, 2008; Horbury et al., 2012) on the one hand, but particularly by new modeling approaches on the other hand (e.g., Zank et al., 1996; Breech et al., 2008; Oughton et al., 2011; Zank et al., 2012). These latter models describe the evolution of turbulent energy density, cross-helicity, and correlation lengths for low-frequency turbulence, as observed in the solar wind, with increasing distance from the Sun. These integral quantities describe the large-scale behavior of turbulence and wave modes, which is a useful approach to circumvent the difficulties that would arise for a complete description of the fluctuations, which is on much smaller scales than typical structures in the heliosphere. Particularly for numerical studies such an approach is desirable because of the reduced required computer resources.

The following publication \textit{Implementing turbulence transport in the Cronos framework and application to the propagation of CMEs} (Wiengarten et al., 2015, W15)
describes my efforts to extend the Cronos setup with a respective turbulence transport model. Besides the general aim to model and understand the evolution of turbulence in the heliosphere, another aim is to utilize the results to augment the calculation of transport parameters in the SDE modeling.

All the above-mentioned turbulence transport models have the drawback that they use prescribed solar wind conditions (usually constant speed and Parker field geometry), but it is desirable – particularly in the light of my previous work – to have a self-consistently computed background solar wind, i.e. a coupling of turbulence transport and MHD equations as described in Section 2 of W15. The basic idea is to decompose the magnetic and velocity fields in the MHD equations into respective mean and fluctuating components, which after applying appropriate averaging schemes leads to the so-called Reynolds-averaged MHD equations (see Usmanov et al. (2011) for a thorough description). In comparison with the usual MHD equations they also comprise of terms involving the fluctuations, which requires additional evolution equations for these quantities. Namely, these are the total turbulent (magnetic plus kinetic) energy density and the energy density difference, from both of which the particular magnetic and kinetic components can be computed. Furthermore, the so-called cross-helicity describes the ratio between inward and outward propagating modes. Turbulence cascades in the solar wind and is eventually dissipated into heat, where the rate of dissipation is controlled by the so-called correlation lengths, whose evolution is also described by additional equations in these models.

While most modeling attempts concentrated on the resulting turbulence distribution in the heliosphere for idealized solar wind conditions, thereby neglecting a self-consistent coupling with the Reynolds-averaged MHD equations, such a coupled approach was first taken by Usmanov et al. (2011). To become familiar with this subject and test Cronos’ ability to be correspondingly extended (Section 2 of W15), I started with a feasibility study and compared with these authors’ results (Section 3 of W15). In due course and after discussions with A. Usmanov, some errors were found in their model, which I subsequently corrected in my paper.

Another inherent drawback of the Usmanov model was its restriction of applicability to regions in the heliosphere, where the solar wind speed is much higher than the Alfvén speed. As in my previous work employing the WSA model this condition is not fulfilled towards the inner boundary, I sought to extend the model further to be applicable to these regions as well. A respective more general turbulence transport model was recently presented by Zank et al. (2012) with further refinements in Dosch et al. (2013) and Adhikari et al. (2015). This model has been implemented in a still simplified manner here, but see Chapter 5 for a full implementation of that model. As compared to the model of Usmanov et al. (2011) it allows for the inner boundary location to be located closer to the Sun, and it properly incorporates turbulence generation via shear (Section 4 of W15). However, the Zank model has
thus far been solved for idealized solar wind conditions only. Therefore, a significant improvement provided in W15 is the self-consistent coupling of this model with the Reynolds-averaged MHD equations.

These extensions allowed for a subsequent novel application of the model to a CME propagation scenario (Section 5 of W15). The results revealed that, on the one hand, turbulence does not act back strongly on the large-scale quantities describing the CME, so that general studies of CME propagation need not be extended in this direction. On the other hand, CMEs have a strong effect on the turbulence quantities. These effects are as manifold as the CME structure is complex, with partially increased and decreased turbulence levels. A subsequent investigation of the effects of such complicated turbulence distributions on the energetic particle propagation will be quite interesting.

Another extension applied to the code setup is a conservative treatment of the co-rotating reference frame as opposed to the formerly applied realization with the required fictitious forces as source terms. This is described in more detail in an addendum in Section 4.4.
4.2 Wiengarten et al. (2015)

Implementing turbulence transport in the Cronos framework and application to the propagation of CMEs

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IMPLEMENTING TURBULENCE TRANSPORT IN THE CRONOS FRAMEWORK
AND APPLICATION TO THE PROPAGATION OF CMEs

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ABSTRACT

We present the implementation of turbulence transport equations in addition to the Reynolds-averaged magnetohydrodynamic equations within the Cronos framework. The model is validated by comparisons with earlier findings before it is extended to be applicable to regions in the solar wind that are not highly super-Alfvénic. We find that the respective additional terms result in absolute normalized cross-helicity to decline more slowly, while a proper implementation of the mixing terms can even lead to increased cross-helicities in the inner heliosphere. The model extension allows us to place the inner boundary of the simulations closer to the Sun, where we choose its location at 0.1 AU for future application to the Wang–Sheeley–Arge model. Here, we concentrate on effects on the turbulence evolution for transient events by injecting a coronal mass ejection (CME). We find that the steep gradients and shocks associated with these structures result in enhanced turbulence levels and reduced cross-helicity. Our results can now be used straightforwardly for studying the transport of charged energetic particles, where the elements of the diffusion tensor can now benefit from the self-consistently computed solar wind turbulence. Furthermore, we find that there is no strong back-reaction of the turbulence on the large-scale flow so that CME studies concentrating on the latter need not be extended to include turbulence transport effects.

Key words: magnetohydrodynamics (MHD) – methods: numerical – shock waves – solar wind – Sun: magnetic fields – turbulence

Supporting material: animations

1. INTRODUCTION

In a recent publication (Wiengarten et al. 2014), we presented results for inner-heliospheric solar wind conditions from simulations based on observational boundary conditions derived from the Wang–Sheeley–Arge (WSA; Arge & Pizzo 2000) model. The obtained three-dimensional (3D) configurations provide the basis for subsequent studies of energetic particle transport. For a long time, the standard approach to couple the solar wind dynamics to the transport of charged energetic particles has been to parameterize all transport processes in terms of “background” quantities such as the large-scale solar wind velocity and heliospheric magnetic field strength. This was particularly true for the treatment of spatial diffusion (see, e.g., Potgieter 2013). Only in recent years were so-called ab initio models developed, in which the diffusion coefficients are formulated explicitly as functions of small-scale, low-frequency turbulence quantities such as the magnetic field fluctuation amplitude or the correlation length (e.g., Parhi et al. 2003; Pei et al. 2010; Engelbrecht & Burger 2013). This significant improvement has been possible, on the one hand due to the development of turbulence transport models that, most often, describe the evolution of turbulent energy density, cross-helicity, and correlation lengths for low-frequency turbulence, as observed in the solar wind, with increasing distance from the Sun; see, e.g., the review in Zank (2014). On the other hand, our present-day knowledge about turbulence in the solar wind (see, e.g., the reviews by Matthaeus & Velli 2011; Bruno & Carbone 2013) has increased tremendously since the first measurements (Coleman 1968; Belcher & Davis 1971) thanks to highly sophisticated analyses (e.g., Horbury & Osman 2008; Horbury et al. 2012).

After the pioneering papers by Tu et al. (1984) and Zhou & Matthaeus (1990a, 1990b, 1990c) and the first systematic studies of the radial evolution of turbulence quantities (Zank et al. 1996), major progress has only been achieved in recent years. First, Breech et al. (2008) improved the previous modeling by considering off-ecliptic latitudes. Second, in Usmanov et al. (2011) this turbulence model was extended to full time dependence and three spatial dimensions. In the same paper the turbulence evolution equations were simultaneously solved along with a large-scale magnetohydrodynamic (MHD) model of the supersonic solar wind. While Usmanov et al. (2012, 2014) extended this study further with the incorporation of pickup ions and electrons as separate fluids, as well as an eddy-viscosity approximation to self-consistently account for turbulence driven by shear, Oughton et al. (2011) undertook another extension of the modeling by considering not only one but two, mutually interacting, incompressible components, namely quasi-two-dimensional turbulent and wave-like fluctuations. The effect on turbulence due to changing solar wind conditions in the outer heliosphere during the solar cycle have recently been addressed by Adhikari et al. (2014).

All of the mentioned models have one limitation in common, namely the condition that the Alfvén speed $V_A$ is significantly lower than that of the solar wind $U$, which precludes their application to the heliocentric distance range below about 0.3 AU. The turbulence in this region and its consequences for the dynamics of the solar wind have been studied on the basis of the somewhat simplified transport equations for the wave power spectrum and the wave pressure (e.g., Tu & Marsch 1995; Hu et al. 1999; Vainio et al. 2003; Shergelashvili & Fichtner 2011). The Alfvén speed limitation in the more detailed models was very recently removed with a new, comprehensive approach to the general problem of the
transport of low-frequency turbulence in astrophysical flows by Zank et al. (2012); see also Dosch et al. (2013). Not only are the derived equations formally valid close to the Sun in the sub-Alfvénic regime of the solar wind, but they also represent an extension of the treatment of turbulence by non-parametrically and quantitatively considering the evolution of the so-called energy difference in velocity and magnetic field fluctuations, and by explicitly describing correlation lengths for sunward- and anti-sunward-propagating fluctuations as well as for the energy difference (sometimes also referred to as the residual energy).

In our previous modeling (Wiengarten et al. 2014) we derived inner boundary conditions beyond the Alfvénic critical point at 0.1 AU by means of the WSA model. This approach matches a potential field solution for the coronal magnetic field to the observed photospheric magnetograms, and the resulting magnetic field topology can be linked empirically to the corresponding solar wind speed for every open field line (Wang & Sheeley 1990). We performed simulations of the inner-heliospheric solar wind conditions for several Carrington rotations. Subsequently, the resulting time-dependent 3D configuration is used to study the transport of charged energetic particles by means of stochastic differential equations (A. Kopp 2015, private communication). Within that study, the transport coefficients required for the latter model have so far been estimated from the large-scale quantities provided by the ideal MHD equations (see discussion above). In order to obtain more realistic transport coefficients for the study of propagation of charged energetic particles, we extend our previous modeling by solving the 3D time-dependent turbulence transport equations self-consistently coupled to the Reynolds-averaged MHD equations. Such an approach was taken by Usmanov et al. (2011) and will provide the starting point for our modeling. In a first step we validate our implementation by comparing with these authors’ findings. The turbulence transport equations used there can also be obtained from the more general turbulence transport equations of Zank et al. (2012) by applying respective simplifications. The Usmanov model neglects the Alfvén velocity and is therefore only applicable to highly super-Alfvénic solar wind regimes and we remove this constraint by retaining the respective terms of the derived equations formally valid close to the Sun in the sub-Alfvénic regime of the solar wind, therefore only applicable to highly super-Alfvénic solar wind conditions and we remove this constraint by retaining the respective terms of the derived equations.

The paper is organized as follows. In Section 2 we present the turbulence transport equations and the respective coupling to the ideal MHD equations. Details are outsourced to the Appendix. Section 3 is used to validate our implementation by comparing with the respective results of Usmanov et al. (2011). We present the extensions we apply to the model and demonstrate their effects in Section 4. In Section 5 we move the inner boundary closer to the Sun and show results for both quiet and CME-disturbed cases. We conclude with a summary and an outlook on future improvements in Section 6.

2. EQUATIONS AND CODE SETUP

We follow the approach of Usmanov et al. (2011) to incorporate the evolution equations of small-scale turbulence quantities into the framework of the MHD code Cronos (see Appendix C for details concerning the code). As we will seek to inject CMEs at an inner boundary of 0.1 AU, the assumption of highly super-Alfvénic solar wind conditions is not justifiable everywhere. The turbulence transport equations are extended to keep terms associated with the Alfvén velocity, which can be derived from a simplified model by Zank et al. (2012; see Appendix A), while we employ the coupling between small-scale and large-scale equations as given in Usmanov et al. (2011). The turbulence transport equations for the considered case are then

\[
\begin{align*}
\partial_t Z^2 + \nabla \cdot (UZ^2 + V_i Z^2 \sigma_c) &= \frac{Z^2}{2} (1 - \sigma_0) \nabla \cdot U + 2V_i \cdot \nabla (Z^2 \sigma_c) \\
&+ Z^2 \sigma_0 \hat{B} \cdot \nabla \hat{U} \\
&- \frac{aZ^2}{\lambda} (\sigma_c) + \langle z^+ \cdot S^+ \rangle - \langle z^- \cdot S^- \rangle \\
&- \frac{\partial_i(Z^2 \sigma_c) + \nabla \cdot (UZ^2 \sigma_c + V_i Z^2)}{2} \\
&= \frac{Z^2}{2} \sigma_c \nabla \cdot U + 2V_i \cdot \nabla Z^2 + Z^2 \sigma_0 \nabla \cdot V_i \\
&- \frac{aZ^2}{\lambda} (\sigma_c) + \langle z^+ \cdot S^+ \rangle - \langle z^- \cdot S^- \rangle \\
&\frac{\partial_i(\rho \lambda) + \nabla \cdot (U \rho \lambda)}{\lambda} = \rho \hat{B} [Z^2(\sigma_c) + \langle z^+ \cdot S^+ \rangle(1 - \sigma_c) + \langle z^- \cdot S^- \rangle(1 + \sigma_c)]
\end{align*}
\]

In Section 2 we present the turbulence transport equations and the respective coupling to the ideal MHD equations. Details are outsourced to the Appendix. In Section 3 we validate our implementation by comparing with the respective results of Usmanov et al. (2011). We present the extensions we apply to the model and demonstrate their effects in Section 4. In Section 5 we move the inner boundary closer to the Sun and show results for both quiet and CME-disturbed cases. We conclude with a summary and an outlook on future improvements in Section 6.
with $f^z := \sqrt{1 - \sigma_c^2} \left[ \sqrt{1 + \sigma_c} \pm \sqrt{1 - \sigma_c} \right]$ where the following moments of the Elsässer variables (described below) are used:

$$Z^2 := \frac{\left( z^+ \cdot z^+ \right) + \left( z^- \cdot z^- \right)}{2} = \left( u^2 \right) + \left( b^2 / \rho \right) \quad (4)$$

$$Z^2 \sigma_c := \frac{\left( z^+ \cdot z^+ \right) - \left( z^- \cdot z^- \right)}{2} = 2 \left( u \cdot b / \sqrt{\rho} \right) \quad (5)$$

$$Z^2 \sigma_D := \left( z^+ \cdot z^- \right) = \left( u^2 \right) - \left( b^2 / \rho \right) \quad (6)$$

Here, $Z^2$ is twice the total energy per unit mass of the fluctuations, $\sigma_c$ is the normalized cross-helicity, $\sigma_D$ is the normalized difference between the magnetic and kinetic energy of the fluctuations per unit mass, also known as residual energy. As done in previous studies, we assume an observationally inferred constant value for the energy difference $\sigma_D = -1/3$ (Tu & Marsch 1995) and reserve an extension to include a variable energy difference (Zank et al. 2012) for future studies. Furthermore, $\lambda$ is the correlation length, $V_\parallel = B_0 / \sqrt{\rho}$ is the normalized Alfvén velocity, $\alpha = 2\hat{\theta} = 0.8$ are the Karman–Taylor constants, and terms involving sources of turbulence $S^z$ are discussed in subsequent sections.

The Elsässer variables $z^\pm := u \pm b / \sqrt{\rho}$, where $u$ and $b$ denote the fluctuations about the mean fields $U$ and $B$, describe the inward- ($z^+$) and outward- ($z^-$) propagating modes with respect to the mean magnetic field so that $z^\pm$ is anti-parallel/parallel to it. $B_0$ denotes the unit vector in the direction of the mean magnetic field.

The turbulence transport Equations (1)–(3) are implemented in the framework of the CRONOS code as additional equations to be solved alongside the Reynolds-averaged, normalized ideal MHD equations in the corotating frame of reference with respective coupling terms to account for the effects of turbulence on the large-scale MHD quantities in analogy to Usmanov et al. (2011):

$$\partial_t \rho + \nabla \cdot \left( \rho \mathbf{V} \right) = 0 \quad (7)$$

$$\partial_t \left( \rho \mathbf{U} \right) + \nabla \cdot \left[ \rho \mathbf{V} \mathbf{U} + \rho \mathbf{I} \mathbf{1} - \eta \mathbf{B} \mathbf{B} \right] = -\rho \mathbf{g} + \mathbf{U} \times \mathbf{E} \quad (8)$$

$$\partial_t \mathbf{B} + \nabla \times \left( \mathbf{BV} - \mathbf{VB} \right) = 0 \quad (9)$$

$$\partial_t \mathbf{e} + \mathbf{V} \cdot \left[ c \mathbf{V} + \frac{1}{2} \left( \mathbf{B} \mathbf{B} / 2 + \mathbf{q} \mathbf{n} \right) \mathbf{U} - \left( \mathbf{U} \cdot \mathbf{B} \right) \mathbf{B} - \mathbf{V}_A \rho \mathbf{Z} \mathbf{Z} / 2 + \mathbf{q} \mathbf{n} \right]$$

$$= -\rho \mathbf{g} \cdot \mathbf{U} \cdot \nabla \rho = \left( \frac{Z^2 \sigma_c}{2} V_A \cdot \nabla \rho + \frac{\rho Z^2}{2} \right)$$

$$+ \mathbf{U} \cdot \left( \mathbf{B} \cdot \nabla \right) \left( \eta - 1 \right) \mathbf{B} - \rho \mathbf{V}_A \cdot \nabla \left( Z^2 \sigma_c \right) \quad (10)$$

with $\rho = \left( \rho + \left| \mathbf{B} \mathbf{B} / 2 + \mathbf{p}_c \right| \right)$, $\rho_c = (\sigma_c + 1) \rho Z^2 / 4$ and $\eta = 1 + \sigma_D \rho Z^2 / (2\rho B^2)$ for the considered case of transverse and axisymmetric turbulence. Equations (7)–(9) are identical to those of Usmanov et al. (2011), while the above form of the energy Equation is derived in Appendix B. Furthermore, $\rho$ is the mass density, $\mathbf{U}$ and $\mathbf{V} = \mathbf{U} - \Omega \times \mathbf{r}$ denote the fluid velocity in the rest and corotating frame, respectively, $\mathbf{B}$ is the mean magnetic field, $p$ is the scalar temperature, $\mathbf{g} = (GM_\odot / r^2) \mathbf{e}_z$ describes the Sun’s gravitational acceleration, and $\Omega = \Omega_\odot$ is the Sun’s angular rotation speed with $\Omega = 14.71^d / d$ (Snodgrass & Ulrich 1990). The energy density $\epsilon = \rho U^2 / 2 + B^2 / 2 + \eta / (\gamma - 1)$ is used without both the gravitational potential and the turbulent energy component $\rho Z^2 / 2$, which are instead attributed by means of the right-hand-side source terms in Equation (10); see Appendix B. An adiabatic equation of state is used with $\gamma = 5/3$, while, due to the inclusion of Hollweg’s heat flux (Hollweg 1974, 1976) $q_{\text{fl}} = (3/4)p \mathbf{V}$, the effective value of the adiabatic index $\gamma_{\text{eff}} = 13/9$ is close to observationally inferred values (Totten et al. 1995).

We use spherical coordinates $(r, \theta, \phi)$ with the origin being located at the center of the Sun. Thus, $r$ is the heliocentric radial distance, $\theta \in [0, \pi]$ is the colatitude or polar angle (with the north pole corresponding to $\theta = 0$) and $\phi \in [0, 2\pi]$ is the azimuthal angle.

The above sets of equations are both given in their normalized form, so that for instance no factors of $4\pi$ or $\mu_0$ occur with the magnetic energy density.

CRONOS employs a semi-discrete finite-volume scheme with Runge–Kutta time integration and adaptive time-stepping, allowing for different approximate Riemann solvers. Although we make use of its conservative features by implementing as many terms as possible as divergence of fluxes, a number of source terms remain. In cases where source terms involve differentiation we apply second-order accurate central finite differences. The solenoidality of the magnetic field is ensured via constrained transport, provided the magnetic field is initialized as divergence-free. Besides the code’s support of Cartesian, cylindrical, and spherical (including coordinate singularities) coordinates, it also allows for non-equidistantly spaced grids, e.g., a spatially varying cavity of the Sun, and as long as all coordinate planes remain orthogonal.

3. MODEL VALIDATION

To validate our implementation we compare our results with those of Usmanov et al. (2011). In order to have an equivalent set of equations the following adoptions have to be made to Equations (1)–(3): neglecting the Alfvén velocity and employing only the isotropization of newly born pickup ions as source for turbulence, i.e.,

$$\left\langle z^z \cdot S^z \right\rangle_{\text{pui}} = \frac{E_{\text{pui}}}{2} = \frac{1}{2} \frac{f_D U V_A n_H}{n_0 \tau_{\text{ion}}} \exp \left( -L_{\text{ov}} / r \right). \quad (11)$$

Here, $f_D = 0.25$ is the fraction of pickup-ion energy transferred into excited waves, $n_H = 0.1 \text{ cm}^{-3}$ is the interstellar neutral hydrogen density, $\tau_{\text{ion}} = 10^8 \text{ s}$ is the neutral ionization time at 1 AU, $L_{\text{ov}} = 8 \text{ AU}$ is the characteristic scale of the ionization cavity of the Sun, and $n_w = 5 \text{ cm}^{-3}$ is the solar wind density at 1 AU. Although neglected in the turbulence transport equations, here $V_A = B_0 / \sqrt{\rho}$, and $U$ is the solar wind speed.

The background solar wind results from an untilted dipole configuration for which the boundary conditions at 0.3 AU have been fitted to be close to the ones of Usmanov et al. (2011), as can be seen in Figure 1. Thus we have a tenous and hot high-speed wind at high latitudes, while the equatorial region is occupied by a dense and cold slow-speed solar wind. The magnetic field corresponds to a Parker spiral configuration with a change of sign at the equator, resulting in a flat current-sheet there. The turbulence quantities are set accordingly to
Figure 1. Boundary conditions at 0.3 AU (black lines) in comparison with those of Usmanov et al. (2011; red lines).

Figure 2. Results in meridional slices for (top left to bottom right): magnetic field strength $B$, radial velocity $V_r$, temperature $T$, number density $n$, turbulent energy density $Z^2$, normalized cross-helicity $\sigma_C$, correlation length $\lambda$, and turbulence levels $\delta B/B$. 

higher values in the fast wind, decreasing to smaller values in the slow wind (see also Figure 2 for an overview).

Our boundary conditions approximate those used by Usmanov fairly well except for the transition of the magnetic field at the current sheet, which is much sharper in our case. The radial initialization is also the same as Usmanov’s.

The computational domain in this case covers the radial range from 0.3 to 100 AU with 300 cells of linearly increasing radial cell size $\Delta r \in [10, 230] R_\odot$. Rotational symmetry allows us to use just one active cell (plus ghost cells) covering the azimuth $\phi$, and the polar angle is covered with 180 cells of uniform size. The simulation is advanced in time until a steady state is reached—which is basically the time that the slowest solar wind parcels need to reach the outer boundary. A quantitative comparison with the Usmanov results is presented in Figure 3. Shown are the radial variations of the large-scale quantities in the six left panels and the turbulence quantities in the right panels, respectively taken at colatitudes of $0^\circ$ (solid line), $30^\circ$ (dashed), $60^\circ$ (dotted), and $90^\circ$ (dash-dotted). Note that the red curves are not those shown in Usmanov et al. (2011), but have been obtained from A. Usmanov (2015, private communication) after some differences had been discovered: first, the temperature curve shown in their original paper is in disagreement with the respective curves for number density and pressure. Second, their implementation of the term $\mathbf{B} \cdot (\mathbf{B} \cdot \mathbf{V}) \mathbf{U}$ in spherical coordinates failed to include all geometrical source terms.

Our results are generally in good agreement with the newly obtained reference values, but some small deviations exist that will be addressed when briefly describing the results below: the magnetic field strength (top left) decreases as $1/r^2$ at the poles, where it is purely radial, while for lower latitudes the azimuthal component decreases as $1/r$ becomes dominant. Slight differences with regard to the reference case are present as a result of the different boundary conditions. This is more clearly visible in the panel for the Alfvén velocity (bottom left), however, the asymptotic values are in very good agreement. The total turbulent energy $Z^2$ (top right) decays gradually within about 10 AU, after which the turbulence generation via pickup ions becomes important and flattens the profiles. Since the pickup-ion source term is proportional to $V_A$ there is a latitude dependence resulting in a later onset of profile flattening toward high latitudes. The match between the results is excellent in the high-speed wind region, while the results at the equator beyond 10 AU are off. This is because of our constrained transport scheme involving staggered grids, where the magnetic field is stored on respective cell surfaces and the other quantities at cell centers. The current sheet is implemented best with an even number of cells in polar angle so that there is actually no cell in which $B = 0$. This in turn gives no zero pickup-ion term (by means of a non-vanishing $V_A$ entering), which explains the...
higher values for the total turbulent energy at the equator. The cell-centered quantities are actually located at half-integer values, so that in Figure 3 our results are respectively offset by a half degree from those of Usmanov, which can also be expected to give some minor deviations.

The dissipated energy is transferred into heat so that the temperature (or pressure, related through number density (middle panels)) is higher than would be the case for an adiabatically cooling wind for given $\gamma$. This is also reflected in slightly higher terminal radial velocities (left center), where the equatorial wind is faster than in the reference case because of the dissipated higher turbulent energy as mentioned above. The cross-helicity gives the ratio between inward- and outward-propagating modes. As we have an inwardly directed mean magnetic field in the considered upper hemisphere, only the anti-parallel $\mathbf{z}^\perp$ modes can escape the sub-Alfvénic region below about $20 R_\odot$, so that $C_{\delta}$ is close to unity. As new turbulence—specifically also parallel-propagating modes $\mathbf{z}^\parallel$—are generated in the outer heliosphere the ratio between the modes goes to zero. The interesting feature of increased cross-helicity between 1 and 10 AU is due to the additional mixing term $\mathbf{B} \cdot (\mathbf{B} \cdot \nabla) \mathbf{U}$, which introduces a measure for the efficiency of diffusion between slow and fast solar wind as indicated in Equation (3). The breaks at about 10 AU are again caused by the pickup-ion term, indicating that sources of turbulence tend to decrease the correlation length, which will also be addressed when including shear driving below.

The overview presented in Figure 2 also shows the ratio of turbulent magnetic field to mean magnetic field $\delta B / B$ as an additional quantity, which can be calculated via

$$\delta B^2 = \langle b^2 \rangle = \frac{Z^2}{2} (1 - \sigma_D) \quad (12)$$

for given (constant) $\sigma_D$. This quantity bears great importance for the transport of energetic particles in the heliosphere as it is a measure for the efficiency of diffusion (see, e.g., Manuel et al. 2014). The results show that although the turbulent energy is low in polar regions, the magnetic field strength there diminishes more rapidly and results in high diffusion levels that gradually decrease toward the ecliptic.

4. MODEL EXTENSION

It is stated in Usmanov et al. (2011) that their model does not seem to require additional source terms to account for the effects of turbulence driven by shear. However, as acknowledged in Usmanov et al. (2014), this is not the case. Furthermore, this is also pointed out in Appendix A of Zank et al. (2012), where it is noted that these kind of turbulence transport models do not capture turbulence driven by shear terms due to the imposed structural similarity closure relations, such that instead these terms have to be rationally accounted for via additional source terms. Usmanov et al. (2014) incorporated shear effects with an eddy-viscosity approximation, which we intend to adopt in our implementation for future studies as well. For now we include the required terms in a similar fashion as in Zank et al. (1996) and Breech et al. (2008), but in improvement to these models we compute the gradients in the solar wind speed self-consistently from the background field via

$$\langle \mathbf{C} \cdot \mathbf{S} \rangle_{\mathbf{U}} = \frac{1}{2} \mathbf{Z} \mathbf{C}_{\delta} \left[ \begin{array}{c} \frac{1}{r} \frac{\partial \theta}{\partial \theta} + \frac{1}{\sin(\theta)} \frac{\partial \phi}{\partial \phi} \end{array} \right] |\mathbf{U}|. \quad (13)$$

We use a value of $\mathbf{C}_{\delta} = 0.5$, which is commonly taken at high latitudes (no shear) to match observational results (Breech et al. 2005). Previous studies (e.g., Breech et al. 2008; Engelbrecht & Burger 2013) have estimated typical values for gradients in the solar wind speed and absorbed them in the definition for $\mathbf{C}_{\delta}$ so that it is varying with position. Here, we treat $\mathbf{C}_{\delta}$ as a constant and get an equivalent expression for $\mathbf{C}_{\delta}$ as indicated in Equation (13).

Figure 4 shows a comparison of simulations using the above setup with and without the shear term in meridional slices at different heliocentric distances (solid: 1 AU; dashed: 10 AU). The black (red) lines show the results (not) including the shear term, while the blue lines are taken from Breech et al. (2008). As expected, differences arise mainly in the transition region between slow and fast solar wind (at about 70°–80°), which gives rise to shear. Considering the 1 AU slices (solid lines) first, it can be seen that the shear term leads to (otherwise absent) enhancements in turbulent energy, which are comparable to the enhancements in the Breech results, where the latter are at slightly lower colatitudes due to different modeling of the transition region. Meanwhile, the cross-helicity is now strongly decreased in this region due to the newly generated turbulence, which is also qualitatively visible in the Breech data, who however used lower boundary values for the cross-helicity so that it is initially lower. While the correlation length is enhanced in the Breech model, it is decreasing in the shear region in our model. This is due to our inclusion of the term in the respective Equation (3) for the correlation length, whereas mentioned above with regard to the pickup-ion source term, the generation of turbulence leads to decreased correlation lengths. The shear term is absent in the evolution equation for $\lambda$ in the Breech model, where it is assumed that shear drives turbulence at all scales. As our starting point for the turbulence transport equations is the model by Zank et al. (2012), who include this term also in the correlation length equation, we will maintain it as well. While at 1 AU the resulting temperature enhancement is similar to the one in Breech (different boundary values again cause an overall lower temperature here), the results at larger radial distances show some differences: in our model the turbulent energy just barely peaks at the transition region and the temperature is only slightly enhanced as well, whereas in the Breech model the peak becomes ever more pronounced. This is the result of an interplay between the generation of turbulence due to shear, which weakens with radial distance, and its dissipation controlled by the correlation length. A more detailed study addressing the effect of shear on the correlation length might be in order to clarify proper modeling. We want to
mention though that Ulysses data for solar minimum conditions (plate 6 in McComas et al. 2000) do not seem to show evidence for a strongly enhanced temperature in this region.

The model can be readily extended to include terms involving the Alfvén velocity. We maintain the same boundary conditions as before and the results are compared to the ones neglecting Alfvén velocity in Figure 5. The effect on the large-scale quantities is negligible and, thus, not shown. The turbulence quantities also show only minor differences: the turbulent energy tends to be up to about 1.5 times higher at high latitudes and the correlation length is almost unaffected. Near the equator the results are almost identical for all quantities. The normalized cross-helicity also tends to stay about 10% larger when including the additional terms. These deviations occur close to the inner boundary, where the Alfvén speed is highest, and the resulting higher cross-helicity values are convected to larger radial distances. This effect is expected to be more prominent when moving the inner boundary closer to the Sun, as will be done in the subsequent section. For an inner boundary at about 0.3 AU as considered so far, the neglect of the Alfvén velocity terms is therefore justifiable to some extent, but the effect of enhanced cross-helicity could be incorporated in models neglecting these terms by increasing the boundary values accordingly.

5. APPLICATION TO THE INNER HELIOSPHERE AND TRANSIENT STRUCTURES

The turbulence transport Equations (1)–(3) now also accomodate the effect of shear driving by means of Equation (13) so that the model can be applied to solar wind transients with arbitrary gradients in solar wind speed. In Section 5.2 we apply the above set of equations to a “toy-model” CME and study the results in comparison to the model not including turbulence. Furthermore, including terms involving the Alfvén velocity enables us to move the inner boundary closer to the Sun. In the following the inner boundary is located at 0.1 AU, which is usually just beyond the Alfvén critical radius. This is a suitable choice for the following reasons: (i) The turbulence transport model is only partly appropriate for sub-Alfvénic regions such as the corona or the heliosheath. Specifically, the dissipation terms are subtle to model for low-beta regions and still need to be properly adapted for such cases.
Coronal MHD models are much more complex and are computationally quite expensive. A simplified model of the corona is the WSA model that is frequently used to derive boundary conditions for heliospheric MHD simulations such as in our previous work (Wiengarten et al. 2014) or in the ENLIL code (Odstrcil et al. 2004), which is in operation at the space weather prediction center. Here, the interface between WSA and MHD is usually located at 0.1 AU, so that especially for future purposes, where we will aim to perform the simulations with input from the WSA model, this would be the obvious choice. (iii) When applying our model to interplanetary disturbances such as CMEs, it is desirable to catch as much of their evolution self-consistently, which demands to put the inner boundary as close to the Sun as possible. Given the above caveats, this currently cannot be done in a more self-consistent manner by triggering a reconnection event at the coronal base (as in, e.g., Manchester et al. 2005; Kozarev et al. 2013), but instead an estimate for CME properties at intermediate distances has to be found (see Section 5.2). In what follows the simulation domain is restricted to the radial extent $r \in [0.1, 1.2]$ AU and we do not cover the polar coordinate singularities to avoid small time steps. Therefore, $\theta \in [0.1, 0.9] \pi$. Furthermore, to save computing time the azimuthal extent is restricted to $\varphi \in [\pi, 1.5] \pi$ as the center of the CME will be located at $[\theta_{CME}, \varphi_{CME}] = [0.5, 1] \pi$, and during its subsequent evolution it does not reach the outer azimuthal boundaries in this setup. The applied resolution is $[\Delta r, \Delta \theta, \Delta \varphi] = [0.5 R_S, 1^\circ, 1^\circ]$ corresponding to gridcells per direction as $[N_r, N_{\theta}, N_{\varphi}] = [480, 144, 180]$.

5.1. Quiet Solar Wind

We first describe the quiet background solar wind, into which a CME will be injected. CMEs occur more frequently during periods of solar maximum, which is characterized by a highly tilted current sheet and disappearance of the region of fast polar solar wind, so that instead a slow wind is present at all latitudes. For simplicity, and since we leave out the polar coordinate singularity, we resort to a simple flat current sheet. This also allows us to keep the analysis of the results relatively tractable.

We estimated respective boundary conditions at 0.1 AU for the large-scale quantities from typical values used in our previous work employing the WSA model (Wiengarten et al. 2014). The boundary values and the resulting radial evolution at selected colatitudes are shown in Figure 6 (black lines), where for orientation the findings of Usmanov et al. (2011; red lines) from 0.3 AU onwards are shown as well. The resulting configuration is similar to the equatorial slow-speed region from the previous section but with slightly enhanced speeds, higher temperature, and lower density, while the magnetic field is the same as before. For the turbulent energy

![Figure 6. Results for the quiet solar wind at different colatitudes in the same format as Figure 3.](image-url)
and the correlation length we use boundary values that also
give similar radial profiles as shown previously, but for the cross-helicity it should be assumed that just beyond the
Alfvénic critical radius there are almost only forward-
propagating modes, so that \(|\eta_0|\) should be close to unity and we choose \(|\eta_0|(0.1 \text{ AU}) = 0.95\). As shown above, including
the Alfvén velocity terms in the model tends to retain cross-
helicity values closer to unity, and since there are no additional
sources of turbulence so far the cross-helicity now remains
larger at and beyond 0.3 AU in contrast to the Usmanov values.

5.2. Perturbation by a CME

5.2.1. Initialization

As the computational domain does not extend down to the
corona, where CMEs are thought to be triggered via
reconnection events, we do not use an injection scheme that
inserts out-of-equilibrium flux ropes as done in coronal models
(e.g., Manchester et al. 2005; Kozarev et al. 2013), but we
estimate typical CME properties at the intermediate distance of
\(r_\text{in} = 0.1 \text{ AU}\) from simulations performed by Kleimann et al.
(2009). We find that the shape of the CME in these simulations
remains similar to the initialized one, as was also reported in
previous studies and motivated the Cone model (Zhao et al. 2002),
which is also used to initiate CMEs in the ENLIL setup
(Odstrcil et al. 2004). The almost radial propagation of
CMEs through the corona allows for an easy geometrical
estimation of its properties a few solar radii away from the Sun.
While for space weather forecasting studies such estimates are
based on observations, here we consider a “toy model” with
idealized properties. We first define the normalized angular
distance of a given point \((\theta, \varphi)\) on the spherical inner boundary
to the center of the CME onset site \([\theta, \varphi]_{\text{cme}} = [0.5, 1] \pi\) as

\[
a = \arccos \left[ X_{0,\text{cme}} \sin(\theta) \cos(\varphi) + Y_{0,\text{cme}} \sin(\theta) \sin(\varphi) + Z_{0,\text{cme}} \cos(\theta) \right] / \delta_{\text{cme}},
\]

where \([X, Y, Z]_{0,\text{cme}} = \left[ \sin(\delta_{\text{cme}}) \cos(\varphi_{\text{cme}}), \sin(\delta_{\text{cme}}) \sin(\varphi_{\text{cme}}), \cos(\delta_{\text{cme}}) \right]\) are the Cartesian coordinates of the site’s center,
and \(\delta_{\text{cme}} = \pi/8\) denotes its angular radius. Within this circular
patch characterized by \(a(\theta, \varphi) \approx 1\), we raise the large-scale
fluid quantities during the CME initialization according to
\([v_y, T, n]_{\text{cme}} = [80, 4 \, T, 1.5n_{\text{quiet}} \cos(0.5 \pi \cdot a)] f(\tau)\), so that
the enhancement peaks at the center and decreases toward the
edges of the circular area. For the time dependence we choose a
linearly decreasing function \(f(\tau)\) from maximal values at \(t_{\text{cme}}\)
back to quiet values at \(t_{\text{cme}} + \delta_{\text{cme}}\) with a duration of
\(\delta_{\text{cme}} = 5t_0\), where our normalization value for time \(t_0 = 3191\)
\(\text{s. Furthermore, the onset time } t_{\text{cme}} = 200t_0 \text{ is chosen as such as}
that the initial quiet conditions have reached a steady state.

Although the magnetic field strength could be simply raised as
the other quantities, this would not change the fields
topology (Parker spiral), which we assume to be affected
qualitatively by the CME’s onset. We therefore prescribe an
additional strong \(B_\phi\) component as to get field lines wrapping
around the central region of the CME. To preserve the
solenoidality constraint we directly prescribe the vector

\[
A = A_0 \begin{pmatrix} 0 \\ -B_0r_0^2 \sin(\theta)(\varphi + \Omega/V_r) \\ -B_0r_0 \cos(0.5 \pi \cdot \phi) f(\tau) \end{pmatrix},
\]

where \(A_0\) gives rise to the Parker spiral magnetic field, while
\(A_0\) results in the desired field lines wrapping around the
CME (see Figure 7).

Meanwhile, we leave the turbulence quantities at the quiet
solar wind boundary values. This is probably not a realistic
assumption as the evolution in the sub-Alfvénic region should
have an impact on the turbulence quantities as well. However,
on the one hand there is little to no observational data of
 turbulence associated with CMEs this close to the Sun, and on
the other hand, prescribing respective estimates as boundary
conditions for the turbulence different from the quiet wind ones
would make it more difficult to analyze the self-consistent
evolution of these quantities beyond 0.1 AU, i.e., the influence
of different boundary conditions and the evolution due to the
governing equations would be impossible to disentangle.

5.2.2. Results and Impact on Turbulence Quantities

An overview of the resulting 3D structure is shown in
Figure 7. The field lines show the typical Parker spiral pattern
far away from the CME, while close by they wrap around it.
The CME can be partitioned into a compact central core region
containing the high-speed ejecta and a surrounding sheath
region bounded by a shock driven by the CME. Due to the
wealth in structure involved, we show results in two-
dimensional (2D) slices. First, we present meridional slices at
\(\varphi = \pi\) in Figure 8 so that they coincide with the azimuthal
symmetry axis of the initial CME. The evolution in time is
available as an animation in the supplementary material. Here,
we show an adapted snapshot of the animation at \(t_{\text{cme}} = 32.5t_0\)
after initialization, which is the time at which the sheath region
reaches 1 AU. The core and sheath region are most clearly seen

Figure 7. 3D visualization of the CME with magnetic field lines. The center sphere is the inner boundary, while the computational domain is clipped at the equator and made opaque. The color coding is for radial speed and shows the sheath and core region of the CME (see text), while the whitish opaque shape is the contour of \(V_r = 650 \text{ km s}^{-2}\) that shows the 3D extent of the core region of the CME.

(An animation of this figure is available.)
in the large-scale quantities (top row), but in particular in the radial velocity data, whereas in most of the quantities more complex structures are visible as well. In general, structural variations occur mainly close to or within the elongated core region, while the almost circular sheath region is rather homogeneous in comparison. The sheath region is characterized by modest enhancements compared to the quiet conditions (visible beyond $\approx 1\ AU$) in density and magnetic field strength, while strong enhancements of $v_{r,\text{sheath}} \approx 700\ \text{km}\ \text{s}^{-1}$ and $T_{\text{sheath}} \approx 10^7\ \text{K}$ are found. The turbulent energy is also increased in this region, and also more so than the magnetic field strength, which follows from the visible enhancements in $\delta B/B$. The cross-helicity is slightly reduced, while the correlation length seems to exhibit almost no changes within the sheath region.

The core region partly overlaps with the current-sheet affected equator. The current sheet is not ideally resolved, which would require adaptive mesh refinement, which, however, is not yet available in the Crinos framework. Therefore, close to the current sheet we get strips of increased or depleted values that are overestimated in this model, but this does not affect the results offset from the equator too much.

While the sheath region is clearly discernible and has the same extent in all quantities, the core region is not similar in all quantities. The patch containing the highest velocity values reflects different behavior in the other quantities, where basically two regions can be distinguished: on the one hand there is a compression at the leading edge, also toward higher latitudes, with respective elevations in magnetic field strength, density, and turbulent energy, while on the other hand a rarefaction region trails the core, where depleted values are present. Besides these compressional effects there is clearly a distinct band of high turbulent energy due to shear around the edges of the high-speed central region. Respective structures are also visible in the panels for the correlation length and for the cross-helicity, where the latter is generally speaking closer

Figure 8. Results including turbulence at $t = 32.5 t_0$ after CME injection in meridional slices at $\theta = \pi$.

(An animation of this figure is available.)
to zero in most parts affected by the CME but also shows some additional structure, probably due to the complex magnetic field geometry. Finally, the panel for $\delta B/B$ reveals enhanced values in the sheath and around the core region, while the rarefaction region exhibits reduced turbulence levels. The respective effects on the perpendicular and parallel mean free path of energetic particles is twofold, as the former is proportional to $\delta B/B$, while the latter is antiproportional to it. This can lead to counterintuitive results, where the presence of enhanced turbulence can even facilitate the transport of energetic particles as found by Guo & Florinski (2014) for CIRs.

While the meridional slices are symmetric with respect to the equatorial current sheet, this cannot be expected for azimuthal slices because of the symmetry breaking in the spiral structure of the magnetic field. Figure 9 shows respective results in azimuthal slices at $\theta = 85^\circ$, where this colatitude is chosen in order to show the behavior not directly at the current sheet, whose influence is overestimated in this model. These slices are oriented in accordance with the orientation in Figure 7. From the field lines shown there, it is clear that the magnetic field topology is different at the upper edge of the CME, where the field lines are compressed in a sense according to the initial bending direction of the Parker spiral, as compared to the lower edge where field lines are compressed in a sense opposite to the spiral bend. While many features remain similar to the ones described above for the meridional perspective, there are some additional features due to the symmetry breaking: the core region’s tail is bent toward the lower edge, while the sheath region is rather unaffected, i.e., remains quite symmetric in the hydrodynamic quantities ($V_r, T, n$), but as discussed above the magnetic field compression in the sheath region is stronger at the upper edge, which also affects the turbulence quantities: at the upper edge of the core region there is an additional feature of reduced cross-helicity and enhanced turbulence, which is also reflected by a respective feature in temperature, whereas these structures are absent at the lower edge. A striking azimuthal structure for the diffusion levels is found, as the...
upper edge of the CME including the sheath region there shows relatively small values, while toward the nose and the lower edge the diffusion levels are markedly higher. This represents an intriguing feature for a subsequent study of energetic particle propagation.

To the best of our knowledge the observations of turbulence in or associated with CMEs are rather limited and use data obtained at 1 AU (e.g., Ruzmaikin et al. 2010). The first study that derived quantitative estimates of magnetic turbulence levels near CME fronts was presented by Subramanian et al. (2009). Interestingly our findings are within the limits provided by these estimates.

5.2.3. Impact of Turbulence Quantities on CME

In the previous section we described the impact of disturbances in the large-scale flow via a CME on the turbulence quantities. We now study the effect of the turbulence quantities on the disturbed large-scale flow by comparing the simulations discussed above with simulations where the turbulence is switched off, but the remaining setup is maintained.

We omit showing 2D slices as above since the results remain remarkably similar. Instead, Figure 10 shows radial profiles for the large-scale quantities at $\varphi = \pi$ and colatitudes of 85° (solid lines) and 75° (dashed lines) for the case with (black lines) and without turbulence (red lines). The deviations are very small in almost all regions, but a notable difference is the extent of the sheath region, which is marked, e.g., by the largest temperature values. The additional heating due to enhanced turbulence there results in a slightly more extended sheath region, but the effect can be considered small enough so that it is negligible for general CME propagation studies.

6. SUMMARY AND OUTLOOK

In this paper we presented our implementation of turbulence transport coupled to the Reynolds-averaged ideal MHD equations in the framework of the CRONOS code. We followed the work of Usmanov et al. (2011) and validated our findings by comparing results with these authors’ findings. Their original model was extended to be applicable to regions of solar wind speeds that do not have to greatly exceed the Alfvén speed, which we achieved by simplifying the more general turbulence transport equations of Zank et al. (2012). It was shown that beyond radial distances of 0.3 AU the neglect of such terms is usually justified, but including them results in a slower decrease of normalized cross-helicity values, i.e., the generation of backward-propagating modes is somewhat inhibited. This effect is stronger when moving the inner boundary of the simulations closer to the Sun, where the Alfvén speed is no longer small compared to the solar wind speed. Some additional terms that were inappropriately absent in the Usmanov et al. (2011) model have also been included in the present work: (i) The effect of turbulence driven by shear was introduced via respective ad-hoc terms, whose strength was estimated from comparisons with the work of Breech et al. (2008). Such an ad-hoc approach has to be taken because the structural similarity assumption, commonly made to achieve closure in the turbulence transport equations, prevents the self-consistent formulation of shear driving. Recently, Usmanov et al. (2014) removed this constraint by employing an eddy-viscosity approximation, which we plan to include in the future as well. (ii) The mixing term $\vec{B} \cdot (\vec{B} \cdot \nabla) \vec{U}$ was now correctly implemented, which results in a (latitude-dependent) effect on the normalized cross-helicity, which is now even increasing toward about 10 AU, after which turbulence driven by
TURBULENCE TRANSPORT EQUATIONS

The turbulence transport equations used in Usmanov et al. (2011) can be derived from the more general model of Zank et al. (2012) with the simplifying assumptions of a single correlation length \( \lambda = \lambda_f = \lambda_d/2 \) and a choice of the structural similarity parameters \( a = 1/2, b = 0 \) corresponding to axisymmetric turbulence along the mean magnetic field direction, i.e., \( \hat{\mathbf{a}} = \hat{\mathbf{B}} \). In not neglecting the Alfvén velocity and considering the corotating frame of reference we get from Equations (35), (37), and (38) of Zank et al. (2012):

\[
\partial_t Z^2 + \nabla \cdot \nabla Z^2 + \frac{Z^2}{2} \nabla \cdot \mathbf{U} = -V_A \cdot \nabla \left(Z^2 \sigma_c + Z^2 \sigma_d \nabla \cdot \mathbf{V}_A\right)
\]

\[
= -\frac{2\lambda_f^2}{\lambda_{Zank}} + (z^+ - z^-) + \langle z^+ - z^- \rangle
\]

\[
\partial_t Z^2 + \nabla \cdot \nabla Z^2 + \frac{Z^2}{2} \nabla \cdot \mathbf{U} = -V_A \cdot \nabla Z^2 + \frac{Z^2 \sigma_c}{2} \nabla \cdot \mathbf{U}
\]

\[
= -\frac{2\lambda_f^2}{\lambda_{Zank}} + (z^+ - z^-) + \langle z^+ - z^- \rangle
\]

\[
\partial_t \lambda_{Zank} + \nabla \cdot \nabla \lambda_{Zank} = \frac{2\lambda_f^2}{\lambda_{Zank}^2} \frac{1}{\sqrt{1 - \sigma_c^2}} \pm \frac{1}{\sqrt{1 - \sigma_c^2}} \frac{1}{\lambda_{Zank}^2} \cdot \left(\langle z^+ \cdot S^+ \rangle \pm \langle z^- \cdot S^- \rangle \right) \left(1 + \sigma_c \right)
\]

with \( f^z = \frac{1}{\sqrt{1 - \sigma_c^2}} \left[ \frac{1}{\sqrt{1 + \sigma_c}} \pm \frac{1}{\sqrt{1 - \sigma_c}} \right] \) where the following moments of the Elsässer variables \( z^x \equiv u \pm bf/\sqrt{\rho} (u \text{ and } b \text{ denoting the fluctuations about the mean fields } U \text{ and } B) \) are used:

\[
Z^2 \equiv \langle z^+ \cdot z^+ \rangle + \langle z^- \cdot z^- \rangle
\]

\[
= \langle u^2 \rangle + \langle b^2/\rho \rangle \quad (\equiv E_T)
\]

\[
Z^2 \sigma_c := \langle z^+ \cdot z^- \rangle - \langle z^- \cdot z^- \rangle
\]

\[
= 2 \langle u \cdot b/\sqrt{\rho} \rangle \quad (\equiv E_C)
\]

\[
Z^2 \sigma_d := \langle z^+ \cdot z^- \rangle = \langle u^2 \rangle - \langle b^2/\rho \rangle \quad (\equiv E_D)
\]

where the last equality is to clarify the change of notation from Zank et al. (2012). These authors absorbed a factor of two into the definition of the correlation length \( \lambda_{Zank} = 2\lambda_{dij} \). To make use of the conservative scheme in the CRONOS code we rewrite the above equations in the fashion of \( \partial_X + \nabla \cdot F_X = S_X \). Removing the factor of two in the

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correlation length we obtain

\[ \sigma Z^2 + \nabla \cdot (UZ^2 + V_A Z^2 \sigma_c) = \frac{Z^2(1 - \sigma_c)}{2} \nabla \cdot U + 2V_A \cdot \nabla (Z^2 \sigma_c) + Z^2 \sigma_B \cdot (\hat{B} \cdot \nabla)U \]

\[ - \frac{aZf^+(\sigma_c)}{\lambda} + (\sigma^+ \cdot S^+)^2 + (\sigma^- \cdot S^-)^2 ] (22) \]

\[ \partial_t (Z_2 \sigma) + \nabla \cdot (UZ_2 \sigma + V_A Z_2) = \frac{Z_2 \sigma_c}{2} \nabla \cdot U + 2V_A \cdot \nabla \sigma + Z^2 \sigma_B \cdot \nabla \sigma_A \]

\[ - \frac{aZf^-(\sigma_c)}{\lambda} + (\sigma^+ \cdot S^+)^2 + (\sigma^- \cdot S^-)^2 ] (23) \]

\[ \partial_t (\rho \lambda) + \nabla \cdot (U \rho) = \rho \beta \left[ Z^f + \left( \sigma_c \right) \right] \]

\[ - \frac{\lambda}{\alpha Z^2} \left( (\sigma^+ \cdot S^+)(1 - \sigma_c) + (\sigma^- \cdot S^-)(1 + \sigma_c) \right) \]

Here, we have also made the following adaptions in order to obtain the slightly different dissipation terms used by Usmanov et al. (2011), whose model we use to validate our implementation: involving the Karman–Taylor constants \( a = 2\beta = 0.8 \) in the dissipation terms and neglecting additional factors of \( 1 - \sigma_c \) on the right-hand side of Equation (18) (due to different modeling of this evolution equation, here it is taken from Breech et al. 2008).

On neglecting Alfvén velocity terms and using only the isotropization of newly born pickup ions as source for turbulence, i.e., \( \langle \sigma^+ \cdot S^+ \rangle = E_{\text{ini}}/2 = 0.5 f_s J \nu_{\text{ini}} n_{\text{ini}}/\sigma_0 \tau_{\text{em}} \exp(-L_{\text{em}}/r) \), we arrive at the respective equations used in Usmanov et al. (2011).

APPENDIX B
ENERY EQUATION

The total energy density to be conserved in the coupled MHD—turbulence transport model is

\[ E = \rho U^2/2 + p/(\gamma - 1) + B^2/2 - \rho GM_0/r + B^2/2 \] (25)

accounting for the (rest-frame) kinetic, thermal, magnetic, gravitational, and turbulent energy densities. The resulting conservation equation can be obtained from carrying out a time derivative on (25), which gives after some algebra (see Appendix A of Usmanov et al. 2011)

\[ \partial_t E + \nabla \cdot \left[ VE + U \rho - \eta (U \cdot B)B + q_{\text{in}} \right] = (\sigma^+ \cdot S^+ - \sigma^- \cdot S^-) \rho/2. \] (26)

APPENDIX C
THE CRONOS CODE

The CRONOS code used in this study is a versatile code for the numerical solution of the MHD equations. The code is written in C++ and is fully MPI-parallel. Usage of C++ leads to a high modularity that allows changing core components at runtime or adding new features rather easily.

The code is of second order in space and time. Among the core components are a variety of approximate Riemann solvers that can be chosen by the user according to the model to be simulated. CRONOS solves hydrodynamical (HD) and MHD problems. The corresponding Riemann solvers included in CRONOS are HLL (see Harten et al. 1983), HLLC (HD only, see

\[ \dot{\partial}_t e + \nabla \cdot \left[ Ve + U (p + B^2/2) \right] - (U \cdot B)B + q_{\text{in}} = Q \] (27)

such that on substracting Equation (26) and solving for \( Q \) we obtain

\[ Q = -\partial_t (\rho Z^2/2 - \nabla \cdot \left[ (V (\rho Z^2/2 - \rho GM_0/r) \right] - \nabla \cdot (U p_{\text{in}} - (U \cdot B) B \sigma_B \rho Z^2/(2B^2) \right] \]

\[ + (\sigma^+ \cdot S^+ + \sigma^- \cdot S^-) \rho/2. \] (28)

After some lengthy algebra and involving Equations (1) and (7) this gives

\[ Q = \left[ Z^2 \sigma_c V \cdot V_A - V_A \cdot \nabla (Z^2 \sigma_c) \right] \rho/2 \]

\[ - U \cdot \nabla p_{\text{in}} + U \cdot (B \cdot V) [(\eta - 1) \dot{B} + \rho Z^2/(\eta 2) \]

\[ + \frac{\lambda}{\alpha Z^2} \left( (\sigma^+ \cdot S^+)(1 - \sigma_c) + (\sigma^- \cdot S^-)(1 + \sigma_c) \right) \]

\[ \dot{Q} = -\partial_t (\rho Z^2/2 - \nabla \cdot \left[ (V (\rho Z^2/2 - \rho GM_0/r) \right] - \nabla \cdot (U p_{\text{in}} - (U \cdot B) B \sigma_B \rho Z^2/(2B^2) \right] \]

\[ + (\sigma^+ \cdot S^+ + \sigma^- \cdot S^-) \rho/2. \] (29)

where we also used the vector identity

\[ U \cdot (B \cdot (\eta - 1) \dot{B}) = (V \cdot (\eta - 1) \dot{B} + (B \cdot \dot{B} - U \cdot \dot{B}) \]

\[ (30) \]

Finally, on extracting a flux term viz.

\[ \left[ Z^2 \sigma_c V \cdot V_A - V_A \cdot \nabla (Z^2 \sigma_c) \right] \rho/2 \]

\[ - \rho \lambda \sigma_c V_A \cdot \nabla \rho/2 \]

\[ \left[ Z^2 \sigma_c V \cdot V_A - V_A \cdot \nabla (Z^2 \sigma_c) \right] \rho/2 \]

\[ (31) \]

and adding Hollweg’s heat flux (Hollweg 1974, 1976) we get the final equation

\[ \partial_t e + \nabla \cdot \left[ eV + (\rho + |B|^2/2) \right] U \]

\[ - (U \cdot B)B - V_A \sigma_B \rho Z^2/(\eta 2) + q_{\text{in}} \]

\[ = -\rho V \cdot g - U \cdot \nabla \rho_{\text{in}} + Z^2 \sigma_c V_A \cdot \nabla \rho + \frac{\lambda}{\alpha Z^2} \left( \sigma^- \cdot S^- \right) \]

\[ + U \cdot (B \cdot V) [(\eta - 1) \dot{B}] - \rho V_A \cdot \nabla (Z^2 \sigma_c). \] (32)
Toro et al. 1994), and HLLD (MHD only, see Miyoshi & Kusano 2005).
For MHD simulations the solenoidality of the magnetic field is ensured by using constrained transport (see Brackbill & Barnes 1980, who first applied it to MHD). For the HLL solver the numerical electric field computation is consistently implemented as described in Kissmann & Pomoell (2012; see also in Londrillo & del Zanna 2000, 2004; Ziegler 2011). For the HLLD we implemented the electric field computation as described in Gardiner & Stone (2014), who showed that a computation via a direct averaging of the fluxes resulting from the conservative form of the MHD equations can lead to instabilities.

Since CRONOS is optimized for highly compressible flows, the second-order reconstruction employs slope limiters that can be chosen by the user. Other limiters can be added easily to the simulation framework. Numerical problems are solved on an orthogonal grid, where Cartesian, cylindrical, and spherical coordinates are supported. For such a grid the cell size can be varied along each coordinated direction. The grid is specified by the user and is not changed during the simulation.

The code is used by supplying a simulation module that contains all relevant information for the simulation setup. Apart from the initial conditions, e.g., additional forces can be defined by the user. A feature extensively used in the present study is the option to solve other hyperbolic partial differential equations simultaneously with the system of MHD equations. For this, the specific fluxes of the additional differential equations can also be specified within the user module. In a similar fashion, other types of differential equations can be handled in parallel to the main solver by supplying the corresponding alternative solver. CRONOS offers a standard interface to specify the alternative solver. For the solution in parallel to the main solver an operator-splitting approach is implemented.

The CRONOS code has been applied in a range of different studies ranging from stellar wind simulations to accretion disc models (see Flaig et al. 2011). Verification of the code was done in the context of the different studies. In particular the numerical papers Kissmann et al. (2009) and Kissmann & Pomoell (2012) show that various HD and MHD standard problems are solved correctly by the code.

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4.3 Further development

As described in more detail in the following chapter, there has been a development after discussions with S. Oughton suggesting that the choice of structural similarity parameters for 2D axisymmetric turbulence stated by Zank et al. (2012) might be incorrect, and should be $a = b = 1/2$ instead of $a = 1/2, b = 0$. Since the model presented here was derived in simplifying the respective equations with the latter choice, the severity of the error thus made is investigated and revised results are presented. However, it turned out that the topological changes are small and to some extent even negligible.

Figure 4.2: Comparison of large-scale MHD quantities during a CME passage between the cases $b = 0$ (red lines) and $b = 1/2$ (black) in the same format as Figure 10 in W15, i.e. at two different co-latitudes of $75^\circ$ (dashed) and $85^\circ$ (solid).

The revised set of equations is obtained in analogy with Appendix A and B of W15, but now for $b = 1/2$ and using Equation (5.10) as motivated in the next chapter. This gives an additional term (fourth term on right hand side) in the evolution
4.3. FURTHER DEVELOPMENT

equation for the cross-helicity

$$
\frac{\partial}{\partial t}(Z^2\sigma_C) + \nabla \cdot (U Z^2\sigma_C + V_A Z^2) = \frac{Z^2\sigma_C}{2} \nabla \cdot U + 2V_A \cdot \nabla Z^2 + Z^2\sigma_D \nabla \cdot V_A
$$

$$
+ 2b \frac{Z^2\sigma_D}{\sqrt{\rho}} \hat{B} \cdot (\hat{B} \cdot \nabla)\hat{B} - \frac{\alpha Z^3 f^-(\sigma_C)}{\lambda}
$$

$$
+ \langle z^+ \cdot S^+ \rangle - \langle z^- \cdot S^- \rangle, \quad (4.1)
$$

while the remaining turbulence transport as well as large-scale MHD equations remain unchanged on keeping $a = 1/2$.

Figure 4.3: Meridional contour plots of large-scale MHD and turbulence quantities for $b = 1/2$ in the same format as Figure 8 in W15.

As the additional term is proportional to the Alfvén-velocity, it drops out for the model validation performed in Section 3 of W15, which neglected such terms for the case $||U|| \gg ||V_A||$ valid beyond some 0.3 AU of heliocentric distance. The term would have appeared in the following Section 4 of W15 though, where the model was extended. However, as the extended model was first applied to regimes of highly
super-Alfvénic winds too, where these terms have little effect, the additional term hardly changed the results at all so that they are not shown here.

It becomes more interesting for the simulations of the very inner heliosphere including a CME (Section 5 in W15), as here the Alfvén speed is not negligible compared to the solar wind speed. Figures 4.2 and 4.3 show the newly obtained results, which are in the same format as Figures 10 and 8 in W15, respectively. The line plots compare the large-scale MHD quantities only, and there is obviously almost no change at all. This is in agreement with the findings in W15 that the turbulence quantities have little to no effect on the large-scale flow, so that small changes in the turbulence quantities are even less recognizable in the large-scale quantities. The contour plots also remain remarkably similar, but on close inspection the absolute values of the turbulence quantities have changed noticeably, so that Figure 4.4 shows normalized differences for the turbulence quantities calculated via \( \frac{X_{1/2}}{X_0} - 1 \cdot 100 \), where \( X \) stands for the respective quantity with the subscripts denoting the value of \( b \), and the resulting value is in per cent. It can be seen that the total turbulent energy density is about 35% lower away from the CME, while close-by changes are much smaller (about 1%). This transfers directly to \( \delta B/B \) as well, where the difference is only about 20% though. Also, the (absolute) cross helicity is about 10% lower, but can spike within the CME, and the correlation length is about 20% larger.

It can be concluded that the additional term has quite an effect in the very inner heliosphere, but not beyond some 0.3 AU. However, especially since the results directly at the CME are only slightly affected, the general findings presented in W15 remain valid.
4.4 Addendum - Conservative treatment of the co-rotating frame of reference

It is often desirable to perform the simulations in a co-rotating frame of reference to simplify boundary conditions. Implementing the resulting fictitious (Coriolis-, centrifugal-, and Euler) forces as source terms can lead to instabilities and non-conservation of angular momentum (Kley, 1998; Mignone et al., 2012), in particular for large heliocentric distances, because the azimuthal velocity component increases linearly with distance. The force terms can, however, be partially included in the time derivative and flux function of the hyperbolic momentum equation, which amounts to a quasi-conservative treatment and results in the following set of equations. These are equivalent to the original ideal MHD equations with fictitious forces as source terms, such that the new set

\[
\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho v) = 0 \tag{4.2}
\]

\[
\frac{\partial}{\partial t} (\rho u) + \nabla \cdot \left[ \rho vu + (p + \|B\|^2/2)\mathcal{I} - BB \right] = -\rho \Omega \times u \tag{4.3}
\]

\[
\frac{\partial}{\partial t} e + \nabla \cdot \left[ e v + (p + \|B\|^2/2)u - (u \cdot B)B \right] = 0 \tag{4.4}
\]

replaces Eqs. (1.1–1.3), and Ohm’s law (1.6) is now

\[
E + v \times B = 0 . \tag{4.5}
\]

Here, \( v \) denotes the velocity in the co-rotating frame, which is related to the inertial frame velocity \( u \) via

\[
v = u - \Omega \times r . \tag{4.6}
\]

This can be derived as follows: using the latter relation and the vector identities

\[
\nabla \cdot (FG) = G \nabla \cdot F + (F \cdot \nabla)G, \quad (F \cdot \nabla)(\Omega \times r) = \Omega \times F,
\]

where \( F \) and \( G \) are arbitrary vectors, and \( \nabla \cdot (\Omega \times r) = 0 \), it can be shown that

\[
\frac{\partial}{\partial t} (\rho v) + \nabla \cdot [\rho vv] + 2\rho \Omega \times v + \rho \Omega \times (\Omega \times r) = \frac{\partial}{\partial t} (\rho u) + \nabla \cdot [\rho vu] + \rho \Omega \times u , \tag{4.7}
\]

so that the non-conservative momentum equation is reproduced. On using Equation (4.3) one gets for the time derivative of the inertial frame total energy

\[
e = p/(\gamma - 1) + \rho \|u\|^2/2 + \|B\|^2/2
\]

the above energy equation

\[
\frac{\partial}{\partial t} e + \nabla \cdot \left[ e v + (p + \|B\|^2/2)u - (u \cdot B)B \right] = 0 \tag{4.8}
\]

instead of the time derivative of the co-rotating frame total energy

\[
e = p/(\gamma - 1) + \rho \|v\|^2/2 + \|B\|^2/2,
\]

which yields

\[
\frac{\partial}{\partial t} e + \nabla \cdot \left[ (e + p + \|B\|^2/2)v - (v \cdot B)B \right] = \\
- v \cdot (2\rho \Omega \times v + \rho \Omega \times (\Omega \times r)) . \tag{4.9}
\]
Chapter 5

Extended turbulence transport model

The next step towards a more sophisticated turbulence transport model is taken by implementing the full set of equations as given by Zank et al. (2012), which now also involves a variable energy difference $\sigma_D$, as well as a corresponding correlation length $\lambda_D$ and separate correlation lengths for the forward and backward propagating modes $\lambda^\pm$. Section 5.1 describes the necessary alterations to the original equations in order to be implemented in the CRONOS framework for a more adequate formulation exploiting the conservative features of the code. The implementation is validated in Section 5.2 by comparing with the work of Adhikari et al. (2015), who applied a number of simplifications, however. After successful validation, it is then possible to extend the model further by considering additional terms that have been left out thus far (Section 5.3).

5.1 Model formulation

In analogy with the previous chapter, these equations are reformulated in the co-rotating frame of reference. The assumed symmetry of the turbulence is arbitrary for now by maintaining the general form of the structural similarity parameters $a, b$. Furthermore, instead of the evolution equations for the correlation lengths $\lambda_D$ and $\lambda^\pm$, it was found that the corresponding equations for the integral scales defined as

\[
L^\pm \equiv \lambda^\pm Z^2 (1 \pm \sigma_C)
\quad \text{and} \quad
L_D \equiv \lambda_D Z^2 \sigma_D
\]

are numerically better suited and are used for the computations. This was found to be particularly the case for $L_D$, because in some cases $\lambda_D \to \infty$ while $\sigma_D \to 0$ (see Figure 5.3). The turbulence transport equations solved in CRONOS can then
be written as

\[ \partial_t Z^2 + \nabla \cdot (VZ^2 + V_A Z^2 \sigma_C) = (Z^2/2) \nabla \cdot U + 2V_A \cdot \nabla (Z^2 \sigma_C) 
- (2a - 1/2)Z^2 \sigma_D \nabla \cdot U 
+ 2aZ^2 \sigma_D \hat{n} \cdot (\hat{n} \cdot \nabla)U 
- Z^3 \sqrt{1 - \sigma_C^2} \left[ \frac{\sqrt{1 + \sigma_C}}{\lambda^+} + \frac{\sqrt{1 - \sigma_C}}{\lambda^-} \right] 
+ (z^+ \cdot S^+) + (z^- \cdot S^-) \]  

(5.2)

\[ \partial_t (Z^2 \sigma_C) + \nabla \cdot (VZ^2 \sigma_C + V_A Z^2) = (Z^2 \sigma_C/2) \nabla \cdot U + 2V_A \cdot \nabla Z^2 
+ Z^2 \sigma_D \nabla \cdot V_A 
+ (2bZ^2 \sigma_D/\sqrt{\rho}) \hat{n} \cdot (\hat{n} \cdot \nabla)B 
- Z^3 \sqrt{1 - \sigma_C^2} \left[ \frac{\sqrt{1 + \sigma_C}}{\lambda^+} - \frac{\sqrt{1 - \sigma_C}}{\lambda^-} \right] 
+ (z^+ \cdot S^+) - (z^- \cdot S^-) \]  

(5.3)

\[ \partial_t (Z^2 \sigma_D) + \nabla \cdot (VZ^2 \sigma_D) = (Z^2/2)(\sigma_D - 4a + 1) \nabla \cdot U 
- Z^2 \sigma_C \nabla \cdot V_A + 2aZ^2 \hat{n} \cdot (\hat{n} \cdot \nabla)U 
- (\sigma_C V_A \cdot \nabla Z^2 - V_A \cdot \nabla (Z^2 \sigma_C)) \sqrt{1 - \sigma_C^2} 
- (2bZ^2 \sigma_C/\sqrt{\rho}) \hat{n} \cdot (\hat{n} \cdot \nabla)B 
- Z^3 \sigma_D \left[ \frac{\sqrt{1 + \sigma_C}}{\lambda^+} + \frac{\sqrt{1 - \sigma_C}}{\lambda^-} \right] 
+ (z^- \cdot S^+) + (z^+ \cdot S^-) \]  

(5.4)

\[ \partial_t (\rho L^\pm) + \nabla \cdot (V \rho L^\pm) = \rho \left[ \pm \nabla \cdot V_A + \nabla \cdot (U/2 \pm V_A) \right] L^\pm 
- ((a - 1/4) \nabla \cdot U \mp \nabla \cdot V_A/2) L_D 
+ (a \hat{n} \cdot (\hat{n} \cdot \nabla)U 
\pm (b/\sqrt{\rho}) \hat{n} \cdot (\hat{n} \cdot \nabla)B \right] L_D \]  

(5.5)

\[ \partial_t (\rho L_D) + \nabla \cdot (V \rho L_D) = -\rho \left[ \nabla \cdot (\nabla L_D/2) + \nabla \cdot V_A (L^+ - L^-) 
+ \sqrt{L^+ - L_D} \nabla L^- - \sqrt{L^- - L_D} \nabla L^+ 
+ [(2a - 1/2) \nabla \cdot \nabla \cdot U 
- 2a \hat{n} \cdot (\hat{n} \cdot \nabla)U](L^+ + L^-) 
+ (2b/\sqrt{\rho}) \hat{n} \cdot (\hat{n} \cdot \nabla)B \right] [L^+ - L^-] \]  

(5.6)

As some of the involved quantities have been introduced in the previous chapter already, there are a few repetitions in what follows in order to have a complete description of the model here.

The Elsässer variables are \( z^\pm := u \pm b/\sqrt{\rho} \) with \( u \) and \( b \) denoting the fluctuations about the mean inertial velocity \( (U) \) and magnetic \( (B) \) fields, while \( \rho \) is the mass density and all quantities and equations are given in their normalized form. The
following moments of the Elsässer variables are used above:

\[ Z^2 := \frac{1}{2} (z^+ \cdot z^+) + (z^- \cdot z^-) = \langle u^2 \rangle + \langle b^2 / \rho \rangle \]

(5.7)

\[ Z^2 \sigma_C := \frac{1}{2} (z^+ \cdot z^+) - (z^- \cdot z^-) = 2 \langle u \cdot b / \sqrt{\rho} \rangle \]

(5.8)

\[ Z^2 \sigma_D := (z^+ \cdot z^-) = \langle u^2 \rangle - \langle b^2 / \rho \rangle \]

(5.9)

Thus, \( Z^2 \) is twice the total (kinetic plus magnetic) energy per unit mass of the fluctuations, \( \sigma_C \) is the normalized cross-helicity, and \( \sigma_D \) is twice the normalized energy difference in the fluctuations per unit mass, also known as residual energy. Furthermore, \( V_A = B / \sqrt{\rho} \) is the Alfvén velocity, and terms involving sources of turbulence \( S^\pm \) are discussed in subsequent sections. Note that the dissipation term (second last line) in the equation for \( Z^2 \sigma_D \) is not the one used by Zank et al. (2012) (based on a model of Müller and Grappin (2005)), but the ones introduced by Dosch et al. (2013), which has also been used in Adhikari et al. (2015), because the original dissipation term was found to lead to unphysical results both in the present setup as well as in others (N. Pogorelov, priv. comm.).

The terms involving the structural similarity parameter \( b \) in the original equations of Zank et al. (2012) have been rewritten above (S. Oughton, priv. comm.) on using the identity

\[ 2 \nabla \cdot V_A + \frac{1}{\rho} \{ V_A \cdot \nabla \rho - (\hat{n} \cdot V_A)(\hat{n} \cdot \nabla \rho) \} = 2\hat{n} \cdot (\hat{n} \cdot \nabla) V_A - \frac{2}{\sqrt{\rho}} \hat{n} \cdot (\hat{n} \cdot \nabla) B , \]

(5.10)

which follows from using the product rule on \( V_A = B / \sqrt{\rho} \) via

\[ \hat{n} \cdot (\hat{n} \cdot \nabla) V_A = \frac{1}{\rho} \hat{n} \cdot (\hat{n} \cdot \nabla) B - \frac{1}{2\rho} (\hat{n} \cdot V_A) (\hat{n} \cdot \nabla) \rho \]

(5.11)

combined with

\[ 2 \nabla \cdot V_A = -\frac{1}{\rho} V_A \cdot \nabla \rho . \]

(5.12)

Equation (5.10) can be applied to Equations (42) and (43) in Zank et al. (2012) for the energy density of the forward and backward propagating modes \( z^\pm \), which allows for a direct comparison with the corresponding Equations (21) and (22) of Matthaeus et al. (1994). On performing this comparison, it becomes obvious that the case \( a = b = 1/2 \) corresponds to 2D axisymmetric turbulence, while Zank et al. (2012) states that \( a = 1/2, b = 0 \) in that case. Regardless of this, the axisymmetry is usually imposed along the direction of the mean magnetic field so that \( \hat{n} = \hat{B} \). For isotropic turbulence, \( a = 1/3, b = 0 \) holds, while \( \hat{n} = 0 \) in this case, which, however, is not considered in the following.
The turbulence transport Equations (5.2) – (5.6) are implemented in the framework of the CRONOS code as additional equations to be solved alongside the Reynolds-averaged MHD equations in the co-rotating frame of reference with respective coupling terms to account for the effects of turbulence on the large-scale MHD quantities (see Wiengarten et al., 2015, (W15)):

\begin{align*}
\partial_t \rho + \nabla \cdot (\rho \mathbf{V}) &= 0 \\
\partial_t (\rho \mathbf{U}) + \nabla \cdot [\rho \mathbf{VU} + \bar{p} \mathbf{1} - \eta \mathbf{BB}] &= -\rho (\mathbf{g} + \Omega \times \mathbf{r}) \\
\partial_t \mathbf{B} + \nabla \cdot [\mathbf{VB} - \mathbf{BV}] &= 0 \\
\partial_t e + \nabla \cdot [e \mathbf{V} + (p + |\mathbf{B}|^2/2) \mathbf{U} - (\mathbf{U} \cdot \mathbf{B}) \mathbf{B} - \mathbf{V}_A \rho Z^2 \sigma_C/2 + q_H] &= -\rho \mathbf{V} \cdot \mathbf{g} - \mathbf{U} \cdot \nabla p_w - \frac{Z^2 \sigma_C}{2} \mathbf{V}_A \cdot \nabla \rho - \rho \mathbf{V}_A \cdot \nabla (Z^2 \sigma_C) \\
&+ \frac{\rho}{2} Z^3 \sqrt{1 - \sigma_C^2} \left[ \frac{\sqrt{1 + \sigma_C}}{\lambda^+} + \frac{\sqrt{1 - \sigma_C}}{\lambda^-} \right] \\
&+ \mathbf{U} \cdot (\mathbf{B} \cdot \nabla) [(\eta - 1) \mathbf{B}] + \rho Z^2 \sigma_D (a - 1/2) \nabla \cdot \mathbf{U}
\end{align*}

with \( \bar{p} = (p + |\mathbf{B}|^2/2 + p_w) \), \( p_w = (\sigma_D + 1)\rho Z^2/4 \) and \( \eta = 1 + \sigma_D \rho Z^2/(2B^2) \) for transverse and axisymmetric turbulence, while \( p_w = (\sigma_D + 3)\rho Z^2/12 \) and \( \eta = 1 \) for isotropic turbulence. Equations (5.13) – (5.16) are equivalent to those of W15, while the energy equation now also retains the structural similarity parameter \( a \). Furthermore, \( \mathbf{V} = \mathbf{U} - \Omega \times \mathbf{r} \) is the fluid velocity in the co-rotating frame, \( p \) is the scalar thermal pressure, \( \mathbf{g} = (GM_\odot/r^2)\mathbf{\hat{r}} \) is the solar gravitational acceleration, and \( \Omega = \Omega_e \) is the Sun’s angular rotation velocity with \( \Omega = 14.71^\circ/d \) (Snodgrass and Ulrich, 1990). \( e = \rho \mathbf{U}^2/2 + B^2/2 + p/(\gamma - 1) \) is the energy density without the turbulent energy component \( \rho Z^2/2 \), which is instead included by means of the source terms in Equation (5.16). An adiabatic equation of state is used with \( \gamma = 5/3 \) while, due to the inclusion of Hollweg’s heat flux (Hollweg, 1974, 1976) \( q_H = (3/4)p \mathbf{V} \), the effective value of the adiabatic index (see also Usmanov et al., 2011) is \( \gamma_{eff} = 13/9 \), which is close to observationally inferred values.

### 5.2 Model validation

In W15 the code was validated by comparing with the results of Usmanov et al. (2011), who solved a reduced set of turbulence transport equations alongside the Reynolds-averaged MHD quantities. As the coupling of the turbulence to the MHD equations from my previous work is retained, only the implementation of the new extended set of turbulence transport equations (5.2) – (5.6) had to be validated. These equations have been solved numerically by Adhikari et al. (2015), where the calculations were restricted to the ecliptic plane \( \vartheta = \pi/2 \), neglected Alfvén velocity for the outer heliosphere calculations, constant solar wind velocity \( \mathbf{U} = 400 \text{km/s} \mathbf{\hat{r}} \), and the shear-mixing term \( \mathbf{B} \cdot (\mathbf{B} \cdot \nabla) \mathbf{U} \) was left out. Furthermore, the structural similarity parameters were adopted as \( a = 1/2, b = 0 \) in that work. Therefore, to
5.2. MODEL VALIDATION

validate the implementation these simplifying assumptions are also taken for now. In accordance with Adhikari et al. (2015) the following expressions for the turbulence source terms due to stream shear and isotropization of pickup ions are used:

\[
\langle z^+ \cdot S^+ \rangle = C_{\text{sheat}} \frac{\Delta U_{\text{sheat}}}{r} Z^2 (1 + \sigma_C) + \frac{\dot{E}_{\text{pui}}}{2} (5.17)
\]

\[
\langle z^- \cdot S^- \rangle = C_{\text{sheat}} \frac{\Delta U_{\text{sheat}}}{r} Z^2 (1 - \sigma_C) + \frac{\dot{E}_{\text{pui}}}{2} (5.18)
\]

\[
\langle z^- \cdot S^+ \rangle + \langle z^+ \cdot S^- \rangle = 2C_{\text{sheat}} \frac{\Delta U_{\text{sheat}}}{r} Z^2 \sigma_D (5.19)
\]

with a tuning factor \( C_{\text{sheat}} = 7.25 \), the difference between fast and slow speed streams at 0.29 AU is \( \Delta U_{\text{sheat}} = 350 \) km/s and

\[
\dot{E}_{\text{pui}} = \frac{f_D n_H U A}{n_{sw} \tau_{\text{ion}}} \exp \left( -\frac{L_{\text{cav}}}{r} \right) (5.20)
\]

where \( f_D = 0.25 \) is the fraction of pickup ion energy transferred into excited waves, \( n_H = 0.1 \) cm\(^{-3}\) is the interstellar neutral hydrogen density, \( \tau_{\text{ion}} = 10^6 \) s is the neutral ionization time at 1 AU, \( L_{\text{cav}} = 8 \) AU is the characteristic scale of the ionization cavity of the Sun, and \( n_{sw} = 5 \) cm\(^{-3}\) is the solar wind density at 1 AU adopted in this model. Although neglected in the governing equations, \( V_A = 50 \) km/s here. The fixed inner boundary values are \( Z_0^2 = 7134 \) (km/s)\(^2\), \( \sigma_{C,0} = 0.9 \), \( \sigma_{D,0} = -0.004 \), \( \lambda_{D,0} = 0.0204 \) AU, \( \lambda_{0}^+ = 0.000779 \) AU and \( \lambda_{0}^- = 0.00143 \) AU. Note: Adhikari et al. (2015) use a different definition for the cross-helicity (see Equation (10) there) resulting in a positive cross-helicity for a positive (outwardly directed) radial magnetic field. Here, an inwardly directed field with the usual definition for cross-helicity as given above is adopted, thus also getting positive cross-helicity values. However, the associated correlation lengths have to be reversed, i.e. \( \lambda^\pm = \lambda_{\text{Adhikari}}^\mp \).

The computational domain covers the radial range from 0.29 AU to 100 AU with 2400 cells of increasing radial cell size \( \Delta r \in [0.4, 43] \) \( R_C \). This extremely high resolution in particular at the inner boundary was necessary to retain a stable solution due to the imposed strong shear terms. Rotational symmetry allows to use just one cell covering the azimuth \( \varphi \), and since for this test case the Alfvén velocity (and, thus, the magnetic field) is neglected, there is also no preferred direction along the polar angle, so that a fairly low resolution can be applied in \( \vartheta \). Steep gradients near the inner boundary due to large dissipation terms require (global) time-steps that have to be considerably smaller than the usual constraint of the CFL condition calculated from the smallest cell-size and the characteristic velocities \( v_c \) there. While usually a value of \( \text{cfl}_{\text{thresh}} = 0.4 \) can be chosen in \( dt = \text{cfl}_{\text{thresh}} \cdot \min(\Delta x_i/v_c) \) it was necessary to reduce it to \( \text{cfl}_{\text{thresh}} = 0.03 \). Such a time-step constraint can also be computed self-consistently with methods such as sub-cycling, where several sub-steps for the source terms are taken in-between a larger MHD time-step. However, since a time-step reduction was found only to be necessary in the first few inner radial cells, it
was chosen to increase $c f_l_{\text{thresh}}$ after a steady state was reached in these cells, which takes a relatively short time only.

Figure 5.1: Comparison of my results (black curves) with Adhikari et al. (2015) (red) for the turbulent energy $Z^2$ (top left), the normalized cross-helicity $\sigma_C$ (top right), turbulent energy density for forward and backward propagating modes $z^\pm$ (left center) and respective correlation lengths $\lambda^\pm$ (right center), the residual energy $\sigma_D$ (bottom left) and its correlation lengths $\lambda_D$ (bottom right).

The results (black lines) and the reference solution of Adhikari et al. (2015) (red lines) are shown in Figure 5.1 for the turbulent energy density $Z^2$, the normalized cross-helicity $\sigma_C$, turbulent energy density for forward and backward propagating modes $z^\pm$ and respective correlation lengths $\lambda^\pm$, residual energy $\sigma_D$ and its correlation length $\lambda_D$. The turbulent energy dissipates with increasing radial distance, and is transferred into heat (temperature not shown here). The rate of dissipation is controlled by the correlation lengths $\lambda^\pm$. Because of the low boundary values of the latter, the initial dissipation is very strong. In the outer heliosphere beyond the ionization cavity turbulence is generated by isotropization of pickup ions and the turbulent energy density becomes almost constant. The cross-helicity gives the ratio of forward ($z^+$) to backward ($z^-$) propagating modes, where the orientation is anti-parallel to the mean magnetic field. Thus, for an inwardly directed mean magnetic field, only backward propagating modes can escape the sub-Alfvénic solar wind regime below the Alfvén critical point, and the cross-helicity $\sigma_C \lesssim 1$ towards
the inner boundary. With the generation of turbulence in the supersonic solar wind, also forward propagating modes are generated and equipartition is reached with increasing radial distance, i.e. $\sigma_C \to 0$ and $z^+ = z^-$. The residual energy gives the difference between the kinetic and magnetic fluctuations’ strength. In case of equipartition the turbulence is called Alfvénic and $\sigma_D \approx 0$. An interesting result of Adhikari et al. (2015) is that the magnetic fluctuations become increasingly dominant out to about 10 AU, whereas beyond this point the fluctuations become more Alfvénic again. The correlation lengths control the rate of dissipation of turbulent energy. The correlation length of the forward propagating modes $\lambda^-$ is initially longer (i.e. the dissipation is weaker) than for the backward propagating modes, because the backward modes contain the higher energy. With increasing radial distance and turbulence generation the correlation lengths both rise gradually and become equal beyond about 10 AU due to the equipartition of the respective modes. The correlation length of the residual energy is steadily increasing, gradually out to 10 AU and more rapidly thereafter, as the residual energy tends toward zero, and increasingly less energy is ‘dissipated’ into the energy difference.

The excellent agreement between my results and the reference values demonstrates the correct implementation, so that it can now be proceeded to include additional terms left out thus far.

5.3 Model extensions

The calculations can easily be extended on the basis of the general equations of the previous section that have been fully implemented. In the following, the general effects of including these terms are demonstrated. For a sophisticated tuning of the parameters (boundary conditions, strength of the shear and pickup ion driving) a thorough comparison with spacecraft data would be required. This could not be achieved during the work for this thesis, but it should be a mandatory next step.

An arguable approach was taken by Adhikari et al. (2015) concerning the shear driving (Equations (5.17)–(5.18)), as the chosen form for the shear- generated turbulence is respectively proportional to the forward and backward propagating modes, so that in this case the initially stronger backward propagating modes are further enhanced. This leads to the initial increase in the cross-helicity (top right panel in Figure 5.1). If instead a shear driving term that is proportional to the total turbulent energy density is chosen, the respective source terms become

$$\langle z^+ \cdot S^+ \rangle = C_{\text{shear}} \frac{\Delta U_{\text{shear}}}{r} Z^2 + \frac{\dot{E}_{\text{pui}}}{2}$$  

(5.21)

$$\langle z^- \cdot S^- \rangle = C_{\text{shear}} \frac{\Delta U_{\text{shear}}}{r} Z^2 + \frac{\dot{E}_{\text{pui}}}{2}.$$  

(5.22)

Otherwise maintaining the previous setup, the results with the new shear terms are shown in Figure 5.2, which are quite similar to the reference case. However, the
cross-helicity is now monotonically decreasing and the steep gradients at the inner boundary are more gradual now, which seems to be more realistic. Also, the value for the energy difference is now closer to $-1/3$ at 1 AU as seen in observations (see W15 and references therein). Therefore, the new source terms are probably better suited, however, a thorough tuning of $C_{\text{shear}}$ is still necessary as well as a latitude-dependent value for the difference between fast and slow streams $\Delta U_{\text{shear}}$, because this term mimics CIRs that are mainly present at equatorial latitudes only. Furthermore, the pickup ion source term can also be augmented (Isenberg, 2005). Such advances should be incorporated in future modeling.

Another simulation has been performed, in which as a first step the magnetic field, and thus terms involving $V_A$, are taken into account. The magnetic field is prescribed as in W15, i.e. in the form of a Parker spiral, but in a mono-polar fashion (inwardly directed at all latitudes) to avoid the influence of a current sheet. It comes as no surprise that the results are barely changing (and are, thus, not shown) in this outer-heliospheric scenario, where the approximation $U \gg V_A$ is valid. However, this result is a respective validation of this frequently made assumption. In the following, terms involving $V_A$ are always taken into account.

A more interesting extension (again otherwise maintaining the setup from the previous section, i.e. old shear terms) involves the shear-mixing term $\hat{B} \cdot (\hat{B} \cdot \nabla) U$, for
which the magnetic field is also not neglected. (The magnitude of $B$ is irrelevant for this term, however). It was already shown in W15 that this term is latitude-dependent, so that in Figure 5.3 the radial evolution at selected co-latitudes differs now. This becomes obvious from simplifying this term for the present underlying assumption of a constant solar wind speed and Parker spiral magnetic field, yielding

$$\mathbf{B} \cdot (\mathbf{B} \cdot \nabla) \mathbf{U} \approx \left( \frac{B_\varphi}{B} \right)^2 \left( \frac{U}{r} \right)$$

so that via $B_\varphi$ a dependence on latitude is introduced. Accordingly, the effects of this term are most clearly seen at equatorial latitudes (dashed-dotted). Furthermore, while within about 2 AU the azimuthal magnetic field component is still small, it becomes dominant beyond – due to its $1/r$ dependence as opposed to the $1/r^2$ one of the radial component – which explains that differences occur mainly beyond 2 AU.

As compared with the reference case, major discrepancies are now found for the cross-helicity, which does not approach zero in the outer heliosphere, the stronger so towards the ecliptic. Thus, an equipartition between forward and backward propagating modes is not reached, as can also be seen from the center panels for the respective turbulent energy densities and correlation lengths. Furthermore, the energy difference quickly goes to zero as soon as pickup ion driving sets in, and the respective correlation length diverges (which made the computation with $L_D$ instead of $\lambda_D$ necessary, as mentioned above).

A more elaborate analysis of the effects of this additional term is again beyond the scope of this work, however, its influence is evident and not negligible.
As outlined in Section 5.1, there is doubt about the chosen value $b = 0$ for 2D axisymmetric turbulence, and instead a value of $b = 1/2$ is deemed appropriate. This introduces a similar term as the previously described one into play, namely $\rho^{-1/2} \hat{B} \cdot (\hat{B} \cdot \nabla) B$, and yet another simulation was performed incorporating only this change as compared to the reference case. As with the previous term, its effects become evident only beyond about 2 AU, where the magnetic field becomes increasingly perpendicular to the flow direction. The results as shown in Figure 5.4 are quite intriguing as they show increases in the turbulent energy density, but no equipartition between forward and backward propagating modes (indeed, $\sigma_C \to 1$) and also no equipartition between kinetic and magnetic fluctuations as $\sigma_D \to \text{const.} \neq 0$.

Finally, a setup was considered in which all the additional terms presented in this section were included, and the results are shown in Figure 5.5. As one was tempted to believe that such a seemingly complete model would result in reasonable results, the found behavior is rather disappointing. Particularly a strong increase in the turbulent energy density and no equipartition between forward and backward propagating modes is in conflict with the common conception based on observational data. Furthermore, this simulation became unstable beyond some 70 AU (see center panels).

Besides the aforementioned next steps that should be taken, there is also criticism to

Figure 5.4: *Same as Figure 5.1 with $b = 1/2$.*
5.3. MODEL EXTENSIONS

Figure 5.5: Same as Figure 5.1 with $b = 1/2$, shear-mixing term and new source terms.

these kind of models taking into account 2D turbulence only, because especially the pickup ion isotropization in the outer heliosphere rather drives Alfvén waves (slab turbulence). It is often assumed for modeling of diffusion coefficients based on the magnetic fluctuations that the ratio between the two is $\delta B_{2D}/\delta B_{\text{slab}} \approx 4$ (i.e. 80% 2D, 20% slab; Bieber et al., 1996), so that the slab component is smaller but not negligible. Models of turbulent transport usually consider only one or the other, but there are also approaches for combined theories, such as the two component model by Oughton et al. (2011). In the framework of a planned upcoming project with S. Oughton, this model will also be implemented in CRONOS and investigated in the near future.

Nevertheless, considerable progress is expected to be made from this general implementation of the model of Zank et al. (2012), as in the present setup it can be solved for the first time in 3D and also in a time-dependent manner, and it can also be coupled self-consistently to more realistic background solar wind conditions, particularly to the observations based simulations driven by the WSA model (Wiesengarten et al., 2014). For the latter, it will be necessary to devise empirical formulas for the turbulence values at the inner boundary in a similar fashion as in the current WSA setup, i.e. depending on coronal conditions quantified by, e.g., the flux tube expansion factor.
Chapter 6

Modeling of astrospheres

6.1 Overview

Global heliospheric models – focusing on the interaction between the solar wind and the ISM – and respective MHD simulations with the CRONOS code are another major topic in our working group. For the heliosphere such a numerical setup was developed by J. Kleimann, and in a recent paper (Röken et al., 2015) these simulations were compared to a new analytic description for the magnetic field in the vicinity of the heliopause.

In recent years, observational advancements (e.g. Hubble Space Telescope, Wide-field Infrared Survey Explorer (WISE) mission) allowed for all-sky surveys measuring dust emission (mostly infrared; e.g., Groenewegen et al., 2011) or the Lyman-α line (Linsky and Wood, 2014) associated with bow-shocks around other stars. It can be concluded that these stars are also emitting a stellar wind interacting with the ISM, consequently forming a respective astrosphere depicting the same bullet-like shape as the heliosphere, and also containing structures such as a termination shock, an astropause, astrosheaths and the already observed bow-shock (an overview is given in Section 2 of Scherer et al., 2015, S15). Therefore, many findings about the solar wind and our heliosphere can be transferred to other stars and their astrospheres, and the numerical setup devised for the heliosphere is already principally suited for respective investigations.

Care must be taken though, as the interstellar environment around those stars is most likely different from our local environment, and the processes driving a stellar wind may be very different from the thermally/wave-driven solar wind (see Lamers and Cassinelli (1999) for an overview). For example, the wind emitted by hot (O/B-)stars is line driven, and the energy transfer within these stars is completely radiative, so that it is still an open question whether a respective stellar magnetic field is present (although some examples have recently been found (Hubrig et al., 2015)). The resulting stellar wind velocities can be as high as several thousand km/s, and these stars’ astrospheres can be several parsecs wide. Interestingly, the
much cooler M-dwarf stars have also been shown to emit such fast stellar winds, and as these stars have an almost completely convective interior, they are magnetically very active and a considerable amount of the mass loss is probably attributable to flares and CMEs. For nearby stars, it is even possible to infer their photospheric magnetic field distribution (Donati et al., 2008). Respective data has been used in, e.g., Vidotto et al. (2011, 2015); Vidotto (2014) on the basis of solar and heliospheric numerical models with a focus on M-dwarfs with orbiting exoplanets to investigate possible interactions between these stellar winds and planetary magnetospheres. An effective shielding against the stellar wind’s influence should be regarded as an important factor for habitability. Similarly, the size of a respective astrosphere and its capability to shield planets from cosmic rays may also be important, so that global astrospheric models for these cases are a possible interesting future direction in our group.

A different goal was pursued in the publication Cosmic rays in astrospheres (Scherer et al., 2015) presented in this chapter, where the focus is on hot stars, because the associated astrospheres are huge cavities that modulate the cosmic ray flux through them and might therefore be responsible for tiny-scale anisotropies in all-sky maps of the GCR flux. This work was done in co-operation with colleagues of the Astronomical Institute at the Ruhr University Bochum, who provided observational data for the investigated O-star $\lambda$ Cephei, from which some of its stellar wind parameters could be derived, while some educated guesses have to be made for observationally inaccessible quantities like the wind’s temperature (Section 4 of S15). Together with these inner boundary conditions, outer boundary conditions in the chosen spherical setup need to be chosen according to the ISM values (also educated guesses), and special attention has to be paid to make sure that outflow in the tail direction is ensured.

The chosen set of equations to describe this scenario in this case is hydrodynamic and assumes a single (proton) fluid. More sophisticated models including magnetic fields and a multi-fluid approach – particularly accounting for interstellar neutrals – are currently being implemented. One important effect that neutrals or partially ionized heavy elements have on the plasma flow in the outer astrosheath is that they can effectively cool the plasma via Coulomb collisions, a process for which the length scale is smaller than the extent of the astrosheath and, thus, has to be taken into account (as opposed to the heliosphere, where this effect is negligible). Respective cooling terms can be introduced in the hydrodynamic equations without the necessity for an explicit multi-fluid approach. Meanwhile, heating terms were also considered, such as photo-ionization due to the large photon flux emitted by the star. Both heating and cooling are discussed in Section 3 of S15.

The resulting MHD configuration was then used as input to an SDE model to analyze cosmic ray fluxes modulated by this astrosphere (Section 5 of S15). This was done in co-operation with our colleagues from South Africa. The results demon-
strated that cosmic rays are strongly influenced at lower energies, but also at very high energies in the TeV range a small modulation of a few per mille was found as compared to cosmic rays not encountering this astrospherical obstacle. Such tiny-scale anisotropies in all-sky maps of measured high-energy cosmic ray fluxes at Earth are observed, e.g. with the IceCube experiment (see Figure 6.1), so that one possible explanation might be the modulation via nearby large astrospheres as considered here.

Figure 6.1: IceCube cosmic ray map for the 400 TeV energy band showing tiny-scale anisotropies (taken from Abbasi et al., 2012, The IceCube Collaboration).
6.2 Scherer et al. (2015)

**COSMIC RAYS IN ASTROSPHERES**

*Astronomy & Astrophysics*

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Cosmic rays in astrospheres

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ABSTRACT

Context. Cosmic rays passing through large astrospheres can be efficiently cooled inside these “cavities” in the interstellar medium. Moreover, the energy spectra of these energetic particles are already modulated in front of the astrospherical bow shocks.

Aims. We study the cosmic ray flux in and around λ Cephei as an example for an astrosphere. The large-scale plasma flow is modeled hydrodynamically with radiative cooling.

Methods. We study the cosmic ray flux in a stellar wind cavity using a transport model based on stochastic differential equations. The required parameters, most importantly, the elements of the diffusion tensor, are based on the heliospheric parameters. The magnetic field required for the diffusion coefficients is calculated kinematically. We discuss the transport in an astrospheric scenario with varying parameters for the transport coefficients.

Results. We show that large stellar wind cavities can act as sinks for the Galactic cosmic ray flux and thus can give rise to small-scale anisotropies in the direction to the observer.

Conclusions. Small-scale cosmic ray anisotropies can naturally be explained by the modulation of cosmic ray spectra in huge stellar wind cavities.

Key words. stars: winds, outflows – cosmic rays – hydrodynamics

1. Introduction

Recently, simulations of astrospheres around hot stars have gained new interest, see for example Decin et al. (2012), Cox et al. (2012), Arther (2012), van Marle et al. (2014). These authors modeled astrospheres using a (magneto-)hydrodynamic approach, either in 1D or 2D. In this work, such astrospheric models are used for the first time to estimate the cosmic ray flux (CRF) through it. Because of the large spatial extent of O star astrospheres (wind bubbles), these objects can efficiently cool the spectrum of Galactic cosmic rays (GCR). Especially λ Cephei is an interesting example, being the brightest runaway Of star in the sky (type O6If(n)p). We estimate the CRF at different energies for λ Cephei as an example of an O star astrosphere using stochastic differential equations (SDE; Strauss et al. 2013) to solve the GCR transport equation. Runaway O and B stars are common and part of a sizable population in the Galaxy, a significant number of which show bow-shock nebulae (e.g., Huthoff & Kaper 2002). In Sect. 3 we discuss the radiative cooling functions, while in Sect. 4 we show the astrosphere model results. In Sect. 5 we estimate the CRF.

2. Large-scale structure of astrospheres

Winds around runaway stars, or in general, stars with a nonzero relative speed with respect to the surrounding interstellar medium (ISM), develop bullet-shaped astrospheres.

The hydrodynamic large-scale structure is sketched in Fig. 1, the notation of which is described below.

The hypersonic stellar wind (Mach numbers $Ma \gg 1$) undergoes a shock transition to subsonic velocities at the termination shock (TS) in the inflow direction. Then a tangential discontinuity, the astropause (AP), is formed between the ISM and the stellar wind, where the velocity normal to it vanishes: there is no mass transport through the AP. Other quantities such as the tangential velocity, temperature, and density are discontinuous, while the thermal pressure is the same on both sides. If the relative speed, or the interstellar wind speed as seen upstream in the rest frame of the star, is supersonic in the ISM, a bow shock (BS) exists. If the relative speed is subsonic, there will be no BS, see Table 1 for the stellar parameters and for the stellar-centric model distances of the TS, AP, and BS. The region between the BS and AP is called outer astrosheath, the region between the AP and TS the inner astrosheath. The AP around the inflow direction at the stagnation line is sometimes called the nose, while the region beyond the downwind TS is called the astrotail. The latter can extend deep into the ISM. The region inside the TS is called the inner astrosheath.

In the downwind direction, the termination shock forms a triple point (T), from which the Mach disk (MD) extends down to the stagnation line; this is the line through the stagnation point and the star. A tangential discontinuity (TD) emerges down into the tail. A reflected shock (not shown here) also extends from the triple point toward the TD.
### 3. Cooling and heating

As a result of the large dimensions of O star atmospheres and their outer astrosheath, the plasma can effectively be cooled by Coulomb collisions. In this process, an electron in an atom (molecule) will be excited, and after returning to a lower energy state, the re-emitted photon will carry away the energy (Sutherland & Dopita 1993, and references therein). This can lead to an effective cooling of the shocked ISM (ISM$_2$ in Fig. 1).

Several cooling functions are discussed in the literature (e.g., Rosner et al. 1978; Mellema & Lundqvist 2002; Townsend et al. 2009; Schure et al. 2009; Reitberger et al. 2014). The differences in the cooling functions are caused by different abundances and different levels of approximation. Because we do not know the abundances in the ISM surrounding $\lambda$ Cephei, we use here the analytic representation by Siewert et al. (2004), which lies in between all the other cooling functions mentioned above, and can therefore be considered as a useful principal representation.

Mainly the hot shocked ISM is affected, while the stellar wind gas is not. The reason for this is that the number densities in the shocked ISM are higher by a factor of 3.6, which is the compression ratio between the shocked and unshocked ISM, and that it is by a factor $10^2$ hotter, that is, $T_{\text{ISM, shocked}} \approx 2.5 \times 10^5$ K. In this region most of the mentioned cooling functions yield similar values. Inside the inner astrosheath, that is, the region between the AP and the TS, the number density is on the order of $n = 10^{-3}$ cm$^{-3}$ and the velocities are on the order of $v = 600$ km s$^{-1}$, and thus the cooling length scale, depending on $v$ and $n$, becomes huge and is neither important there nor inside the TS, see below.

The heating length scale only depends on the number density $n$ and also increases to scales much larger than the distances inside the AP. Therefore, as a result of the huge ram pressure of the stellar wind inside the TS, we can, from a dynamical point of view, safely neglect heating and cooling, because it does not influence the adiabatic expansion of the stellar wind. Moreover, the thermal pressure is negligible compared with the ram pressure in the inner astrosphere. With the help of the momentum equation, we can uniquely determine the shocked thermal pressure, which dominates in the inner astrosheath.

In the following we always assume quasi-neutrality $n_e = n_p = n$, where $n_e$, $n_p$ are the electron and proton number densities, respectively. Furthermore, we neglect the contribution of heavy ions. In Table 1 we summarize the parameters of $\lambda$ Cephei derived from observations and the characteristic distances of its model atmosphere. The parallax translates into a tangential velocity of $41.1$ km s$^{-1}$, which together with the radial velocity of $75.1$ km s$^{-1}$ gives a total speed of $85.5$ km s$^{-1}$. Our hydrodynamic model is three-dimensional (for later use), and in view of the uncertainties of the ISM state, we have chosen a set of parameters as given in Table 2. The standard procedure in modeling is to choose one axis as the inflow direction (here the $x$ axis). As long as the ISM is homogeneous, with a vanishing magnetic field, and the stellar wind is spherically symmetric, the atmosphere is symmetric around the inflow direction.

The derived inner boundary conditions for the model are estimated from the mass-loss rate and the terminal velocity and taken at $0.03$ pc. They are presented in Table 3 together with those of the ISM.

As stated above, the cooling acts differently in the subsonic regions from the way it does in the supersonic regions because in the former the thermal pressure $P$ is dominant, while in the latter it is the ram pressure $pv^2/2$, where $p$ and $v$ are the mass density (mainly protons, but helium or other elements may contribute...
to the mass density) and bulk speed, respectively. While in the following we discuss only protons, we can add, for example, helium, which leads to partial densities, temperatures, and pressures for which the approximations made below can be separated. We are interested in the shortest characteristic length, which is in the subsonic case inversely proportional to the number densities, and thus the protons dominate.

In the hypersonic case, the estimation below can differ by up to 40% when including helium. This would then also require including helium as a new species in the Euler energy equations (including different species, see Scherer et al. 2014), which would violate our assumption of a single fluid. The interaction of other species concerning the energy loss by Coulomb collisions is, however, already included in the cooling functions, so that we can continue with the single-fluid equations consisting of protons including the cooling term for a first analysis.

From the stationary energy equation we obtain in the subsonic region with the assumption \( n m p v^3 / 2 \ll P \):

\[
\nabla \cdot \left( \frac{\gamma}{\gamma - 1} P + \frac{1}{2} n m p v^2 \right) v = \frac{\gamma P v}{(\gamma - 1) n L_{\text{cool},s}} \approx \frac{5 k n T v}{L_{\text{cool},s}} = -n^2 \Lambda(T),
\]

where \( \gamma = 5/3 \) is the adiabatic index, \( m_p \) the proton mass, \( P = 2 n k T \), \( k \) is the Boltzmann constant, \( v \), \( T \) the bulk velocity and temperature of the plasma flow, and \( \Lambda \) the cooling function. Taking the absolute values in Eq. (1) and replacing \( \nabla \) by the inverse subsonic cooling length, \( L_{\text{cool},s} \), can be estimated as

\[
L_{\text{cool},s} \approx \frac{5 k n T}{n \Lambda(T)},
\]

and the subsonic cooling time

\[
\tau_{\text{cool},s} = \frac{L_{\text{cool},s}}{v} = \frac{5 k T}{n \Lambda(T)}. \tag{3}
\]

This cooling time is up to a factor 3 the same as that given in Sutherland & Dopita (1993). For supersonic interstellar flows, that is, \( \rho_{\text{ISM}} v_{\text{ISM}}^2 / 2 \gg \gamma / (\gamma - 1) P \), it follows:

\[
\nabla \cdot \left( \frac{\gamma}{\gamma - 1} P + \frac{1}{2} n m p v^2 \right) v \approx O\left( \frac{m_p n m^3}{2 n L_{\text{cool},h}} \right),
\]

and we derive the supersonic (index \( h \)) “hypersonic” to distinguish it from the subsonic one) cooling length \( L_{\text{cool},h} \) and time \( \tau_{\text{cool},h} \)

\[
L_{\text{cool},h} \approx \frac{m_p v^3}{2 n \Lambda(T)} \quad \text{and} \quad \tau_{\text{cool},h} = \frac{m_p v^2}{2 n \Lambda(T)}. \tag{4}
\]

For the heating function by photo-ionization and some suplemental heat source we use the approach by Reynolds et al. (1999), see also Kosiński & Hanasz (2006). The heating rate for photo-ionization depending on electron collisions is limited by recombination and is thus proportional to \( n_e^2 \), while additional heating terms that can include photoelectric heating by dust, dissipation of turbulence, interactions with cosmic rays are proportional to \( n_c \).

\[
\Gamma = n_e^2 G_0 + n G_1, \tag{6}
\]

with the constants \( G_0 = 10^{-24} \text{ erg cm}^3 \text{ s}^{-1} \) and \( G_1 = 10^{-25} \text{ erg s}^{-1} \) (Kosiński & Hanasz 2006). Replacing the right-hand side of Eq. (1) by \( \Gamma \), we obtain

\[
L_{\text{heat},s} = \frac{5 k T v}{n G_0 + G_1} \quad \text{and} \quad L_{\text{heat},h} = \frac{m_p v^3}{2 (n G_0 + G_1)}, \tag{7}
\]

and the heating times \( \tau_{\text{heat},s}, \tau_{\text{heat},h} \) by dividing the respective heating lengths by the speed \( v \).

We can estimate the cooling and heating lengths and times for the shocked ISM (ISM2), and analogously for the shocked stellar wind SW2 (see Fig. 1). The results are displayed in Table 3 together with the characteristic lengths and times for the hypersonic ISM (ISM1), because it is also cooled. For the ISM the dependence of the cooling and heating lengths is shown in Fig. 2. The vertical line denotes the temperature at which the ram pressure equals the thermal pressure. Left of this line the hypersonic length scales from Eqs. (5) and (7) are displayed, while on the right the subsonic scales are shown (Eqs. (2) and (7)).

The supersonic parameters are number density \( n = 11 \text{ cm}^{-3} \) and a speed of \( v = 80 \text{ km s}^{-1} \) while for the subsonic parameters, the density was multiplied by the compression ratio \( s = 3.62 \) and the speed was divided by \( s \) using the Rankine-Hugoniot relations.

Figure 2 shows that in the subsonic case for temperatures above \( \approx 5 \times 10^5 \text{ K} \) the heating scale length is always longer than that for the cooling. Thus cooling is more efficient than heating for the discussed functions and parameters. In the supersonic case \( T < 5 \times 10^5 \text{ K} \), the heating scale lengths are only longer down to temperatures of \( \approx 10^4 \text{ K} \) while for temperatures below \( \approx 4 \times 10^2 \text{ K} \) the cooling scale length is more important. Thus, above \( \approx 4 \times 10^2 \text{ K} \) cooling is more efficient than heating, and below this, heating is important. We can read from this figure that the length scale for cooling of the shocked ISM temperature \( T \approx 2.5 \times 10^5 \text{ K} \) is \( \approx 0.01 \text{ pc} \). From the model we see that the BS to AP distance is 0.17 pc, which is more than ten times the cooling length \( L_{\text{cool},s} \). This strong cooling is balanced by the fact that at least at the stagnation line the shocked ram pressure (1/2)\( \rho_{\text{ISM}} v^2_{\text{ISM}} \) has to be converted into thermal pressure toward the astropause, through which mass flux is zero.

It is also evident from Fig. 2 that if the temperature falls below \( \approx 4 \times 10^2 \text{ K} \) the flow again becomes supersonic.

Different values of the number density \( n \) or speed \( v \) or different cooling or heating functions change the characteristic lengths, but the principle estimates for the dynamics of the flow field remain the same.

In the stationary case, where no relative speed between the star and the ISM exists, one should take for the speed \( v \) that of

---

**Table 3.** Some characteristic numbers using the cooling function from Siewert et al. (2004).

<table>
<thead>
<tr>
<th>( T ) [K]</th>
<th>( v ) [km s(^{-1})]</th>
<th>( n ) [cm(^{-3})]</th>
<th>( L_{\text{cool},s} )</th>
<th>( \tau_{\text{cool},s} )</th>
<th>( L_{\text{heat},s} )</th>
<th>( \tau_{\text{heat},s} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>ISM(_2)</td>
<td>10(^6)</td>
<td>20</td>
<td>40</td>
<td>25 kAU ( \approx ) 0.12 pc</td>
<td>6 kyr</td>
<td>248 AU ( \approx ) 10(^3) pc</td>
</tr>
<tr>
<td>SW(_2)</td>
<td>10(^6)</td>
<td>10(^3)</td>
<td>10(^{-3})</td>
<td>51 kAU ( \approx ) 250 kpc</td>
<td>242 Myr</td>
<td>1241 kAU ( \approx ) 6 Mpc</td>
</tr>
<tr>
<td>ISM(_1)</td>
<td>10(^{4})</td>
<td>80</td>
<td>10</td>
<td>56 kAU ( \approx ) 0.3 pc</td>
<td>3.3 kyr</td>
<td>2.8 MAU ( \approx ) 14 pc</td>
</tr>
</tbody>
</table>
4. Atmosphere model

The hydrodynamic model for the star $\lambda$ Cephei is made in 3D; the third dimension is needed for future comparison with models including bipolar winds or magnetic fields. The boundary conditions are given in Table 2. While the stellar mass loss and the terminal speed can be determined by observations, the stellar wind temperature as well as the interstellar parameters are sophisticated guesses. The model solves the Euler equations for $\lambda$ Cephei using the Cronos MHD code as described in Kissmann et al. (2008), Kleimann et al. (2009), and Wiengarten et al. (2013). The results are displayed in Fig. 3 for the proton number density of $\lambda$ Cephei. In Fig. 3 the wiggles along the AP caused by the thermal instabilities can be clearly recognized. They are due to the cooling functions.

This model provides the underlying plasma structure needed as input for the transport equation discussed below. The model is solved on a spherical grid with a resolution of 0.005 pc in radial dimension, and $2^\circ$ and $3^\circ$ in $\theta$ and $\varphi$ dimension, respectively. The large distance of the outer boundary is needed because during the evolution of the atmosphere it becomes much broader than shown in Fig. 3 and finally shrinks to the state shown here after ca. 170 kyr.
5. Cosmic ray fluxes

To model the flux of GCRs, the Parker transport equation

\[
\frac{\partial f}{\partial t} = -\mathbf{v} \cdot \nabla f + \nabla \cdot (\mathbf{K} \cdot \nabla f) + \nabla \cdot (\mathbf{v} \cdot \nabla f) + \frac{\nabla \cdot \mathbf{v}}{3} \ln P
\]

has been frequently used in the literature (see Potgieter et al. 2001, and reference therein). In this equation, \( f \) is the (nearly) isotropic GCR distribution function, \( \mathbf{v} \) the bulk plasma flow, \( \mathbf{K} \) the diffusion tensor (including, in a 3D geometry, separate components directed parallel and perpendicular to the mean magnetic field), and \( P \) is the particle rigidity. As an initial approach, spherical symmetry is assumed, so that the Parker equation reduces to

\[
\frac{\partial f(r, t)}{\partial t} = -v \frac{\partial f}{\partial r} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa \frac{\partial f}{\partial r} \right) + \frac{P}{3r^2} \frac{\partial}{\partial r} \left( r^2 v \right) \frac{\partial f}{\partial \ln P},
\]

where \( r \) is radial distance and \( \kappa \) is the effective radial diffusion coefficient. In this work, Eq. (9) is solved by transforming it into the equivalent set of SDEs

\[
\frac{d \mathbf{r}}{d \mathbf{r}} = \frac{1}{r^2} \frac{\partial}{\partial \mathbf{r}} \left( r^2 \kappa \right) - \mathbf{v} \right) \right) d \mathbf{v} + \sqrt{2k_r}dW,
\]

\[
dP = \frac{\frac{P}{3r^2} \frac{\partial}{\partial \mathbf{r}} \left( r^2 v \right) \frac{\partial f}{\partial \ln P}}{d \mathbf{r}},
\]

which is then integrated numerically (Strauss et al. 2011), where the solution of the 1D equation along \( r \) can be found in Strauss et al. (2011).

These equations are coupled to the simulated HD geometry by reading in the modeled values of \( \mathbf{v} \) and \( \mathbf{V} \) (governing energy changes) directly from the HD simulations (along the stagnation line) and solving for the GCR flux using essentially a test particle approach. The magnetic field enters the computations via the diffusion coefficient \( \kappa \). In the 1D scenario, the geometry of \( B \) does not enter the calculations, although for an azimuthal field (the case inside the TS), \( \kappa_\perp \approx \kappa_L \), thus reducing to a diffusion coefficient perpendicular to the mean field. As a boundary condition for the GCR flux, a local interstellar spectrum is specified at the edge of the computational domain. The GCR differential intensity is related to the distribution function by \( J = P^2 f \).

Based on experience gained from modulation studies inside the heliosphere, \( \kappa \) can be decomposed into a radial and energy dependence: \( \kappa = \kappa_r(r) \kappa_{S}(P) \), where, for this study

\[
\kappa_1(r) = \begin{cases} \kappa_\text{sw} & \text{if } r < r_{\text{BS}} \\ \kappa_\text{ISM} & \text{if } r \geq r_{\text{BS}} \end{cases}
\]

with \( r_{\text{BS}} \) the radial position of the BS and where \( \kappa_{\text{ISM}} \) is independent of position and \( \kappa_{\text{sw}} = \kappa_0 B_0/B \). \( \kappa_0 \) is a normalization constant, usually specified near the inner boundary, and \( B_0 \) is a constant included for dimensional consistency. Assuming that the astrospheric magnetic field is about 80 times higher than the heliospheric field (Naze 2014), a value of 0.027 kpc^2 Myr^\text{--}1 is used, scaling up the heliospheric diffusion coefficient by about 2 orders of magnitude for this astrospheric case. The \( B^2 \) radial dependence is based on the results of Engelbrecht & Burger (2013), but approximated in such a fashion because in situ observations are, of course, not available. The energy dependence of \( \kappa_\text{sw} \) is taken from Büsching & Potgieter (2008)

\[
\kappa_2(P) = \begin{cases} \left( \frac{P}{P_0} \right)^{-0.6} & \text{if } P > P_0 \\ \left( \frac{P}{P_0} \right)^{-0.48} & \text{if } P \leq P_0 \end{cases}
\]

Fig. 5. Modulation of 1 GeV particles in \( \delta \) Cephei along the stagnation line for different stellar and interstellar mfp. The mfp are shown in the lower panel and the colors correspond to those in the upper panel. The mfp used is, in general, not known, we study the behavior of three different values inside \( \delta \) Cephei and three different values of the interstellar mfp.

5.1. Mean free path

The structure of the atmosphere can be recognized in the lower part of Fig. 5 by the respective jumps in the mfps (from the right, which is the inflow direction): the BS (1.1 pc), AP (0.93 pc) and TS (0.66 pc), represented by the vertical dotted lines. The TS is marked by a sharp decrease of the mfp, the AP by a change of the slope, and finally the BS by the sharp drop at the ISM side. The resulting differential flux (DF) for 1 GeV particles along the stagnation line is displayed in Fig. 6. In all cases the modulation, that is, the decrease in the differential intensity DI, starts far away in front of the BS, a feature that was discussed by Scherer et al. (2011), Herbst et al. (2012), and Strauss et al. (2013) for the case of the heliosphere.

This outer atmospheric modulation depends on the ratio between the parallel and perpendicular diffusion coefficient and vanishes for high ratios. Thus, for an appropriate choice of the transport parameters, the modulation of GCRs starts in front of the atmosphere and then rapidly decreases at the atmospheric BS. It is also evident that in contrast to the heliosphere, the GCRs are modulated directly behind the BS: this is due to the cooling effects, which shrink the region between the AP and BS to 0.17 pc and are a barrier-like feature for the cosmic rays (Potgieter & Langner 2004).

In the lower part of Fig. 5 we plot the mfp used in the modeling. The inner mfp (\( \lambda_{\text{sw}} \)) obtained from the model are then divided or multiplied by a factor two and three to demonstrate its influence. A small \( \lambda_{\text{sw}} \) strongly increases the modulation, and the
flux of 1 GeV particles almost vanishes inside the AP. Increasing \( \lambda_{\text{w}} \) by the same factor leads to a nearly vanishing modulation. Changing the interstellar \( \lambda_{\text{ISM}} \) from 50 pc to 100 pc and 500 pc does not change the DI remarkably. These variations show the effects expected from theory. Especially for short mfp inside the atmosphere the GCR spectra are efficiently cooled. The 20\% modulation in front of the atmosphere is presumably caused by the sharp drop of the mfp between the AP and the BS.

From Fig. 5 we can also see that most of the modulation – up to a factor 5 or even more – occurs between the BS and the AP (depending on the transport parameters). Thus, because astrospheres are large volumes surrounding the star, the GCR spectrum can be observed far away from large astrospheres. This prediction will be improved by further modeling and studying the distribution of hot stars in the Galaxy.

At the BS, the mfp falls to quite low values, rises sharply at the AP, and finally jumps again at the TS. In the inner astrosheath the mfp increase continuously toward the shock because we assumed that the magnetic field is inversely proportional to the speed \( v \) as for the Parker spiral field in the heliosphere (Potgieter et al. 2001). Thus at the stagnation line, the speed must vanish at the AP because this is a tangential discontinuity with no mass flow through it. Inside the TS, the magnetic field increases with \( r \) in the direction to the star, and the mfp decreases. Because of the strong compression of the outer astrosheath, the mfp diminishes to an even lower value, which then forms a barrier for the cosmic ray transport.

This qualitative behavior is theoretically well understood and confirmed by observations in the heliosphere, except for the additional modulation in the outer astrosheath. The latter differs because of the cooling function. Thus, the cooling function has a direct influence on the cosmic ray transport.

### 5.2. Energy dependence

In Fig. 6 we study the behavior of the GCR flux at different energies. The 1 GeV particles are modulated by a factor of almost five, while for higher energies this factor becomes smaller, as expected. But even for the highest energies of 10 to 100 TeV, a small modulation of a few per mille (1 per mille \( = 0.1\% \)) outside of the BS is visible.

In Fig. 6 we plot the DIs for different energies, from 1 GeV to 100 TeV in logarithmic steps of ten. In the upper panel the lower energies (form 1 to 10 GeV) are strongly modulated, while for the 10 GeV and 1 TeV particles the DI is only diminished by a few percent (middle panel). The lower panel shows the modulation of the 10 and 100 TeV particles, which is in the per mille range or even much lower for the 100 TeV particles, which are hardly affected. All energies are modulated ahead of the BS, and thus the modulation volume is larger than that of the atmosphere. The DI of the TeV particles can be increased by diminishing the mfp inside the atmosphere or can become less by increasing the mfp; this is not shown in Fig. 6. The mfp is based on that in the heliosphere, and the modulations displayed in Fig. 6 are based on it.

### 5.3. Observational evidence

Small-scale modulations of a few per mille in the TeV range are observed with, for example, the IceCube experiment (e.g., Abbasi et al. 2012, and references therein). In particular, their Fig. 5 shows a resolution of 3°, which cannot resolve the atmosphere of \( \lambda \) Cephei with angular diameter 0.2°. Nevertheless, the pixels show variations that may be attributed to local GCR fluctuations, provided the statistics in the pixels is large enough and the astrospheres are close enough. Because runaway O/B stars or OB associations are quite frequent in the Galaxy (Huthoff & Kaper 2002), their local disturbance of the GCR spectrum can explain small-scale variations in the GCR flux. \( \lambda \) Cephei was only used as an example, but the above holds true in general for all large astrospheres.

Our simulations may help to understand these variations. The variation in the DIs can be increased or decreased by choosing a smaller or larger mfp inside the astrosphere, therefore a better estimate of their magnetic fields is needed, which can help to understand their turbulence levels.

For the higher energies a modulation outside the atmosphere can also be observed, where the “astrosphere of influence” is roughly twice the BS distance for bullet-shaped astrospheres like that of \( \lambda \) Cephei. This holds true in the direction of the inflowing ISM, while it is more complicated in other directions. These details will be explored in future. We studied here only protons, but because the transport coefficients depend on rigidity, the behavior of other species can roughly be estimated. For helium, for instance, a similar behavior is expected as for the protons shifted by a factor of two in Fig. 6. At these high energies the rigidity has roughly the same value as the particle energy. This means that multiplying the rigidity by a factor of 2 is the same as doing it in the particle energy. Therefore, helium is slightly less modulated when passing through astrospheres than the protons.

If there were a few large astrospheres (or stellar wind bubbles) in the direction toward an observer, the GCR spectrum would be slightly cooler than in other directions. This can contribute to the understanding of the small-scale anisotropies present in the IceCube data (Abbasi et al. 2012). The parameter set for the supersonic wind and ISM are chosen to be close to the observed values, but for modeling purposes we worked with rounded values. In addition, for the transport model we took the turbulence levels based on that of the heliosphere. Both of these aspects need further attention, but the
principal effect remains: large stellar astrospheres can affect the local interstellar cosmic ray spectra.

6. Conclusion

Based on our models, we studied the transport of GCRs in an astrosphere. We have shown that even ahead of an astrosphere, where the mfp is still undisturbed, a cooling of the GCR spectra occurs because particles are trapped by scattering into the astrosphere, in which they can be effectively cooled. The “atmosphere of influence” around the modeled astrospheres is roughly twice its hydrodynamic dimension. Thus, stellar wind bubbles (astrospheres) can cool the Galactic spectrum, and small anisotropies are expected in the direction to an observer.

As a result of its effect in compressing the outer astrosheath, the cooling function directly influences the GCR modulation in this region. Additionally, the cooling and heating functions require high resolutions for global models because of their characteristic length scales. They also give a rough estimate whether the surrounding ISM is also affected during the calculations.

The modulation in astrospheres affects particles up to 100 TeV. This can help to understand the anisotropies on small angular scales, for example, by the IceCube experiment, among others. The angular extent of ζ Cephei’s astrosphere is too small to be resolved by these experiments because of its large distance (∼650 pc). Nevertheless, nearby hot stars or stellar associations can have a larger angular extent and may possibly be observed. In our simulations we saw an effective cooling of the GCR spectrum. Thus, the conclusion is that small-scale cosmic ray anisotropies may be explained by the modulation in such huge cavities.

Because the model is fully 3D, the modulation or other parameters along a line of sight toward Earth can in principle be theoretically determined. Here we demonstrated that large astrospheres can modulate the Galactic cosmic ray spectrum quite significantly, and no homogeneous spectrum over all directions can be expected. To calculate the modulation of GCRs along a line of sight or at Earth requires more sophisticated methods than discussed here, but this is being developed.

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Chapter 7

Summary and outlook

This thesis focuses on the modeling of the inner-heliospheric solar wind by numerically solving the equations of magnetohydrodynamics (MHD). Consequently, the first chapter starts with a descriptive overview of the respective protagonists, namely the Sun with its magnetic field, emanating and shaping the turbulent solar wind that interacts with the interstellar medium to form the heliosphere, and the application of the solar findings to other stars and their astrospheres (Section 1.1). Furthermore, aspects of sub-dividing the heliospheric environment for modeling purposes are given, before the main numerical tool used in this work – the state-of-the-art MHD code Cronos – is described in Section 1.2.

The remaining chapters are respectively based on the publications I authored during my PhD, with respective introductions, additional details and afterthoughts leading to subsequent fields of activity.

Chapter 2 – including my initial first-author publication *MHD simulation of the inner-heliospheric magnetic field* (Wiengarten et al., 2013) – presents the application of the Cronos code to the modeling of the solar wind based on observational input data. The required extensions to the code for adequately describing the solar wind include the introduction of solar rotation and solving the full energy equation, which was validated by reproducing the analytic models of Parker (1958) and Weber and Davis (1967).

Although these latter models have been very successful in describing the large-scale solar wind and the heliospheric magnetic field, they are too simple for reproducing more complex conditions, especially those involving transient events such as co-rotating interaction regions (CIRs) or coronal mass ejections (CMEs). Therefore, in a collaboration with colleagues from the Max Planck Institute for Solar System Research (MPS) in Katlenburg-Lindau (now in Göttingen), maps of the radial magnetic field at the heliobase for solar minimum and maximum conditions served as inner boundary conditions for my subsequent MHD simulations. These maps are the result of a coupled solar surface flux transport (SFT) and a coronal potential field model as described in Jiang et al. (2010), which allow for an adequate description
CHAPTER 7. SUMMARY AND OUTLOOK

of the usually unobservable far side of the Sun, as well as a reconstruction of the solar magnetic field for times before the space age by using sunspot group data from earlier times. Previously, the CRONOS code was operated with analytic prescriptions for initial and inner boundary conditions only, so that new routines to read-in and interpolate the input data on arbitrary grids had to be devised. Moreover, a method for a divergence-free initialization of the magnetic field was developed. Besides the directly provided magnetic field data, the remaining MHD quantities had to be derived as well, which follow from the coronal magnetic field topology – fast wind from coronal holes and slow wind from their boundaries – as described by respective models relying on the inverse relation between flux-tube expansion factor and resulting solar wind speed (Wang and Sheeley, 1990). Here, the model of Detman et al. (2011) was adopted.

Simulations were performed on computing clusters at our institute for typical solar minimum and maximum conditions. Initially, the obtained results were deemed as realistic as they were roughly compared to spacecraft data and agreed with the general topologies expected for the respective phases in the solar cycle. Later on, a more detailed comparison with spacecraft data showed that the magnetic field data used in this work were unsuitable, and the coronal magnetic field modeling was subsequently performed in a different manner by myself, as described next.

The work presented in Chapter 3 was done in the framework of a joint project with the Universities of Kiel and in Potchefstroom, South Africa, on the influence of CIRs on the propagation of energetic particles, with the goal to use a CIR disturbed background solar wind configuration resulting from my MHD simulations as input to a stochastic differential equation (SDE) model for the transport of energetic particles in the heliosphere. Whereas the publication Cosmic Ray transport in heliospheric magnetic structures. I. Modeling background solar wind using the Cronos magnetohydrodynamic code (Wiengarten et al., 2014) describes the respective MHD modeling, the subsequent SDE modeling paper on energetic particle propagation is currently in preparation.

A first mandatory task was to show that the CRONOS code is able to correctly compute CIR structures, which was achieved by reproducing previous numerical results of Pizzo (1982). Our colleagues from Kiel proposed the time period around August 2007 during the ascending phase of solar cycle 23 for a detailed comparison with spacecraft measurements. Besides favorable solar wind conditions with a stable CIR configuration, this time is also preferential due to a unique spacecraft constellation with the just previously launched Stereo-A/B spacecraft trailing and leading Earth on its orbit at 1 AU, and Ulysses crossing the equatorial plane during its third fast-latitude scan.

The required potential field modeling of the solar corona providing the boundary conditions for the MHD simulations had to be performed in a different fashion as compared to my previous work, because the input data used there were found to be incorrect. Instead, the potential field source surface (Altschuler and Newkirk, 1969) coupled with the Schatten current sheet model (Schatten, 1971) was implemented,
because the employed so-called Wang-Sheeley-Arge (WSA; Arge and Pizzo, 2000; Arge et al., 2003) model for deriving the resulting solar wind speeds is tuned to the usage of GONG magnetograms in these potential field approaches. For the analysis of the resulting coronal field topology I developed a sophisticated field line tracing algorithm, which was also necessary to derive the resulting solar wind speeds. The inner boundary conditions for the remaining MHD quantities were set via empirical formulas that contain a number of tunable parameters, for which a best fit to observations was performed. My results show good agreement with spacecraft data, allowing to expect insights for energetic particle propagation from the ongoing SDE modeling.

For the latter it is desirable to have the MHD results extending to large distances, i.e., to the termination shock in order to remain in the supersonic part of the heliosphere. Such simulations require not only huge computer resources, but it is also mandatory to apply time-dependent boundary conditions to account for changes in the corona during the long propagation time of about a year that the solar wind needs to reach the termination shock. Although first steps in these directions have been taken by applying such boundary conditions, it will be necessary to apply for computing time at supercomputing facilities to keep the required simulation time within reasonable limits. This will be particularly necessary for a coupling with outer-heliospheric models to describe the interaction with the interstellar medium (ISM).

While the SDE modeling in our group focuses on Galactic Cosmic Rays and Jovian electrons, similar studies for solar energetic particles are of interest as well. Such an investigation, for which the current results from my MHD simulations are principally suited at least in the supersonic solar wind, is planned in collaboration with W. Dröge at the University of Würzburg. However, a coronal model describing not only the magnetic field (as provided by my potential field solutions), but also the evolving solar wind would be more appropriate, which could be achieved with an MHD model of the solar corona. This could be a future direction of work that would provide a more self-consistent treatment of the corona in comparison with the empirically derived solar wind based on the coronal potential field solutions used in this thesis.

Another possibility of exploiting my results is an investigation of space weather effects, i.e. impacts on the Earth’s magnetosphere and man-made objects.

The employed transport coefficients in the SDE modeling depend not only on the large-scale MHD quantities, but also on the magnetic fluctuations. These cannot be resolved in large-scale MHD simulations, but there are models describing the evolution of integral turbulence quantities such as the total turbulent energy density and the ratio between inward and outward propagating modes. In order to eventually be able to provide these quantities for an improved SDE modeling, a turbulence transport model was implemented alongside the large-scale MHD equations in the CRONOS framework, which is the topic of Chapter 4 based on my publication Implementing turbulence transport in the CRONOS framework and application to the
propagation of CMEs (Wiengarten et al., 2015). I started again by validating the implementation by comparing with previous work of Usmanov et al. (2011). During this comparison, some discrepancies were found that – in discussion with A. Usmanov – could be traced back to errors made by these authors. A corrected model was then used, which was further extended by removing the constraint of being only applicable in regions of highly super-Alfvénic solar wind \((U \gg V_A)\), while I followed the goal to have a model that can eventually be coupled to my previous WSA-driven MHD simulations that start in regions where \(U \geq V_A\). This was achieved by appropriately simplifying a more general model of turbulence transport of Zank et al. (2012), which in the form used here describes the evolution of turbulent energy density, cross-helicity, and correlation lengths for low-frequency turbulence, as observed in the solar wind with increasing distance from the Sun. These integral quantities characterize the large-scale behavior of turbulence (dominated by nonlinear interactions) and wave modes (dominated by propagation effects), which is a useful approach to circumvent the difficulties that would arise for a complete description of the fluctuations, which is on much smaller scales than typical structures in the heliosphere. Particularly for numerical studies such an approach is desirable because of the reduced required computer resources.

My resulting model was then applied to the propagation of CMEs, for which I found that, on the one hand, turbulence does not act back on the large-scale quantities, but, on the other hand, that the CME is a strong driver of turbulence. Therefore, such a model is not required for studies focusing on large-scale CME quantities alone, but it does provide another interesting scenario for a related energetic particle propagation study. While there is only a very limited number of observations of turbulence associated with CMEs, my results are in agreement with estimates provided by Subramanian et al. (2009), however.

Chapter 5 describes the subsequent implementation of the complete model of Zank et al. (2012), i.e. with evolution equations for the energy difference between kinetic and magnetic fluctuations, as well as respective correlation lengths. Thus far, this had been solved neither in 3D nor self-consistently coupled with the MHD equations. A simplified implementation in the ecliptic plane only and neglecting some of the involved terms was done by Adhikari et al. (2015), whose results were compared with for validation purposes here. Afterwards, the complete model was solved, which gave some yet not fully understood results. Consequently, this work is unpublished as of yet, but ongoing. Mandatory next steps are a thorough comparison with spacecraft data and an analysis of the effect of the additional terms, possibly in collaboration with the initiators of these models.

There is also criticism to these kind of models taking into account 2D turbulence only, because especially the pickup ion isotropization in the outer heliosphere rather drives Alfvén waves (slab turbulence). Models of turbulent transport usually only consider one or the other, but there are also approaches for combined theories, such as the two-component model of Oughton et al. (2011), which will also be introduced into the CRONOS code and investigated in the near future.
Furthermore, the model solving the coupled Reynolds-averaged MHD and turbulence transport equations can be fed with inner-boundary conditions derived via the WSA model to advance from the still idealized solar wind conditions applied here to actual conditions during specific periods of time. To do this it will be necessary to devise empirical formulas for the turbulence values at the inner boundary in a similar fashion as in the current WSA setup, i.e. depending on coronal conditions quantified by, e.g., the flux tube expansion factor.

Another line of work in our team is the modeling of the large-scale heliosphere and astrospheres, i.e. the interaction between the solar/stellar wind and the ISM. An analytic model for the interstellar magnetic field in the vicinity of the heliopause was recently presented by Röken et al. (2015), in which it was also compared to numerical results obtained with the CRONOS code by J. Kleimann. This numerical setup was altered by K. Scherer and myself for the application to the astrosphere of the O-star λ Cephei, which, due to the large terminal velocities of the stellar wind, is a cavity of several parsecs in diameter and is thus able to modulate high-energy cosmic rays that pass through it. This was the topic of Chapter 6 based on the paper Cosmic rays in astrospheres (Scherer et al., 2015).

The required computer resources for the simulations performed here are already enormous, and a migration to supercomputing facilities will have to be undertaken, particularly for the planned extensions of the model to incorporate stellar and interstellar magnetic fields, and even a multi-fluid approach.

In conclusion, the work described in this thesis provides the essential extension to the MHD code CRONOS for an adequate modeling of the super-Alfvénic solar wind by basing the simulations on observationally derived input data and including a description for the evolution of turbulence in the heliosphere, which is particularly useful for related energetic particle propagation studies.
Appendix A

Non-equidistantly spaced grids

Refining or coarsening the grid underlying a simulation domain is a desirable feature because it can better resolve interesting features of small scales on the one hand, while on the other hand the computational costs can be significantly reduced by using lower resolutions for areas of low variability. A powerful technique to achieve this goal is the adaptive mesh refinement (AMR) algorithm (Berger and Colella, 1989) that refines or coarsens a grid during run-time according to some prescribable criterion in the simulation data (e.g. gradients in density). Implementing AMR is a challenging task, especially for non-Cartesian geometries and highly-parallelized systems. AMR is currently not implemented in the CRONOS framework, but may be addressed in a future release.

Alternatively, one can consider a grid that, although it is not adapting itself during runtime, can be predefined to be finer or coarser in respective regions depending on the expected scale of changes in the simulation. Currently ongoing is the implementation of so-called logically rectangular grids (Calhoun et al., 2008) into the CRONOS framework (B. Krebl, priv. comm.). A simpler approach that has found its way into the CRONOS framework already is to prescribe the spacing between neighboring grid points for a given direction not to be constant but varying according to some function of the user’s choice. In the two following sections a general overview of these non-equidistantly spaced grids (NESGs) will be given first, followed by considerations important for the case subject to this thesis, namely spherical coordinates and the application to the solar wind.

A.1 General overview

Given a certain direction \( p \in \{x, y, z\}, \{\rho, \varphi, z\}, \{r, \vartheta, \varphi\} \) of the chosen coordinate system, the location of a grid point in that direction depending on that grid points integer index \( i \) \((0 \leq i \leq N_p - 1)\), where \( N_p \) specifies the total number of grid points in that direction, can be calculated via

\[
p(i) = p_{\text{beg}} + f(\xi)(p_{\text{end}} - p_{\text{beg}}).
\]

(A.1)
APPENDIX A. NON-EQUIDISTANTLY SPACED GRIDS

The respective beginning and end of the computational domain in that direction are denoted $p_{\text{beg}}$ and $p_{\text{end}}$. While for convenience $\xi = i/(N_p - 1)$ is introduced. It is obviously mandatory for the grid-generating function $f$ to fulfill $f(0) = 0$ and $f(1) = 1$ in order to get $p(0) = p_{\text{beg}}$ and $p(1) = p_{\text{end}}$. Furthermore, $f(\xi)$ should be a monotonically increasing function so that $0 \leq f \leq 1$. Otherwise grid points could on the one hand be located outside the desired grid extent, i.e. beyond $p_{\text{end}}$ or below $p_{\text{beg}}$, or on the other hand a subsequent grid point $i_2 > i_1$ could be located before the previous one ($p(i_2) < p(i_1)$).

The class of equidistantly spaced-grids can be realized by choosing

$$f_{\text{lin}}(\xi) = \xi,$$  \hspace{1cm} (A.2)

which clearly satisfies the above demands and results in a constant grid point distance

$$\Delta p = p(i + 1) - p(i) = \frac{p_{\text{end}} - p_{\text{beg}}}{N_p - 1}.$$  \hspace{1cm} (A.3)

This is the standard case in the CRONOS setup. Another pre-implemented choice employs an exponential approach via

$$f_{\text{exp}}(\xi) = \left(\frac{p_{\text{end}}}{p_{\text{beg}}}\right)^\xi - 1,$$  \hspace{1cm} (A.4)

resulting in $p(i) = p_{\text{beg}}\left(\frac{p_{\text{end}}}{p_{\text{beg}}}\right)^\xi$, the latter clearly showing the exponential character. Simple algebra gives

$$\Delta p(i) = p(i) \cdot \left(\left(\frac{p_{\text{end}}}{p_{\text{beg}}}\right)^{\frac{1}{N_p - 1}} - 1\right),$$  \hspace{1cm} (A.5)

so that the cell size is linearly increasing in this case.

Both the linear and the exponential realization are visualized in Figure A.1, in which a one-dimensional grid from $p_{\text{beg}} = 1$ to $p_{\text{end}} = 100$ is resolved with $N_{p,\text{lin}} = 100$ grid points, while much less points (see Equation (A.7)) are required for the exponential realization. The left panel shows the grid point location $p(i)$ against the grid point index $i$, where the linear/exponential character of the grid-generating function is evident. The right panel visualizes the variations of grid point distance $\Delta p$ with grid point location $p$, which was shown to be constant/linear for the linear/exponential grid-generating function.

The benefit of such adapted grids is the option to put resolution where it is needed, which results in reduced computational costs due to (i) fewer required grid points and (ii) a possibly enhanced global time-step which is directly proportional to the smallest cell-size in the simulation domain according to the CFL condition $\Delta t \propto \min\{\Delta p_j\}$ (geometrical factors in curvilinear coordinate system have been neglected in this statement).
A.2 Application

In the light of this work there are two aspects that make NESGs a useful tool: on the one hand, heliospheric structures become smeared out (global merged interaction regions) with increasing distance and a coarser grid is applicable, which also reduces the required computer resources. On the other hand the employed spherical grids can contain the polar axis as singularities resulting in increasingly small grid point distances in the azimuthal direction towards the poles\footnote{Alternative approaches to overcoming this problem usually involve compositions of several (rotated) spherical grids, such as, e.g., the Yin-Yang grids (Laukert, 2008), the six-component grid (Feng et al., 2010), or the composite grid (Usmanov et al., 2012). A drawback of these implementations is the required increased overhead due to communication between the grids and respectively more difficult boundary conditions, as well as a loss of conservative properties at the interfaces.}, which is an effect that can also be significantly reduced by choosing an appropriate NESG\footnote{In the first two publications of this thesis this problem was circumvented by leaving out the polar regions as the required features of NESGs and handling of coordinate singularities were not available at the time.}. These two aspects can be addressed by NESGs for the radial coordinate $r$ and the polar angle $\vartheta$. Naturally the question arises whether there exists some suitable function for the azimuthal angle $\phi$ as well. Unfortunately, this is not the case, which can be easily understood by considering the evolution of a CIR (see, e.g., Figure 12 in Wiengarten et al. (2014)), which is obviously not constrained in azimuth but with increasing radial distance covers an ever larger interval, so that a refinement at some specific $\phi$ would not permanently coincide with the CIR. It should also be kept in mind that the grid-generating function can only depend on the respective directions index, and not on some other directions index, i.e. a refinement in $\varphi$ depending on $r$ or $\vartheta$ is not possible, since this would result in non-orthogonal grids. Therefore, for the purposes described in this work, only the $r$ and $\vartheta$ directions can be used in the

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figureA1}
\caption{Illustration of linear and exponential grid-generating functions.}
\end{figure}
context of NESGs, as will be shown in the subsequent sections.

A.2.1 NESG for the radial direction

A modified version of the exponential grid described in Section A.1 is suitable, for which it is also possible to alter the largest cell sizes towards the outer boundary by means of the parameter $a > 0$, where larger values result in exceedingly coarser grids, i.e. the respectively adapted linearly increasing grid point distance (Equation (A.5)) becomes steeper. The grid-generating function in this case reads

$$f_{MODexp}(\xi) = \left( \frac{p_{\text{end}}}{p_{\text{beg}}} \right)^a \xi - 1. \quad (A.6)$$

It is often desirable to fix the smallest cell size $\Delta r|_{r_{\text{beg}}} = r(i = 1) - r(i = 0)$ because the smallest radial cell size usually determines the global time step according to the CFL condition. For fixed $a$ and $\Delta r|_{r_{\text{beg}}}$ the number of grid points becomes

$$N_r = a \ln \left( \frac{r_{\text{end}}}{r_{\text{beg}}} \right) \left[ \ln \left( \frac{\Delta r|_{r_{\text{beg}}}}{r_{\text{end}} - r_{\text{beg}}} \frac{(r_{\text{end}}/r_{\text{beg}})^a - 1}{r_{\text{end}} - r_{\text{beg}}} \right) + 1 \right]^{-1}, \quad (A.7)$$

which has to be rounded to integer values, so that the chosen $\Delta r|_{r_{\text{beg}}}$ will be fulfilled only approximately. Of course $a$ can also be respectively adapted for fixed $\Delta r|_{r_{\text{beg}}}$.

Another important feature that such a grid should provide is the possibility to solve the grid-generating function uniquely for the index $i$. It is easy to show that this is possible for the grids presented in the general overview above, as well as for the grid presented here, yielding

$$i(r) = \frac{N - 1}{a} \ln \left( \frac{r(i) - r_{\text{beg}}}{r_{\text{end}} - r_{\text{beg}}} \left( \frac{r_{\text{end}}}{r_{\text{beg}}} \right)^a - 1 \right) \left[ \ln \left( \frac{r_{\text{end}}}{r_{\text{beg}}} \right) \right]^{-1}. \quad (A.8)$$

This feature is important for the subsequent use of the simulation results in different codes, which need values at intermediate locations, for which the desired quantities have to be interpolated from the stored values at neighboring grid points.

To give an impression of the achievable savings as compared to a linear grid a simulation box is considered as used in Wiengarten et al. (2015) of a radial extent $r \in [0.3, 100]$ AU and a desired smallest cell size at the inner boundary of $\Delta r = 10R_\odot$. A linear grid would require $N_{r,\text{lin}} \approx 2144$, while with $a = 0.55$ the exponential grid comprises of $N_{r,\text{modEXP}} = 300$ with a largest cell size at the outer boundary of roughly 1 AU.

A.2.2 NESG for the polar angle

Instead of leaving out the polar singularity, the idea is to have two cones, each consisting of a large cell at the two polar caps, while maintaining a linear grid for
the remaining cells. The cell centers of the larger polar cells are then separated sufficiently from the polar axis to avoid the undesired small azimuthal cell diameter that would lead to small time steps. A further advantage as compared to leaving out the polar regions is the application of more realistic boundary conditions: while formerly either extrapolating or reflecting boundary conditions had to be applied at the polar angle’s outer boundaries (see Section 1.2.2 and Wiengarten (2011)), the formal inclusion of the polar axis uses boundary conditions via the adjacent, azimuthally opposite (shifted by \( \pi \)) cells of the simulation domain as ghost-cells, which is self-consistent.

Figure A.2: Same as Figure A.1, but for an NESG for the polar angle \( \vartheta \in [0^{\circ}, 180^{\circ}] \) with polar cell sizes \( G = 18^{\circ} \) and an otherwise constant cell size of \( 2^{\circ} \).

The grid-generating function can be derived as follows: first the relative size of the large polar cells \( G \) (for gap) with respect to the extent of the grid in that direction is introduced. Then, the ansatz for a linear function \( f(\xi) = m\xi + b \) is taken, where the slope for the linear part of the grid follows as

\[
m = \frac{\Delta f}{\Delta \xi} = \frac{1 - 2G}{(N_{\text{lin}} - 1)/N_{\text{lin}} - 1/N_{\text{lin}}} = N_{\text{lin}} \frac{1 - 2G}{N_{\text{lin}} - 2} \quad (A.9)
\]

where \( N_{\text{lin}} \) is the number of grid points that would be required to have the whole polar angle covered with a linear grid of the desired constant cell size, e.g. for a cell size \( \Delta \vartheta = 1^{\circ} \), \( N_{\text{lin}} = \pi/1^{\circ} = 180 \). The first and last grid point are set manually by requiring them to be separated by \( G \) from the polar axis, i.e. \( f(1/N_{\text{lin}}) = G \) and \( f(1 - 1/N_{\text{lin}}) = 1 - G \), while the grid generating function for the part of constant cell size is

\[
f(\xi) = N_{\text{lin}} \frac{1 - 2G}{N_{\text{lin}} - 2} \xi + \frac{N_{\text{lin}}G - 1}{N_{\text{lin}} - 2}. \quad (A.10)
\]

The actually required number of grid points then is \( N = hN_{\text{lin}} + 2 \) with

\[
h = f(N_{\text{lin}} - 1/N_{\text{lin}}) - f(1/N_{\text{lin}}) = 1 - 2G.
\]
APPENDIX A. NON-EQUIDISTANTLY SPACED GRIDS

First tests showed that the savings due to the reduced number of grid points can be about 15% in computing time, while the time step can be significantly enhanced up to 500% for a typical value of $G = 0.1\pi$ and $N_{\varphi} = 180$.

A.3 Implementation

The implementation of the new grid-generating functions described above is realized in CRONOS by additional classes as described in the CRONOS Manual (J. Kleimann, priv. comm.). The respective code fragment can be found below, where especially the mirrored ghost-cells for the NESG for the polar angle are of interest.

```cpp
/*** USER SPECIFIED GRID LAYOUTS HERE ***/

/**** EXP GRID ******/

class GridFunction_modEXP: public Interface_GridFunction {
public://class declaration with public functions
  GridFunction_modEXP(REAL, REAL, REAL); //constructor
  virtual REAL get_gridFunc(REAL); //get-function
private://private variables
  REAL domain_begin, domain_end, domain_len; //corresponding to the p's in Eq.(A.1)
  REAL a; //parameter a from Section A.2.1
};

GridFunction_modEXP::GridFunction_modEXP(REAL domain_begin, REAL domain_end, 
  REAL domain_len) {
  this->domain_begin = domain_begin;
  this->domain_end = domain_end;
  this->domain_len = domain_len;
  this->a = value((char*)"stretch_expGrid");
}

// function gives 0 at ratio=0 and 1 at ratio=1
REAL GridFunction_modEXP::get_gridFunc(REAL ratio) {
  //Function return value according to Eq. (A.6)
  return (pow(domain_end/domain_begin,a*ratio)-1.0)/(pow(domain_end/domain_begin,a)-1.0);
}

/**** LIN_POLES GRID with one big cell at poles ******/

class GridFunction_LIN_POLES: public Interface_GridFunction {
public://class declaration with public functions
  GridFunction_LIN_POLES(REAL, REAL, REAL);
  virtual REAL get_gridFunc(REAL);
private://private variables
  REAL domain_begin, domain_end, domain_len; //corresponding to the p's in Eq.(A.1)
  REAL gap; //G
  REAL N; //N_{lin}
};

GridFunction_LIN_POLES::GridFunction_LIN_POLES(REAL domain_begin, REAL domain_end, 
  REAL domain_len) {
  this->domain_begin = domain_begin;
  this->domain_end = domain_end;
  this->domain_len = domain_len;
  this->gap = value((char*)"gap");
  this->N = value((char*)"N_lin");
}

/**** LIN_POLES GRID with one big cell at poles ******/

class GridFunction_LIN_POLES: public Interface_GridFunction {
public://class declaration with public functions
  GridFunction_LIN_POLES(REAL, REAL, REAL);
  virtual REAL get_gridFunc(REAL);
private://private variables
  REAL domain_begin, domain_end, domain_len; //corresponding to the p's in Eq.(A.1)
  REAL gap; //G
  REAL N; //N_{lin}
};

GridFunction_LIN_POLES::GridFunction_LIN_POLES(REAL domain_begin, REAL domain_end, 
  REAL domain_len) {
  this->domain_begin = domain_begin;
  this->domain_end = domain_end;
  this->domain_len = domain_len;
  this->gap = value((char*)"gap");
  this->N = value((char*)"N_lin");
}
```

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A.3. IMPLEMENTATION

this->domain_len = domain_len;
this->gap = value((char*)"gap_poleGrid");

size of large polar cell with respect to grid extent
e.g. gap=0.1 refers to a polar cell size of 0.1*180.0[deg] = 18[deg]

this->N = value((char*)"Nlin_poleGrid");

// function gives 0 at ratio=0 and 1 at ratio=1
REAL GridFunction_LIN_POLES::get_gridFunc(REAL ratio) {
    int adapted = 0; //switch for adapting mapped (opposite/shifted by pi) polar cells
    if (domain_begin < 0.01)
        if (ratio < 0){ //top direction
            ratio = -ratio; //take mirrored (positive) cells value, but return negative f below
            adapted = 1;
        } // Taking a linear function leaving out the polar cells gives Eq. (A.10):
    if (ratio > 1){ //bottom direction
        ratio = 1.0 - (ratio-1.0); //mirror at 1
        adapted = 2;
    } //but has to be set manually to f(0)=0 and f(1)=1
    if (adapted == 1) f=-f;
    if (adapted == 2) f=1.0*(1.0-f);
    return f;
}
Bibliography


BIBLIOGRAPHY


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I thank my whole family and all of my friends for always being there for me and – occasionally – taking my mind off work.
# Curriculum vitae

## Personal data

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<thead>
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<th>Tobias Wiengarten</th>
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## Education

<table>
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<tr>
<th>Date</th>
<th>Degree</th>
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</tr>
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<tbody>
<tr>
<td>since 11/2011</td>
<td>Ph.D.</td>
<td>Ruhr-Universität Bochum</td>
<td>Numerical modeling of plasma structures and turbulence transport in the solar wind</td>
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<td>08/1997 – 06/2006</td>
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<td>Aldegrever Gymnasium Soest</td>
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## Publications


Conference and workshop participations

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<tr>
<td>03/2015</td>
<td><em>DPG Spring-meeting Wuppertal</em>; Talk:</td>
<td>Incorporating Turbulence Transport in the CRONOS MHD framework</td>
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<tr>
<td>02/2015</td>
<td><em>Workshop on Reconnection, Turbulence, and Particles in the Heliosphere</em> in Queenstown, New Zealand; Talk: Coupling Turbulence Transport and WSA-driven MHD simulations</td>
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<td>01/2015</td>
<td><em>Workshop Cosmic Rays in Astrospheres</em> in Bad Honnef</td>
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<td>03/2014</td>
<td>Workshop <em>Cosmic Rays: From the Galaxy to the Heliosphere; a numerical modeling approach</em> in Potchefstroom, Southafrica; Talk: Modeling heliospheric background solar wind using the CRONOS MHD code</td>
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<tr>
<td>01/2014</td>
<td><em>ISSI Team Meeting Heliosheath Processes and Structure of the Heliopause: Modeling Energetic Particles, Cosmic Rays, and Magnetic Fields</em> in Bern, Switzerland</td>
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<tr>
<td>12/2013</td>
<td><em>AGU Fall Meeting</em> in San Francisco, USA; Poster: MHD simulations: Corotating Interaction Regions</td>
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<td>09/2013</td>
<td><em>Space Science Training Week 2013: Data Driven Modeling and Forecasting</em> in Leuven, Belgium; Book award for best formulated research proposal</td>
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<tr>
<td>07/2013</td>
<td><em>8th International Conference of Numerical Modeling of Space Plasma Flows (ASTRONUM 2013)</em> in Biarritz, France; Talk: MHD simulations: Corotating Interaction Regions</td>
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<td>03/2013</td>
<td>527. Wilhelm und Else Heraeus-Seminar: Plasma and Radiation Environment in Astrospheres and Implications for the Habitability of Extrasolar Planets in Bad Honnef; Poster: MHD simulations of the inner heliosphere</td>
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<td>09/2012</td>
<td><em>9th Heidelberg Summer School: Computational Astrophysics</em></td>
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<tr>
<td>03/2012</td>
<td><em>DPG Spring-meeting Stuttgart</em>; Talk: MHD Simulation of the Inner-Heliospheric Magnetic Field</td>
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<td>07/2011</td>
<td><em>Joint Space Weather Summer School 2011</em> in Huntsville, USA</td>
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Soest, July 7, 2015

Tobias Wiengarten