Toward a Quantitative Model for Simulation and Forecast of Solar Energetic Particle Production during Gradual Events. I. Magnetohydrodynamic Background Coupled to the SEP Model

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Abstract
Solar energetic particles (SEPs) are an important aspect of space weather. SEP events possess a high destructive potential, since they may cause disruptions of communication systems on Earth and be fatal to crew members on board spacecraft and, in extreme cases, harmful to people on board high-altitude flights. However, currently the research community lacks efficient tools to predict such a hazardous threat and its potential impacts. Such a tool is a first step for mankind to improve its preparedness for SEP events and ultimately to be able to mitigate their effects. The main goal of the presented research effort is to develop a computational tool that will have the forecasting capability and can serve as an operational system that will provide live information on the current potential threats posed by SEP based on the observations of the Sun. In the present paper we discuss the fundamentals of magnetohydrodynamical simulations to be employed as a critical part of the desired forecasting system.

Key words: solar wind – Sun: coronal mass ejections (CMEs) – Sun: particle emission

1. Introduction
1.1. Potential Threats of Solar Energetic Particles
For our technologically advanced civilization, space plays an increasingly important role. The idea of interplanetary travel and even establishing colonies on the Moon and Mars slowly but steadily transitions from science fiction into the realm of plausibility. However, fascinating as the perspectives could sound, our ability to predict dangers that we may encounter along the way needs to be significantly improved. The dangers themselves, however, are not unknown to us. One of them comes from our Sun in the form of solar energetic particles (SEPs). Triggered by extreme solar events, SEP fluxes may reach values that are damaging to the electronics on board spacecraft and potentially fatal to the crews (e.g., Joyce et al. 2015). Precedents of SEP events of such ominous scale have been recorded in recent history.

During the Apollo program, when astronauts repeatedly visited the Moon, a huge SEP event accompanied the major 1972 August solar storm. The integrated SEP flux produced by this storm could have been fatal for Moon-walking astronauts since the radiation dose from energetic particles penetrating their spacesuits would have exceeded the lethal level (~400 rem in a short period of time). Luckily, during this event the Apollo 16 astronauts were already safely back on Earth, while the crew of Apollo 17 was still preparing for their mission. An SEP event during the historic “giant leap for mankind” lunar landing could have been fatal. NASA, as well as the entire world, was lucky that the Sun “cooperated” with this endeavor.

However, when planning interplanetary human missions, one cannot rely on luck. A mission to Mars and back will take several years, and there is a significant risk of having one or more extreme SEP events that “may expose the crew to doses that lead to acute radiation effects.” The fact that we cannot predict SEP events makes a human mission to Mars a “high-risk adventure” (Jäkel 2004; Hellweg & Baumstark-Khan 2007). Let us come back to Earth and consider the harmful effects of SEP events on assets at Low Earth Orbit (LEO). The terrestrial magnetic field provides some shielding for the International Space Station, as well as the majority of unmanned missions from SEPs. However, extreme SEP events, such as that of 2005 January 20 (e.g., Grechnev et al. 2008; Matthiä et al. 2009), have hard energy spectra, and they are particularly rich in hundreds of MeV to several GeV protons. A significant fraction of flux of the high-energy particles, which have a high penetrating capability, can reach LEO, thus producing significant radiation hazard for human spacecraft. Comparing with the direct threat to human life and health, the SEP effect on unmanned satellites on LEO may seem to be not so important. However, the possible loss of entire satellites with their expensive computers, sensors, and other elements of electronics is not limited to the cost (typically hundreds of millions of dollars) of the satellite itself. Many satellites are integrated into vitally important systems of defense, rescue, and navigation, so the disruption of such systems may have catastrophic consequences.

Even closer to Earth is the ozone (O3) layer in the stratosphere. This layer protects Earth against harmful solar UV and EUV emissions, and the depletion of the ozone layer would increase the number of skin cancer cases in the human population. The higher-energy SEPs can reach the stratosphere. In particular, the SEP event in 1972 August reduced the ozone concentration near the north geomagnetic pole by ~20%; this reduction lasted for ~20 days, i.e., well after the end of the SEP event (Heath et al. 1977). The reason is that very large SEP
events can increase the ionization degree in the stratosphere by more than a factor of 100 over quiet times (see Makhmutov et al. 2009). The increased ionization initiates a chain of chemical reactions that produce so-called “odd nitrogen” molecules, like NO, which cannot be created from the even nitrogen molecule, N₂. Molecules like NO catalyze the ozone decay, and each odd nitrogen molecule can “kill” millions of O₃ molecules.

Among other threats, SEP events and their increased radiation hazard make flight routes over the North Pole more challenging, because of the increased risk of radiation exposure and interference with communication in the high-frequency range (Morris 2007).

We see that some effects of extreme SEP events are only important at higher latitudes near the geomagnetic poles, approximately in the same regions where auroras are often observed. However, during relatively infrequent but more powerful events, such as the Carrington event of 1859, the aurora had been observed as far from geomagnetic poles as in Hawaii, Miami, or Jerusalem (Cliver 2006; Green et al. 2006; Green & Boardsen 2006; Shea et al. 2006; Shea & Smart 2006). For such events, the area in which the ozone layer is depleted may also extend well beyond the polar region, and this would last longer. Air traffic may be interrupted all over the world. We know that such unique events may happen, but we do not know how it would affect modern technology.

These are the main reasons why SEP events are considered as one of the most important aspects of space weather. This explains the need for a predictive technology that is capable of providing a reliable quantitative forecast of SEP events and their impacts.

1.2. Mechanisms of SEP Production

First observations of “solar cosmic rays,” as SEPs were referred to at the time, date back to 1942 (see Forbush 1946) and were immediately linked to solar flares that preceded these particle events. This hypothesis was further supported by observations that followed, and solar flares were considered to be the primary source of SEPs (Meyer et al. 1956). As the number of observed events increased, it became apparent that features of events, such as the aforementioned composition, duration, etc., exhibit a wide variability (Wild et al. 1963). The discovery of coronal mass ejections (CMEs) prompted formulation of a new hypothesis that SEPs are produced by interplanetary shocks that often accompany flares rather than by flares themselves (Kahler et al. 1978; Gosling 1993).

The debate ultimately resulted in the commonly adopted paradigm (e.g., Ruffolo et al. 1998; Reames 1999, 2002; Cliver 2009) that states that SEP events can be divided into two distinct classes: (1) impulsive events and (2) gradual events. The former are caused by solar flares, while the latter are associated with CMEs. Gradual events are prolonged in time and more extended in longitudinal range compared to the impulsive events. Also, SEP composition was found to be a good indicator of the nature of events (Cane et al. 2006), e.g., flare-associated events have Fe/O abundance of ~1 and are electron-rich, while those associated with CME-driven shocks have Fe/O abundance of ~0.1 and are proton-rich.

It should be noted that the pattern above was originally discovered for particles of energies that are limited by ~30 MeV. Such particles are easily detected by instruments outside Earth’s magnetosphere. For this reason, many models focus on this particular part of the particle population. However, the particles that pose the largest threat are those that exceed this energy, and for them the aforementioned pattern is much less clear. Based on compositional and other data, many large SEP events show signatures of both gradual and impulsive events and, thus, do not fully agree with the simple bimodal paradigm (e.g., Cohen et al. 1999; Mazur et al. 1999). Cohen et al. (2008) explain the discrepancy by simultaneous particle production at both flare sites and CME shock fronts, while Tylka et al. (2005) suggest that there is no true separation of events into two distinct categories: the seed suprathermal particle population originates in flares and is then accelerated by CME-driven interplanetary shocks. In both of these explanations, signatures of both types of events naturally arise in large SEP events. These events are frequently associated with so-called ground-level events (GLEs), as most energetic particles have the potential to penetrate Earth’s magnetosphere and ionosphere (Shea & Smart 1990, 1994, 2012; Gopalswamy et al. 2014). Relevant data are provided by measurements performed with neutron monitors. Analysis of properties of GLEs and those of associated solar flares and CMEs (e.g., Gopalswamy et al. 2012; Kahler et al. 2012) confirms that SEP production is likely to involve both types of events. Further observations, e.g., by the AMS-02 instrument (Aguilar et al. 2015), will provide valuable insights into this problem. In our work, we focus primarily on gradual, shock-driven events.

Solar eruptions, including CMEs, are associated with a major restructuring of the coronal magnetic field and the ejection of solar material (~10^{12}−13 kg) and magnetic flux (~10^{15} Wb) into interplanetary space (e.g., Roussev & Sokolov 2006). A shock wave driven by the ejecta can accelerate charged particles to ultrarelativistic energies as a result of Fermi acceleration processes (Fermi 1949). The diffusive shock acceleration (DSA) is a profound mechanism that naturally produces the observed power-law spectra of energetic particles. It was first proposed by Krymsky (1977), Axford et al. (1977), Bell (1978a, 1978b), and Blandford & Ostriker (1978) to explain the origin of galactic cosmic rays (GCRs); however, for the past four decades, this mechanism has been studied extensively also in the context of corotating and traveling interplanetary shocks and has been demonstrated to be well supported by both theory (e.g., Lee 1997; Ng et al. 1999, 2003; Zank et al. 2000) and observations (e.g., Kahler 1994; Tylka et al. 1999, 2005; Cliver et al. 2004).

The most efficient particle acceleration takes place near the Sun at heliocentric distances of 2 ÷ 5 Rₖ, and the fastest particles can escape upstream of the shock, then propagating along the lines of the interplanetary magnetic field (IMF) and reaching Earth shortly after the initiation of the CME (~1 hr).

The theory of DSA is being debated within the community (Reames 1999, 2002; Tylka 2001), since very little is known from observations about the dynamical properties of CME-driven shock waves in the inner corona soon after the onset of an eruption. The main argument against the shock origin is that near the Sun the ambient Alfvén speed is so large, due to the strong magnetic fields there, that a strong super-magnetosonic shock wave is difficult to anticipate (Gopalswamy et al. 2001). How soon after the onset of a CME the shock wave forms, and how it evolves in time, depends largely on how this shock wave is driven by the erupting coronal magnetic fields.
To address the issue of shock origin during CMEs, it is required that real magnetic data are incorporated into a global model of the solar corona (SC), as had been done in, e.g., Roussev et al. (2004). As proposed by Tylka et al. (2005), the shock geometry plays a significant role in the spectral and compositional variability of SEPs above ~30 MeV nucleon\(^{-1}\). Therefore, in order to explain the observed signatures of gradual SEP events, global models of solar eruptions are required to explain the time-dependent changes in the strength and geometry of shocks during these events. The CME-driven shock continues to accelerate particles, and the shock passage at 1 au is often accompanied by an enhancement of the energetic particle flux. To simulate this effect, the shock wave evolution should be continuously traced while it propagates to 1 au.

1.3. Goal and Content of the Paper

The goal of our current and future research is to develop the computational framework embracing several coupled physical and numerical models, which could quantitatively simulate the SEP production during the gradual events while ultimately achieving a capability to predict the SEP flux and spectrum (or, at least, the probability of dangerously high flux and related radiation hazard).

In the series of two papers we outline the framework and describe its existing components. The present paper is the first in the series, which contains the review of the magnetohydrodynamical (MHD) component of the framework. The second paper will describe the kinetic component of the framework.

Some of the computational models or their couplings are still underdeveloped. Therefore, the paper mostly focuses on presenting the physical and mathematical fundamentals of the integrated model, as well as on the description of the available computational tools and their integration into the framework, rather than on the particular results of the models. Some numerical results here are provided only to illustrate the operation of the models. From the brief discussion above we can summarize which computational tools and technologies are needed to achieve the claimed research goal, and therefore what should be included in the desired computational framework.

First, one needs to simulate a full 3D structure of the IMF prior to CME, which determines the magnetic connectivity and allows us to simulate the SEP transport along the magnetic field lines toward 1 au. One also needs to know the 3D distribution of the solar wind parameters. This ambient solution affects the CME and shock wave travel time to 1 au, and hence the time of SEP enhancement in the course of the shock wave passage. The pre-eruptive structure of the SC should also be known, since it controls the possibility for the shock wave formation at small heliocentric distances, which results in efficient DSA, as well as the magnetic connectivity of the active region (AR), at which CME originates, to the upper SC. To simulate the ambient solution in the SC and inner heliosphere (IH), the Alfvén-wave-turbulence-based solar atmosphere Model (AWSoM) is used as described in this paper in Section 2.1. In order to simulate an ongoing CME and to reach the predictive capability, the model should run faster than the real time; therefore, the AWSoM-R model with this feature is utilized (presented in Section 2.2). The CME-driven shock wave should be simulated starting from the lower altitude. Relevant models are described in Section 3.

The overview of MHD models and tools presented in this paper would not be complete without demonstrating how they fit into the overall framework and what makes them an irreplaceable piece in the puzzle. This requires a summary, however brief, of a particle code utilized in simulations (Section 4). We conclude the paper with the proof-of-concept results obtained with the help of our newly developed SEP forecasting framework (Section 5). Again, a detailed summary of physical models and numerical tools that will be used to describe the kinetic component of the framework are to be considered in the second paper of the series.

2. Alfvén-wave-turbulence-driven MHD Description of the SC and the Solar Wind

2.1. Steady-state SC and Solar Wind

In any predictive model for eruptive solar events, the background steady-state SC and IH are as important as a stage for a performance. If poorly designed, the foundation would compromise the whole facility. Thus, an accurate and carefully validated model for the steady-state background is vital and should not be overlooked or explored superficially. In our work we use a widely accepted paradigm that the solar wind is driven by and the SC is heated by the dissipation in the Alfvén wave turbulence.

2.1.1. Alfvén Wave Turbulence

The concept of Alfvén waves was introduced more than 70 years ago by Alfvén (1942). The importance of the role they play within the solar system was not immediately recognized owing to the lack of relevant observations. Results from Mariner 2 allowed a data-backed study of wave-related phenomena in solar wind. A detailed analysis of these observations can be found in, e.g., Coleman (1966, 1967). This pioneering study culminated in Coleman (1968), a work that stated that Alfvén wave turbulence has the potential to drive solar wind in a way that is consistent with observations at 1 au.

Attention to Alfvén-wave-related phenomena was continuously increasing, and an ever-growing number of studies on interaction of these waves with solar wind plasma and various aspects of associated effects were undertaken. Examples of the earliest efforts to investigate the role of Alfvén waves in solar wind acceleration are Belcher et al. (1969), Belcher & Davis (1971), and Alazraki & Couturier (1971). A consistent and comprehensive theoretical description of Alfvén wave turbulence and its effect on the averaged plasma motion has been developed in a series of works, particularly Dewar (1970) and Jacques (1977, 1978) (see also references therein). More recent efforts to simulate solar wind acceleration utilize the approach developed in these works (e.g., Usmanov et al. 2000). Currently, it is commonly accepted that the gradient of the Alfvén wave pressure is the key driver for the solar wind acceleration.

At the same time, damping of Alfvén wave turbulence as a source of the coronal heating was extensively studied (e.g., Barnes 1966, 1968). Later, it was demonstrated that reflection from the sharp pressure gradients in the solar wind (Heinemann & Olbert 1980; Leroy 1980) is a critical component of Alfvén wave turbulence damping (Matthaeus et al. 1999; Dmitruk et al. 2002; Verdini & Velli 2007). For this reason, many numerical models explore the generation of reflected counter-propagating waves as the underlying cause of the turbulence...
energy cascade (e.g., Cranmer 2010), which transports the energy of turbulence from the large-scale motions across the inertial range of the turbulence spatial scale to short-wavelength perturbations. The latter can efficiently damp owing to the wave–particle interaction. In this way, the turbulence energy is converted to the particle (thermal) energy. Recent efforts of many studies are aimed at developing models that include Alfvén waves as a primary driving agent for both heating and acceleration of the solar wind. Examples are Hu et al. (2003), Suzuki & Inutsuka (2005), Verdi et al. (2010), Matsumoto & Suzuki (2012), and Lionello et al. (2014a, 2014b).

2.1.2. Ad Hoc Coronal Heating Functions and Semi-empirical Models for the Solar Wind Heating

It is important to emphasize that while incorporating the Alfvén-wave-driven acceleration is a matter of including the wave pressure gradient in governing equations (Jacques 1977), there is still no widely accepted approach to describing the coronal heating via Alfvén wave turbulence cascade. A large number of models of SC heating have been constructed over the years. One can trace two major approaches to representing the process: (i) to use an ad hoc heating function to mimic SC heating with heating rate being chosen to better fit observations, and (ii) to use a semi-empirical coronal heating function that is based on aspects of physics of Alfvén waves.

The former approach is utilized, for example, by Lionello et al. (2001, 2009), Riley et al. (2006), Titov et al. (2008), and Downs et al. (2010). This method provides a reasonably good agreement with observations in EUV, X-rays, and white light. The agreement looks particularly impressive for the Predictive Science Inc. (PSI) predictions about the solar eclipse image (Mikić et al. 2007). An important limitation is that models utilizing an ad hoc approach depend on a few free parameters, which need to be determined for various solar conditions. Such an approach has an inherent shortcoming: although it is well suited for typical conditions, it cannot properly account for unique conditions such as those that can take place during extreme solar events.

Another illustration of the ad hoc approach is the semi-empirical model to simulate solar wind. For example, the Wang–Sheeley–Arge (WSA) model, instead of incorporating physical properties of Alfvén waves, utilizes semi-empirical formulæ that relate the solar wind speed to the solar magnetogram and the properties of the magnetic field lines of the potential magnetic field as recovered from the synoptic magnetogram. Its development history may be traced through Wang & Sheeley (1990, 1992, 1995), Arge & Pizzo (2000), and Arge et al. (2003). The major benefit of the model is the opportunity to seamlessly integrate it into a global space weather simulation as was done in Cohen et al. (2007). In this study, the WSA formulæ were used as the boundary condition for the MHD simulator via the varied polytropic gas index distribution (see Roussev et al. 2003b). Models mentioned above successfully explain observations of the solar wind parameters at 1 au.

A number of validation and comparison studies have been published (Owens et al. 2008; Vásquez et al. 2008; MacNeice 2009; Norquist & Meeks 2010; Gressl et al. 2014; Jian et al. 2015; Reiss et al. 2016). However, these models do not fully capture the physics of Alfvén wave turbulence or even disregard it altogether. Even though some models are designed to account for the Alfvén waves’ physics (such as Cohen et al. 2007), none capture every aspect of the interaction of the turbulence with the background flow, which includes both energy and momentum transfer from the turbulence to the solar wind plasma. Thus, none of such models can be used as a fully consistent tool for simulating the solar atmosphere.

2.1.3. Alfvén-wave-turbulence-based Model for the Solar Atmosphere

The ad hoc elements were eliminated from the model for the SC and quiet-time IH by Sokolov et al. (2013). In AWSO the plasma is heated by the dissipation of the Alfvén wave turbulence, which, in turn, is generated by the nonlinear interaction between oppositely propagating waves (Hollweg 1986). Within the coronal holes, there are no closed magnetic field lines; hence, there are no oppositely propagating waves. Instead, a weak reflection of the outward-propagating waves locally generates sunward-propagating waves as quantified by van der Holst et al. (2014). The small power in these locally generated (and almost immediately dissipated) inward-propagating waves leads to a reduced turbulence dissipation rate in coronal holes, naturally resulting in the bimodal solar wind structure. Another consequence is that coronal holes look like cold black spots in the EUV and X-rays images, while the closed-field regions are hot and bright, and the brightest are ARs, near which the wave reflection is particularly strong (see Oran et al. 2013; Sokolov et al. 2013; van der Holst et al. 2014).

The model equations are the following:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0, \tag{1}
\]

\[
\frac{\partial B}{\partial t} + \nabla \cdot (\rho B - Bu) = 0, \tag{2}
\]

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot \left( \rho uu - B B \right) + \nabla \left( P_i + P_e + \frac{B^2}{2 \mu_0} + P_a \right) = -\frac{GM_0}{R^3}, \tag{3}
\]

The notation used in the equations is as follows: \( \rho \) is the mass density, \( u \) is the velocity, \( u = \left| u \right| \) (assumed to be the same for the ions and electrons), \( B \) is the magnetic field, \( B = \left| B \right| \), \( G \) is the gravitational constant, \( M_0 \) is the solar mass, \( r \) is the position vector relative to the center of the Sun, \( R = \left| R \right| \), and \( \mu_0 \) is the magnetic permeability of vacuum. As has been shown by Jacques (1977), the Alfvén waves exert an isotropic pressure (see term \( \nabla P_a \) in the momentum equation). The relation between the wave pressure and wave energy density is \( P_a = (w_i + w_e)/2 \). Here \( w_i \) are the energy densities for the turbulent waves propagating along the magnetic field vector \( (w_i) \) or in the opposite direction \( (w_e) \). The isotropic ion pressure, \( P_i \), and electron pressure, \( P_e \), are governed by the
energy equations:
\[
\frac{\partial}{\partial t} \left( \frac{P_i}{\gamma - 1} + \frac{\rho u^2}{2} + \frac{B^2}{2\mu_0} \right) + \nabla \cdot \left( \rho \frac{\rho u^2}{\gamma - 1} + \frac{\rho B^2}{\mu_0} \right) - B(u \cdot B) + \frac{\nabla \cdot \left( P_i \right)}{\gamma - 1} = - (u \cdot \nabla)(P_i + P_e) + \frac{N_e N_i k_B T_i}{\gamma - 1} \left( \frac{\nu_{ei}}{N_i} \right) \times (T_e - T_i) - \frac{GM_{\odot} \rho \mathbf{R} \cdot u}{R^3} + Q_i,
\]

(4)

where \( T_{e,i} \) are the electron and ion temperatures, \( N_{e,i} \) are the electron and ion number densities, and \( k_B \) is the Boltzmann constant. Other newly introduced terms are explained below.

The equation of state \( P_i = N_e k_B T_i \) is used for both species. The polytropic index is \( \gamma = 5/3 \). The optically thin radiative energy loss rate in the lower corona is given by

\[
Q_{\text{rad}} = N_e N_i \Lambda(T_i),
\]

(6)

where \( \Lambda(T_i) \) is the radiative cooling curve taken from the CHIANTI version 7.1 database (Landi et al. 2013, and references therein). The Coulomb collisional energy exchange rate between ions and electrons is defined in terms of the collision frequency

\[
\nu_{ei} = \frac{2 \sqrt[m_e]{e \varepsilon_0} \varepsilon_0}{3 \pi \gamma \left( 2 \pi k_B T_e \right)^{3/2}}.
\]

(7)

The electron heat flux \( q_e \) is used in the collisional formulation of Spitzer & Härm (1953):

\[
q_e = \kappa_e \mathbf{b} \cdot \nabla T_e, \quad \kappa_e = 3.2 \frac{6 \pi}{\Lambda_C} \left( \frac{2 \pi \varepsilon_0}{m_e e^2} \right)^{5/2} \frac{k_B T_e}{k_B}.
\]

(8)

where \( m_e \) and \( e \) are the electron mass and charge, \( m_p \) is the proton mass, \( \varepsilon_0 \) is the vacuum permittivity, \( \mathbf{b} = \mathbf{B}/B \), and \( \Lambda_C \) is the Coulomb logarithm.

Dynamics of Alfvén wave turbulence and its interaction with the background plasma requires a special consideration. The evolution of the Alfvén wave amplitude (velocity, \( \mathbf{u} \), and magnetic field, \( \mathbf{B} \)) is usually treated in terms of the Elsässer (1950) variables, \( \xi \pm = \mathbf{u} \pm \frac{\mathbf{B}}{\sqrt{\rho \mu_0}} \). The Wentzel–Kramers–Brillouin (WKB) approximation is used to derive the equations that govern transport of Alfvén waves, which may be reformulated in terms of the wave energy densities, \( w_{\pm} = \rho \varepsilon_{\pm}/4 \). Dissipation of Alfvén waves, \( \Gamma_{\pm} w_{\pm} \), is crucial in driving the solar wind and heating the coronal plasma. The dissipation occurs when two counterpropagating waves interact. Therefore, an efficient source of both types of waves is needed, and it is maintained by Alfvén wave reflection from steep density gradients. For this reason, we need to go beyond the WKB approximation, which assumes that wavelength is much smaller than spatial scales in the background. The equation describing propagation of the turbulence, its dissipation, and reflection has been derived in van der Holst et al. (2014):

\[
\frac{\partial w_{\pm}}{\partial t} + \nabla \cdot [(u \pm V_A) w_{\pm}] + \frac{w_{\pm}}{2} (\nabla \cdot u) = -\Gamma_{\pm} w_{\pm} \mp R \sqrt{w_{\pm} w_i}.
\]

(9)

Here the dissipation rate equals \( \Gamma_{\pm} = \frac{2}{L_B \sqrt{w_{\pm} / \rho}} \), and the reflection coefficient is given by

\[
R = \min \left( \frac{\sqrt{\mathbf{b} \cdot (\nabla \times \mathbf{u})^2}}{(|V_A| \cdot \nabla \log V_A^2 \cdot \max(\Gamma_+))} \right) \times \left[ \max \left( 1 - \frac{L_{\text{max}}}{w_i/w_\pm}, 0 \right) \right] - \max \left( 1 - \frac{L_{\text{max}}}{w_i/w_\pm}, 0 \right).
\]

(10)

where \( L_{\text{max}} = 2 \) is the maximum degree of the turbulence “imbalance.” If \( w_i/w_\pm < L_{\text{max}} \), then \( R = 0 \) and the reflection term is not applied.

Now, knowing the dissipation of the Alfvén turbulence, we are able to write the expression for ion and electron heating due to turbulence,

\[
Q_i = f_p (\Gamma_+ w_i + \Gamma_i w_i),
\]

\[
Q_e = (1 - f_p)(\Gamma_+ w_i + \Gamma_i w_i),
\]

(11)

where \( f_p \approx 0.6 \) is a fraction of energy dissipated to ions. Finally, to close the system of equations, we use the following boundary condition for the Poynting flux, \( \Pi \):

\[
\frac{\Pi}{B} = \frac{\Pi_B}{B_B} = \text{const} \approx 1.1 \cdot 10^6 \text{ W m}^{-2} \text{T}.
\]

(12)

The scaling law for the transverse correlation length is

\[
L_d \sim B^{-1/2}, \quad 100 \text{ km} \cdot \text{T}^{1/2} \leq L_d \sqrt{B} \leq 300 \text{ km} \cdot \text{T}^{1/2}.
\]

(13)

2.2. Alfvén-wave-turbulence-based Model for the Solar Atmosphere in Real Time

AWSoM has been demonstrated to be an accurate tool for modeling realistic conditions of solar wind (Oran et al. 2013; Sokolov et al. 2013; van der Holst et al. 2014). However, in terms of computational efficiency, the model is somewhat restrictive. The reason for that deficiency is the extremely fine resolution of the computational mesh close to the solar surface; such fine mesh is needed to resolve the dynamics of Alfvén wave turbulence and ensure the numerical stability. An alternative approach is to reformulate the mathematical problem in the said region. Instead of solving a computationally expensive 3D problem on such a grid, we substitute it with a multitude of much simpler 1D problems along threads that allow bringing boundary conditions up from the solar surface to a height defined by the assumptions below and are the key concept of our Threaded-Field-Line Model (TFLM).

The main assumption in the reformulated problem is that the solar magnetic field may be considered to be potential with high accuracy in a certain range of radii, \( R_{\odot} < R < R_B \). A thread represents a field line. Reduction from 3D to 1D is summarized below; for more details we refer readers to Sokolov et al. (2016). Due to the constraint on the magnetic field divergence, \( \nabla \cdot \mathbf{B} = 0 \), the
magnetic flux remains constant along the thread:

\[ B(s) \cdot A(s) = \text{const}; \]  
(14)

hereafter \( s \) is the distance along the field line, \( B \) is the magnitude of the magnetic field, and \( A \) is the cross-section area of the flux tube in the consideration. Conservation laws are also greatly simplified owing to the fact that in low-beta plasma, velocity is aligned with the magnetic field. Here, assuming steady state, conservation laws take the following form:

Continuity equation:

\[ \frac{\partial}{\partial s} \left( \frac{\rho u}{B} \right) = 0 \quad \Rightarrow \quad \left( \frac{\rho u}{B} \right) = \text{const}. \]  
(15)

Conservation of momentum:

\[ \frac{\partial P}{\partial s} = - b_R GM_\odot \rho \frac{\gamma - 1}{R^2} \quad \Rightarrow \quad P = P_{TR} e^{\frac{\gamma}{\gamma - 1} \frac{GM_\odot \rho}{B^2} \frac{\partial x}{s}}, \]  
(16)

where \( R_{TR} \) is the height of the transition region (TR), \( b_R \) is the radial component of \( B \), terms proportional to \( u^2 \) are neglected, \( f \times B \) is omitted owing to electric current vanishing in the potential field (\( f \times B = 0 \)), and the pressure of Alfvén wave turbulence is assumed to be much smaller than the thermal pressure, \( P_s \ll P \).

Conservation of energy:

\[ \frac{2N_k B}{B(\gamma - 1)} \frac{\partial T}{\partial t} + 2k_B \gamma \left( \frac{N_k u}{B} \right) \frac{\partial T}{\partial s} = \frac{\partial}{\partial s} \left( \frac{\rho u}{B} \right) \frac{\partial (GM_\odot / R)}{\partial s} + \frac{\gamma - 1}{B} \]  
(17)

The term \( \frac{\partial T}{\partial s} \) is retained under the assumption that the electron heat conduction is a relatively slow process. Alfvén wave dynamics is reformulated as well. In Equation (9) we substitute \( w = \left( \frac{1}{T} \right)^{\frac{2}{3}} \mu_B \rho a^2 \):  

\[ \frac{\partial a^2 \pm}{\partial t} + \nabla \cdot (u a^2 \pm) \pm (V_A \cdot \nabla) a^2 \pm = \mp Ra \cdot a \pm + 2 \left[ \frac{\mu B}{L_\perp \sqrt{B^2}} \right] a^2 \perp. \]  
(18)

The equations are additionally simplified since in the lower corona environment \( u \ll V_A \), i.e., waves are assumed to travel fast and quickly converge to equilibrium:

\[ \frac{\partial a^2 \perp}{\partial t} = \mp \frac{R}{V_A} a \perp - 2 \left[ \frac{\mu B}{L_\perp \sqrt{B^2}} \right] V_A a^2 \perp. \]  
(19)

Additionally, we substitute \( d\xi = ds \frac{\mu B}{L_\perp \sqrt{B^2}} \):  

\[ \pm a^2 \perp = \pm \frac{d \xi}{d\xi} \frac{R}{2V_A} a \perp - a \perp a \pm. \]  
(20)

In order to close the system of equations, we need to define the boundary conditions for TFLM. For the “+” wave one needs to provide a value at \( \xi = \xi_+, a_+ \), and for the “−” wave a value at \( \xi = \xi_-, a_- \). Specifically, at the photosphere level, as a result of Equation (12) the dimensionless amplitude of the outgoing wave is equal to 1: \( b_{e|_{R=R_p}} > 0; a_+ = 1 \);

\[ b_{y|_{R=R_p}} < 0; a_-=1. \]  

Boundary conditions at the interface between TFLM and the global corona model (GCM) are

\[ b_{y|_{R=R_0}} > 0: \left( \frac{u}{B} \right)_{\text{TFLM}} = \left( \frac{u}{B} \right)_{\text{GCM}}^2 ; \]  
(21)

\[ b_{y|_{R=R_0}} < 0: \left( \frac{u}{B} \right)_{\text{TFLM}} = - \left( \frac{u}{B} \right)_{\text{GCM}}^2 ; \]  

Thus, TFLM is fully described as a closed mathematical model does not solve the boundary conditions for transverse components of the magnetic field and velocity on top of the TR. To advance the model, as well as to incorporate the observations of the vector magnetic field and transverse velocity at the solar surface, the wave amplitudes should be solved for ingoing and outgoing Alfvén perturbations to relate the observations on the photosphere level to the numerical boundary conditions to be applied on top of the TR. This approach is typical for the hyperbolic system of conservation laws, such as the system of MHD equations that mostly describes the motions in the SC and IH, and we are going to employ it in the near future to incorporate more detailed
3. CME Models in Numerical Simulations

As mentioned above, we focus in our work on gradual SEP events. Events of this kind are characterized by a steadily increasing particle flux, unlike impulsive events, which have an abrupt time profile (Reames 1999). Based on numerous observations (Kahler et al. 1978), it is commonly accepted that gradual, proton-rich SEP events are associated with CMEs. The two phenomena are linked via an interplanetary shock wave, which forms in front of a CME: the shock wave itself results from interaction of a CME with ambient solar wind plasma, and at the same time, as the shock moves outward, it accelerates more and more particles, hence the gradual nature of events.

Thus, properties of gradual SEP events are strongly influenced by CMEs that trigger them. Therefore, in order to successfully design a predictive model for gradual SEP events, we need an accurate model to describe CMEs. Due to the lack of in situ measurements of the shock waves and the excited turbulence in their vicinity, numerical simulations remain the primary means of research. A series of numerical studies employing the theory of DSA were performed in cases of both idealized (Zank et al. 2000; Li et al. 2003; Rice et al. 2003) and realistic (Sokolov et al. 2004; Kóta et al. 2005) CME-driven shock waves.

While there are many models of CME initiation by magnetic-free energy, these simulations are often performed in a small Cartesian box (e.g., Török & Kliem 2005), or using global models with no solar wind (e.g., Antiochos et al. 1999; Fan & Gibson 2004). So far, there have only been a few magnetically driven Sun-to-Earth CME simulations through a realistic interplanetary medium using 3D MHD (see Manchester et al. 2004b, 2005; Lugaz et al. 2007; Tóth et al. 2007). The MHD simulation of Tóth et al. (2007) was able to match the CME arrival time to Earth within 1.8 hr and reproduce the magnetic field magnitude of the event.

In general, the purpose of a CME generator is to enhance locally the free magnetic energy of the existing global (“ambient”) solution describing the steady state of the SC and IH magnetic field, \( B_{\text{amb}}(R) \), by superposing an erupting configuration representing a CME’s ejecta. A choice of a reasonable representation of the latter is still debatable. A simple but convenient way to simulate a magnetically driven CME is to superimpose a magnetic flux rope configuration onto the background state of the SC. Such a magnetic configuration describes an erupting magnetic filament filled with a plasma of excessive density. That filament becomes an expanding flux rope (magnetic cloud) in the ambient solar wind while evolving and propagating outward from the Sun, thus allowing the simulation of the propagation to 1 au of a magnetically driven CME. In this paper, we provide a brief discussion of several approaches to generate CMEs with this technique.

3.1. Magnetized Cone Model

Observations of halo CMEs (e.g., with the LASCO instrument; Brueckner et al. 1995; Plunkett et al. 1998) provided new insights into the geometry of CMEs and its relation with other properties. One can accurately infer the angular width and the central position angle of a halo CME together with the plasma velocity. For example, these observations have revealed that (i) the bulk velocity tends to be radial; and (ii) the angular width, \( 2\Delta \theta \), tends to remain constant as CME propagates through the corona. These persistent features lead to the development of the cone model (Zhao et al. 2002). Having only three free parameters, angular width of a CME and its initial position on the solar surface, the model approximates a CME and its propagation with a cone with apex located at the center of the Sun. It was later improved by Michalek (2006) for arbitrary shapes. The cone model is successfully used at the Community Coordinated Modeling Center (CCMC) and has proved to be an efficient tool for predicting arrival times of CMEs (Vršnak et al. 2014; Mays et al. 2015). Thanks to the model’s accuracy and robustness, it is used together with the WSA model in CCMC’s operational activities. However, by design, the cone model lacks details about the magnetic field carried by a CME. The model may be substantially enriched as we suggest below.

In order for the simulated CME ejecta to truly represent a magnetic cloud, one needs to incorporate magnetic field, controlled by the ambient external field at the location where CME is added, into the model. One possible way to achieve this is to impose a spheromak, i.e., an equilibrium spherical MHD configuration (see the Appendix), around the central point of the cloud, \( \mathbf{R}_c \). Spheromak’s magnetic field is

\[
B_{sk}(r) = \left[ j_1(\alpha_0 r) - \beta_0 \right] (2B_0 + \sigma_0 \alpha_0 [B_0 \times r]) + j_2(\alpha_0 r) \frac{[r \times [r \times B_0]]}{r^2},
\]

where \( j_1 \) and \( j_2 \) are spherical Bessel functions. Here the vector \( B_0 \) is introduced with the magnitude equal to \( B_0 \) directed along the spheromak’s axis of symmetry, \( \sigma_0 = \pm 1 \) is the sign of helicity (we assume \( \sigma_0 = \text{const > 0} \)), and \( \beta_0 = \text{const} \) is the characteristic value of plasma beta. The coordinate vector, \( \mathbf{r} \), originates at the center of configuration, \( \mathbf{R}_c \). We assume no currents outside a spherical magnetic surface \( ||R - R_c|| = r_0 \), which thus bounds the configuration. The radial and toroidal components of the magnetic field turn to zero at the surface; thus, \( j_1(\alpha_0 r_0) = \beta_0 \alpha_0 r_0 \). For a given \( \beta_0 \) this equation relates the configuration size, \( r_0 \), to the extent of magnetic field twisting, \( \alpha_0 \), needed to close the configuration within this size.

One also needs to account for the field, which the currents inside spheromak produce outside the boundary, \( ||R - R_c|| = r_0 \). The calculation of the magnetic moment (see definition in Jackson 1999), m, of the spheromak configuration gives

\[
m = \frac{1}{2} \int_{|r|| \leq r_0} d^3 \mathbf{r} \times \mathbf{j} = \frac{1}{2\mu_0} \int_{|r|| \leq r_0} d^3 \mathbf{r} \times (\nabla \times B_{sk})
\]

\[
= \frac{4\pi r_0^3}{3\mu_0} j_2(\alpha_0 r_0) B_0.
\]

The final expression for \( m \) is obtained via reducing the volume integral to the integral over the spheromak’s surface, at
which \( B_{\text{sh}, r>r_0}(r) = j_\perp (\alpha r_0) |r \times [r \times B]| /r^2 \). The field of magnetic dipole, \( m \), which we admit as the spheromak’s field outside the boundary, equals

\[
B_{\text{sh}, r>r_0}(r) = \frac{\mu_0}{4\pi r^3} \left\{ \frac{3(r \cdot m) r - m}{r^2} \right\} 
= j_\perp (\alpha r_0) \frac{r_0^3}{r^3} \left\{ \frac{(r \cdot B_0) r}{r^2} - B_0 \right\}.
\]

(28)

Now, we provide the full expression for a spheromak superposed onto the ambient field, \( B_{\text{amb}}(r) \):

\[
B(r) = \begin{cases} 
B_{\text{amb}}(R) + B_{\text{sh}, r>r_0}(R - R_0), & \| R - R_0 \| > r_0 \\
B_{\text{amb}}(R) + \frac{2}{3} j_\perp (\alpha r_0) B_0, & \| R - R_0 \| \leq r_0
\end{cases}
\]

(29)

where the uniform field, \( \frac{2}{3} j_\perp (\alpha r_0) B_0 \), is added to the spheromak field for two reasons. First, this preserves the field continuity at \( \| R - R_0 \| = r_0 \), i.e., from both sides of the boundary the field equals \( j_\perp (\alpha r_0) \left\{ \frac{(r \cdot B_0) r}{r^2} - B_0 \right\} \). Second, certain aspects of CME ejecta’s interaction with ambient plasma dictate this correction. Indeed, if an ejecta represents a magnetic cloud, its frozen-in magnetic field effectively replaces the preexisting field, \( B_{\text{amb}} \), at any location, \( R \), it passes. Therefore, the cloud’s internal field, which we assume to be the superposition of the ambient field with the field of the spheromak centered at \( R_\text{cloud} \) (i.e., \( R_\text{cloud} \equiv R_0 \)), must be corrected by the negative of this preexisting field. This reasoning demands that the expression in the square brackets in Equation (29) be exactly zero at \( R_0 \), i.e., \( B_0 \) and \( B_{\text{amb}} \) must be related as

\[
B_0 = -\frac{3}{2j_\perp (\alpha r_0)} B_{\text{amb}}(R_0).
\]

(30)

which ensures both the continuity of the field, Equation (29), and the proximity of the internal field (equality, if the ambient field is uniform), \( B_{\text{amb}}(R) - B_{\text{amb}}(R_0) \), to the equilibrium state \( B_{\text{sh}}(R - R_0) \). Should the field of the superimposed configuration not match the ambient field in direction, the nonzero torque, \( [m \times B_{\text{amb}}] \), acting on the magnetic moment, \( m \), in the field \( B_{\text{amb}}(R_0) \) would tend to align the configuration axis with the external field. Should the configuration field be stronger/weaker than that governed by Equation (30), the ambient field would be too weak/strong to balance the hoop force in the spheromak configuration, so that the latter would tend to expand/shrink. The field in the configuration determined by Equations (29) and (30) is oppositely directed and somewhat stronger than the ambient field. For comparison, the field in the center of the configuration equals

\[
B_{\text{sh}}(R) = 2(1 - \beta_0)B_0 = -\frac{1}{j_\perp (\alpha r_0)} B_{\text{amb}}(R_0).
\]

Magnetic geometry of the described configuration provides a natural explanation of the geomagnetic activity caused by CMEs. Indeed, if the configuration described above passes Earth’s location, the local magnetic field may consequently change from \( B_{\text{amb}}(R_0) \) to \( B_{\text{sh}}(R_0) \) and back, so that all components of the IMF change sign and increase in absolute value by a factor of \( (1-\beta_0) \approx (4/5) \). This is a classical scenario for the magnetospheric storm.

Disregarding the solar gravitational pull and assuming uniform ambient field, the magnetic configuration described above is in a force equilibrium. As demonstrated by Low (1982), once some special distribution of plasma velocity is imposed onto an equilibrium magnetic structure with adiabatic index \( \gamma = 4/3 \), this structure starts to evolve self-similarly, i.e., with the only change in its geometry being the radial motion and uniform expansion (see Sedov 1959; Zel’dovich & Raizer 1967, regarding self-similar solutions). Specifically, we need to assume, and implement in the numerical simulations, the radially diverging initial motion with the radial velocity at each point being proportional to the heliocentric distance:

\[
u|_{t=0} = \frac{U_{\text{CME}} R}{|R|},
\]

where the CME speed, \( U_{\text{CME}} \), may be found from observations. In application to the magnetized cone model this means that superimposing a spheromak with such a velocity profile onto a barometric atmosphere would be consistent with basic principles of the cone model of Zhao et al. (2002): (i) the bulk velocity of the resulting magnetic cloud is radial, and (ii) the shape of the cloud, due to self-similarity, remains constant. As noted above, we neglected the gravity, i.e., the moving magnetic cloud is not in the perfect force equilibrium. Therefore, exact self-similarity cannot be achieved; rather, it is approached when the relative contribution of gravitational force tending to decelerate the cloud is small. Another force tending to decelerate the magnetic cloud is the drag force, which opposes the faster CME motion through the slower-moving ambient plasma. On the other hand, in the nonuniform ambient magnetic field antiparallel to \( B_0 \), the force acting on the magnetic dipole repels it out of the AR, thus accelerating its radial motion. These counteracting forces may partially balance each other, thus resulting in almost steady radial motion as assumed by the cone model.

3.2. Stretched Spheromak Configuration by Gibson–Low

The family of equilibrium configurations given by Equation (26) may be extended with the use of coordinate transformation suggested by Gibson & Low (1998). The arising pressure imbalance perfectly compensates the gravitational force acting on the spheromak’s plasma. The new equilibrium configuration in the heliocentric coordinates, \( R \), with the magnetic field, \( B(R) \), and pressure distribution, \( P(R) \), may be described in terms of the spheromak solution, Equation (26), of the Grad–Shrafovich equations (see the Appendix), \( B'(R') = B_{\text{sh}}(R' - R_0) \) and \( P'(R') = P_{\text{sh}}(R' - R_0) \). For each point \( R \), we take the values of these functions in the point \( R' = (1 + a^2)R, R' = R + a \), which is radial coordinate stretching, an arbitrary constant \( a \) being the distance of stretching. When the stretching transformation is applied, it displaces the magnetic configuration toward the heliocenter and gives it a teardrop-like shape. The magnetic field vector in the course of stretching should be scaled in addition to
plane and then stretched toward the heliocenter by distance corresponding to levels the magnetic
P are transformed as follows:

\[ \text{Figure 1. Equatorial plane of the stretched flux rope for } \beta_0 = 0.02 \text{ (see Figure 5). The original flux rope is shifted by distance 1.6} \beta_0 \text{ along a direction in the equatorial plane and then stretched toward the heliocenter by distance 0.3} \beta_0 \text{ (left) and 0.6} \beta_0 \text{ (right). Magnetic field direction is marked with arrows; the off-plane component of the magnetic field is normalized per } R_0 \text{ (see Equation (26)) and shown by color. Local values of plasma parameter } \beta(r) = \mu_0 P(r)/B^2(r) \text{ are shown with red curves corresponding to levels } \beta = 0.04, 0.08, 0.12, \text{ and 0.16 as marked explicitly.} \]

Now, one can consider the stretched magnetic configuration:

\[ \mathbf{B}(\mathbf{R}) = \frac{R'}{R} \left( \mathbb{I} + \frac{a}{R} \mathbf{e}_R \mathbf{e}_R \right) \cdot \mathbf{B}'(\mathbf{R}') , \tag{31} \]

where \( \mathbf{e}_R = \frac{\mathbf{R}}{R} \) and \( \mathbb{I} \) is the identity matrix. The radial field component, \( B'_R = (\mathbf{B}' \cdot \mathbf{e}_R) \), is thus multiplied by \( \left( \frac{R'}{R} \right)^2 \), all others by \( \frac{R'}{R} \). Thus, the transformed magnetic field is divergence-free. The plasma pressure of the stretched magnetic configuration is defined as

\[ P(\mathbf{R}) = \left( \frac{R'}{R} \right)^2 \left[ P' - \frac{a}{R} \left( 2 + \frac{a}{R} \frac{B'_R^2}{2\mu_0} \right) \right] \tag{32} \]

One can verify an equilibrium condition for the transformed magnetic configuration. The spatial derivatives of \( B'(\mathbf{R}') \) and \( P'(\mathbf{R}') \) are transformed as follows:

\[ \nabla = \left[ \left( 1 + \frac{a}{R} \right) \mathbb{I} - \frac{a}{R} \mathbf{e}_R \mathbf{e}_R \right] \nabla' . \]

\( \nabla' \)

Using the equilibrium condition for a nonstretched configuration, \( \frac{1}{\mu_0} \left[ [\nabla' \times \mathbf{B}] \times \mathbf{B} \right] - \nabla P = F_R \mathbf{e}_R \), where the radial force arising from extra tension of the stretched magnetic field is

\[ F_R = \frac{aR'}{R^3} \left[ \left( 2 + \frac{a}{R} \right) \left( \frac{B'_R^2}{\mu_0 R'} + (\mathbf{e}_R \cdot \nabla') \left( P' + \frac{B'_R^2}{2\mu_0} \right) \right) \right] + \frac{2P'}{R^3} \left[ 3 + 2 \frac{a}{R} \frac{B'_R^2}{\mu_0 R'} \right] . \tag{33} \]

Now, one can consider the stretched magnetic configuration described by Equations (31) and (32) once superposed with some background barometric distribution of pressure, \( P_{\text{bar}}(\mathbf{R}) \), and density, \( \rho_{\text{bar}}(\mathbf{R}) \), which satisfy the hydrostatic equilibrium condition, \( -\nabla P_{\text{bar}} + \rho_{\text{bar}} \mathbf{g} = 0 \), \( \mathbf{g} = -GM_S / R^2 \). The superposed distribution satisfies the equilibrium condition accounting for gravity,

\[ \frac{1}{\mu_0} \left[ [\nabla \times \mathbf{B}] \times \mathbf{B} \right] - \nabla (P + P_{\text{bar}}) + (\rho + \rho_{\text{bar}}) \mathbf{g} = 0 , \tag{34} \]

if the density variation due to the effect of the stressed field is

\[ \rho = \frac{F_R}{\mathbf{g}(\mathbf{R})} . \tag{35} \]

As a result of the transformation, the spherical configuration is stretched toward the heliocenter as shown in Figure 1. When the solution represented by Equations (31), (32), and (35) (the Gibson-Low (GL) flux rope) is superimposed onto the existing corona, the sharper end of the teardrop shape is submerged below the solar surface. In the wider top part of the configuration ("balloon") the density variation in Equation (35) is negative, that is, the resulting density is lower than that of the ambient barometric background. As a result, the Archimedes force acting on this part pulls the whole configuration outward from the Sun. The cavity with the reduced density is often observed in the CME images from the LASCO coronagraphs. Then, in the narrower bottom part of the configuration ("basket"), the excessive positive density simulates the dense ejecta, which is pulled outward from the Sun by the radial tension in the stretched magnetic configuration. Finally, the tip of the configuration with the magnetic field lines both ingoing and outgoing from the solar surface anchored to the negative and positive magnetic spots of a bipolar AR is considered as the source of the CME. Depending on the reconnection rate, either the configuration can keep being magnetically connected to the AR, or it may disconnect and close and then propagate toward 1 au as the magnetic cloud.

The time evolution of the GL flux rope is self-similar (provided that \( \gamma = 4/3 \); see Low 1982). Additionally, this result may be generalized: adjusting the density profile in Equation (35) for effective gravity \( g(R) + aR \) would result in accelerated/decelerated propagation of a CME. A literal requirement for self-similarity of the GL flux rope can hardly be fulfilled in realistic coronae. Indeed, in order for the
configuration to remain in force equilibrium (or to keep the specific shape of the force imbalance to maintain acceleration) and therefore propagate in a self-similar fashion, a specific and unrealistic distribution of the external pressure is needed. Additionally, since the Ampere’s force is nonlinear in magnetic field, superimposing the GL flux rope adds a new effect of the background magnetic field onto the flux rope’s currents, which contributes even more to the force imbalance. The significance of these effects has not been thoroughly studied; however, CME propagation has been shown to be approximately self-similar (e.g., Manchester et al. 2004a, 2004b).

The GL flux rope model has been used for CME initiation in, e.g., Manchester et al. (2004a, 2004b, 2006), Lugaz et al. (2005), and Jin et al. (2017a, 2017b). The recent developments allowed significant simplification of the process of triggering CMEs using the GL model. The product of the effort is the Eruptive Event Generator based on Gibson–Low magnetic configuration (EEGGL) (Jin et al. 2017a), which is discussed in detail in Borovikov et al. (2017).

3.3. Thin Flux Rope by Titov–Demoulin

The approach of TD also stems from consideration of the magnetic field’s topology. A pre-eruptive configuration of the field is reconstructed with three different components, \( B_f \), \( B_p \), and \( B_e \). \( B_f \) is created by a uniform ring current flowing in the emerging flux rope (later the model has been modified in Titov et al. (2014) to include a nonuniform current profile, TDm hereafter), \( B_e \) is the magnetic field of two equal imaginary magnetic charges of opposite signs embedded below the solar surface, and finally \( B_p \) is produced by a constant line current flowing through the said charges.

The TD flux rope model has been used in a number of studies (e.g., Roussev et al. 2003a; Manchester et al. 2008), as well as its modified version, TDm (Linker et al. 2016). Specific examples of CME simulations using the AWSoM model for the SC and IH with a superimposed TD magnetic configuration include Manchester et al. (2012) and Jin et al. (2013).

3.4. Comparison of CME Generators

The three approaches to CME generation in numerical simulations briefly discussed in preceding sections differ in certain aspects. While all are based on equilibrium magnetic configurations, each model utilizes them differently, which affects their properties and applicability range.

The magnetized cone model, first described in the present paper, is yet to be implemented and tested. Like the original cone model, it considers a fully developed CME and, similarly, should be applied well above the lower SC boundary, not to interact with the magnetic field of the AR, or even at the outer edge of the SC. One can notice that the gravitational force is not included in the computation of the flux rope parameters, Equation (29). Therefore, in order for the result of Low (1982) to be applicable, the contribution to the force balance must be negligible. Thus, the model can be a useful tool in operations for forecasting CMEs’ effects on the arrival at Earth rather than in investigation of low corona phenomena such as SEP acceleration.

The GL configuration, also based on the spheromak, was designed to account for gravity’s contribution to force equilibrium and therefore can be applied in the low corona. Note that, according to findings of Low (1982), the GL flux rope necessarily travels outward, i.e., it represents a flux rope that is already at the early stage of eruption, unlike the TD flux rope.

TD-type configuration is substantially different from the other two. It is constructed to be in a static force equilibrium in the local magnetic field. Therefore, the TD flux rope, once imposed, may be expected to relax to steady state and remain stable. In other words, the TD flux rope requires an additional driver to erupt. For example, the magnetic configuration may be constructed in such way that the background (strapping) magnetic field would not be sufficient to stabilize the flux rope and prevent it from erupting. This can be achieved either by applying flux cancellation motion to weaken the partially annihilated overarching field (see, e.g., Linker et al. 2016) or simply by choosing the higher configuration current, \( I \), so that the hoop force (\( \propto I \)) is simply balanced by the Ampere force (\( \propto I \)). Thus, the TD flux rope offers a wider range of opportunities to study various phenomena in the low corona and, in particular, is suitable to trigger SEP acceleration in numerical simulations.

Both the TD and GL flux ropes have been successfully applied in CME simulations (see references above). An extensive comparative study of which of the two represents CME shock geometry more accurately has not been performed and goes beyond the scope of the current work.

4. Interface between MHD and Kinetic Models

4.1. Transport Equation

The transport of energetic particles through the interplanetary space by itself is an important problem in space science. It has been studied since the discovery of the GCRs, the energetic particles originating from beyond the solar system. A comprehensive summary of the problem can be found in the review by Parker (1965). Although results in the said review are obtained in a different context, some can readily be applied for the SEP transport.

The distribution of SEPs is far from Maxwellian; therefore, they should be characterized by a (canonical) distribution function \( F(R, p, t) \) of coordinates, \( R \), and momentum, \( p \), as well as time, \( t \), such that the number of particles, \( dN \), within the elementary volume, \( d^3R \), is given by the following integral: \( dN = d^3R \int d^3p F(R, p, t) \). In a magnetized plasma, it is convenient to deal with the distribution function at the given point, \( R \), in the comoving frame of reference, which moves with the local speed of interplanetary plasma, \( \mathbf{u}(R, t) \), on introducing spherical coordinates, \( (p = |\mathbf{p}|, \mu = \mathbf{b} \cdot \mathbf{p}/|\mathbf{p}|, \varphi) \), in the momentum space with its polar axis aligned with the direction of the magnetic field, \( \mathbf{b} \), with \( \mu \) being the cosine of pitch angle. The normalization integral in these new variables becomes \( dN = d^3R \int_0^\infty p^2 dp \int_0^1 d\mu \int_0^{2\pi} d\varphi F(R, p, \mu, \varphi, t) \). Using this canonical distribution function, one can also define a gyrotropic distribution function, \( f(R, p, \mu, \varphi, t) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi F(R, p, \mu, \varphi, t) \). This function is designed to describe the particle motion averaged over the phase of its gyration about the magnetic field. The isotropic (omnidirectional) distribution function, \( f_0(R, p, \mu, t) = \frac{1}{2} \int_{-1}^{1} df(R, p, \mu, t) \), is averaged over the pitch angle, too. The normalization integrals are \( dN = 2\pi d^3R \int_0^\infty p^2 dp \int_{-1}^{1} df(R, p, t) = 4\pi d^3R \int_0^\infty p^2 dp f_0(R, p, t) \).
The commonly used kinetic equation for the isotropic part of the distribution function has been introduced in Parker (1965):

\[
\frac{\partial}{\partial t} f_0(R, p, t) + (u \cdot \nabla) f_0(R, p, t) - \frac{1}{3} (\nabla \cdot u) \times \frac{\partial}{\partial \ln p} f_0(R, p, t) = \nabla \cdot (\kappa \cdot \nabla f_0(R, p, t)) + S, \tag{36}
\]

where \( \kappa = D_{xx} \mathbf{b} \mathbf{b} \) is the tensor of parallel (spatial) diffusion along the magnetic field and \( S \) is the source term. In this approximation, the cross-field diffusion of particles is neglected.

Equation (36) captures the effect of interplanetary plasma and IMF on the SEP transport and acceleration. The term proportional to the divergence of \( u \) is the adiabatic cooling, for \( (\nabla \cdot u) > 0 \), or the first-order Fermi acceleration in compression or shock waves. According to estimates by Parker (1965), during quiet time the adiabatic scaling of particles' energy from their origin to 1 au is \( \sim (\rho_{1 \text{ au}}/\rho_{\odot})^{n/3} \), where \( n = 2 \) for nonrelativistic particles and \( n = 1 \) for relativistic particles.

Small-scale irregularities also have a significant impact on particle propagation. Their scale is \( 10^5-10^7 \) km, which is comparable to gyroradii of SEPs but very small compared to 1 au. Particles scatter on these irregularities, and on the large scale the particle motion can be described as diffusion, the first term on the right-hand side of Equation (36). Based on Equation (36), Krymsky (1977), Axford et al. (1977), Bell (1978a, 1978b), and Blandford & Ostriker (1978) proposed the DSA mechanism to explain the observed power-law spectra of GCRs.

In the present paper we limit our consideration with the case of the Parker Equation (36) as the model to describe the SEP acceleration and transport. More realistic and accurate models accounting for the pitch-angle dependence for the distribution function are delegated to the companion paper.

4.2. Lagrangian Coordinates and Field Line Advection Model

We adopt Equation (36) as the mathematical approach to the problem of SEP transport. However, this consideration is computationally challenging: a fully 3D propagation of particles requires significant resources. This can be avoided by observing that Equation (36) assumes that the particle motion in physical space consists of the particle guiding center's displacement along the IMF and advection with plasma into which the IMF is frozen. This property allows us to describe the particle propagation in the Lagrangian coordinates. The benefit of this approach is the reduction of a complex 3D problem to a multitude of much simpler 1D problems along magnetic field lines, with no loss of generality.

At the early age of the mechanics of continuous media there were two competing approaches to a mathematical description of the motion of fluids. In Eulerian coordinates, \( R, t \), the distribution of the fluid parameters (density, velocity, temperature, pressure, etc.) at each instant of time, \( t \), is provided as a function of coordinates, \( R \), in some coordinate frame. There is no need to emphasize that any given point, \( R \), is immovable.
while the fluid passes this point with the local flow velocity \( u(R, t) \), so that at each time instant the fluid element at this point differs from that present at this point a while ago. In contrast with this approach, the Lagrangian coordinates, \( R_L \), stay with the given fluid element rather than with the given position in space. While the fluid moves, each moving fluid element keeps unchanged the value of the Lagrangian coordinates, \( R_L \), while its spatial location, \( R(R_L, t) \), changes in time in accordance with the definition of the local fluid velocity:

\[
\frac{DR(R_L, t)}{Dt} = u(R, t).
\]  

Here the partial time derivative at constant Lagrangian coordinates, \( R_L \), is denoted as \( \frac{D}{Dt} \), while the usual notation, \( \frac{\partial}{\partial t} \), denotes the partial time derivative at constant Eulerian coordinates, \( R \). As usual, we choose the Lagrangian coordinates for a given fluid element equal to the Eulerian coordinates of this element at the initial time instant, \( R_L = R|_{t=0} \). For numerical simulations, with any choice of the grid in Lagrangian coordinates, \( (R_{ijL})_t = (R_{ij})_{t=0} \), one can numerically solve the multitude of ordinary differential equations, Equation (37), to trace the spatial location for all Lagrangian grid points in the evolving fluid velocity field, \( u(R, t) \), as long as the latter is known.

An example of application of Lagrangian coordinates to the Parker equation, Equation (36), is FLAMPA (Sokolov et al. 2004).

### 4.3. M-FLAMPA

The geometry of magnetic field lines may become very complex, and they can form intricate patterns as they evolve in time. By pushing and twisting field lines, extreme events, such as CMEs and associated interplanetary shocks, can make the field line topology even more complex. This

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**Figure 3.** Simulated flux of SEP exceeding 10 MeV (GOES channel 2): along the extracted lines from the Sun to 1 au (top) and interpolated between footprints (small blue diamonds) of lines on a 1 au sphere (bottom).

**Figure 4.** Time evolution of simulated flux of SEPs exceeding 10 MeV (GOES channel 2) at 1 au on a single line (solid black line) compared to GOES measurements (dashed black line). Time is measured from the CME initiation (4:00 on 2012 January 23).
makes forecasting the regions affected by SEP events a challenging problem. To address this challenge, one needs to design a computational technique that naturally and efficiently describes this ever-evolving geometry. The Multiple-Field-Line-Advection Model for Particle Acceleration (M-FLAMPA) code was designed to solve this problem. M-FLAMPA allows us to solve the kinetic equation for SEPs along a multitude of IMF lines originating from the Sun, using time-dependent magnetic field and plasma parameters obtained from the MHD simulation. The model is a high-performance extension of the original FLAMPA code (Sokolov et al. 2004), which simulates SEP distribution along a single field line. M-FLAMPA is a major improvement that takes full advantage of modern supercomputers.

M-FLAMPA solves for the gyrotropic SEP distribution function \( f(\mathbf{x}, p, t) \), where \( p \) is the magnitude of the relativistic momentum of energetic particles. The code takes advantage of the fact that particles stay on the same magnetic field line and, therefore, the distribution function may be treated as a function of the distance along the field line, \( s \), rather than a 3D vector \( \mathbf{x} \). Also, coefficients in the governing equations depend only on background plasma parameters and their Lagrangian derivatives (see Section 4.2). This important property reduces the problem of particle acceleration in 3D magnetic field into a set of independent 1D problems on continuously evolving Lagrangian grids. In other words, each field line in the model is treated separately from others, which results in a perfectly parallel algorithm. We note that the same computational technology is applied to the transport equations for the Alfvén wave amplitudes (Sokolov et al. 2009).

M-FLAMPA is directly coupled with SC and IH MHD models via an advanced coupling algorithm within the Space Weather Modeling Framework (SWMF). This technique seamlessly connects field lines between the two distinct computational domains, where lines are extracted based on a concurrently updated solution of solar wind parameters. The line-extracting procedure is augmented with a new interpolation algorithm (Borovikov et al. 2015) that eliminates spurious distortions near grid resolution interfaces that routinely occur in large-scale MHD simulations. The underlying algorithmic innovations ensure that M-FLAMPA can combine the accuracy of realistic MHD simulations with high computational efficiency. Thus, the new technology is well suited for modeling and predicting SEP impacts during extreme solar events.

The integrated model traces magnetic field lines from the MHD models to find the area that is covered by field lines originating from a given area of the solar surface, such as an AR. As described above, each field line is represented by a Lagrangian grid that advects with the background plasma in a time-dependent manner. The relevant data at the location of the grid points are transferred to M-FLAMPA, which in turn calculates the evolution of the energetic particle population by solving the governing kinetic equations.

5. Proof-of-concept Results from the MHD+SEP Coupled Model

5.1. Simulation of SEP Event of 2012 January 23

As a demonstration of our predictive framework’s capabilities, we provide simulation results for the SEP event associated with the observed CME of 2012 January 23. Various aspects of the event have been studied in the literature (e.g., Nesse Tyssøy et al. 2013; Joshi et al. 2013). The simulation is performed as follows: (1) use the magnetogram for late 2012 January (CR 2119) to find a pre-eruptive, steady-state solution for SC and IH; (2) initiate a CME with parameters computed by the EEGGL tool for anticipated CME speed, e.g., as measured by the Stereocat tool or found in the DONKI Space Weather activity archive; and (3) run MHD and particle models concurrently, where the former provides background solar wind parameters for the latter.

We present some results of the simulation below. Figure 2 shows three different snapshots (2 hr apart) of the CME forming in the SC, together with extracted field lines. The CME was initiated at 29°5 latitude and 208°5 longitude in the heliographic rotating coordinate system (HGR) and with anticipated speed \( U_{CME} = 2000 \text{ km s}^{-1} \). Figure 3 shows SEP flux for energies exceeding 10 MeV, which corresponds to NOAA GOES energy channel 2, along extracted field lines and through a 1 au sphere (interpolated between footprints of field lines on that sphere). Finally, Figure 4 demonstrates a comparison of time evolution of SEP flux with GOES measurements.

This simulation has been performed using computational resources of the NASA Pleiades supercomputer. The 6 hr run has been completed in 4.5 hr of CPU time with 480 computational cores (20 Haswell nodes by 24 cores) utilized.

6. Conclusions

The present paper serves the purpose of being a guide into and a reference for our research effort in the field of SEP forecasting. In this paper we have reviewed the physical principles that form the basis of the MHD component of our SEP forecasting framework. These principles serve as a foundation for a large number of computational models (developed over the span of several decades) that allow simulating quiet-time SC and IH, as well as eruptive events in SC and their propagation into IH. Here, however, we have put more focus on those models and tools (specifically, AWSoM, AWSoM-R, EEGGL) that have been or are being implemented in the SWMF (Tóth et al. 2012), which is to host the full SEP forecasting framework. Additionally, we have suggested the concept of a magnetized cone model, which could serve as a simple yet effective eruptive event generator.

The present paper is to be followed by the review of the kinetic component of our full SEP model and will complete its description.

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Appendix

Equilibrium Magnetic Configurations: Spheromak

The equation of MHD equilibrium reads as (Landau & Lifshitz 1960)

\[ \mathbf{j} \times \mathbf{B} - \nabla P = 0, \]

(38)

which we consider in spherical coordinates \((r, \theta, \varphi)\). Here \(\mathbf{B}\) is the vector of the magnetic field, \(\mathbf{j}\) is the electric current, and \(P\) is the plasma pressure. It has been demonstrated (Grad & Rubin 1958; Shafranov 1966) that an axisymmetric equilibrium MHD configuration is governed by a single scalar equation, commonly referred to as the Grad–Shafranov equation. The key concept that allows transforming Equation (38) to this simpler form is that of magnetic surfaces, which are defined as surfaces of constant pressure, \(P\).

From Equation (38), \(\mathbf{j} \cdot \nabla P = 0\) and \(\mathbf{B} \cdot \nabla P = 0\), i.e., a single line of either magnetic field or electric current is entirely confined within a single magnetic surface. Further, magnetic field flux and current functions defined as

\[
\psi(r_\perp, z) = \int_0^{r_\perp} B_r(r_\perp', z) r_\perp' \, dr_\perp', \quad I(r_\perp, z) = \int_0^{r_\perp} j_r(r_\perp', z) r_\perp' \, dr_\perp',
\]

(39)

can both be demonstrated to be constant on a given magnetic surface (here \(r_\perp = r \sin \theta\) and \(z = r \cos \theta\)). Therefore, for an axisymmetric equilibrium configuration, there is a functional dependence between \(\psi, I\), and \(P\): \(I = I(\psi), P = P(\psi)\). Using Ampere’s law, \(\nabla \times \mathbf{B} = \mu_0 \mathbf{j}\), and by introducing the toroidal component of the vector potential, \(\nabla \times \mathbf{A} = \mathbf{B}\), one can relate the current and magnetic flux via the toroidal components of the field and vector potential: \(I = \frac{\mathbf{B}_0}{\mu_0} \mathbf{A}_\varphi, \psi = r_\perp \mathbf{A}_\varphi\). Thus, the total magnetic field may be expressed as

\[
\mathbf{B} = \nabla \times (A_\varphi \mathbf{e}_\varphi) + B_r \mathbf{e}_r = \frac{1}{r_\perp} (\nabla \psi \times \mathbf{e}_r + \mu_0 I \mathbf{e}_\varphi).
\]

(40)

Here \(\mathbf{e}_\varphi\) is the unit vector of the azimuthal (toroidal) direction. Analogously, for the current density vector we have

\[
\mu_0 \mathbf{j} = \nabla \times (A_\varphi \mathbf{e}_\varphi) + B_r \mathbf{e}_r = -\nabla^2 (A_\varphi \mathbf{e}_\varphi) + \mu_0 \frac{d(I \mathbf{e}_\varphi)}{d\psi} / r_\perp.
\]

(41)

Once substitutions of Equations (40) and (41) are performed and a common factor of \(\nabla \psi / r_\perp\) is omitted, the condition of equilibrium, Equation (38), reads

\[
\mathbf{e}_\varphi \cdot \nabla^2 (A_\varphi \mathbf{e}_\varphi) = -\mu_0 r_\perp \frac{dP}{d\psi} - \mu_0 \frac{dI}{d\psi} B_r.
\]

(42)

In the particular case of constant \(dI / d\psi\) and \(dP / d\psi\), by expressing the Laplace operator in spherical coordinates, Equation (42) reduces to the equation describing electromagnetic waves (magnetic dipole and multipole harmonics; see Jackson 1999):

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial A_\varphi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial A_\varphi}{\partial \theta} \right) - \frac{A_\varphi}{r^2 \sin^2 \theta} + \alpha_0^2 A_\varphi = -\mu_0 r \sin \theta \frac{dP}{d\psi},
\]

(43)

where \(\alpha_0 = \mu_0 dP / d\psi\). It may be solved by developing the solution over spherical harmonics: \(A_\varphi = \sum_{\alpha=1}^{\infty} \alpha_0 j_\alpha(\alpha_0 r) P_\alpha(\cos \theta) - \mu_0 \alpha_0^2 r \sin \theta \frac{dP}{d\psi}\), where \(P_\alpha\) are associated Legendre polynomials, \(j_\alpha(x) = \sqrt{\pi / 2\alpha} J_{\alpha + 1/2}(x)\), and \(J_\alpha(x)\) and \(j_\alpha(x)\) are regular and spherical Bessel functions, respectively. For a dipole harmonic we have

\[
A_\varphi = A_{\alpha_0} \left[ j_1(\alpha_0 r) - \frac{\mu_0 r}{\alpha_0^2} \frac{dP}{d\psi} \right] \sin \theta.
\]

(44)

Introducing parameters \(B_0 = \alpha_0 A_{\alpha_0}\) and \(\beta_0 = \mu_0 \alpha_0^2 \frac{dP}{d\psi}\), we obtain the expression for the spheromak’s magnetic field and pressure:

\[
B_{\alpha_0}(r) = \left[ \frac{j_1(\alpha_0 r)}{\alpha_0 r} - \beta_0 \right] \left( 2B_0 + \alpha_0 \alpha_0 B_0 \right) + \frac{j_2(\alpha_0 r) [r \times [r \times B_0]]}{r^2},
\]

(45)

\[
P_{\alpha_0}(r) = \left[ \frac{j_1(\alpha_0 r)}{\alpha_0 r} - \beta_0 \right] \frac{\beta_0 \alpha_0^2 [r \times B_0]^2}{\mu_0}.
\]

(46)

Here the vector \(B_0\) is introduced with the magnitude equal to \(B_0\) directed along the polar axis of the spherical coordinate system, and \(\alpha_0 = \pm 1\) is the sign of helicity (we assume \(\alpha_0 > 0\)). At the center of configuration the magnetic field equals \(B_{\alpha_0}|_{r=0} = 2(\frac{1}{3} - \beta_0)B_0\), which for low-beta plasma differs only by a numerical factor of ~0.7 from \(B_0\). In Equations (45)–(46), the coordinate vector, \(r\), originates at the center of configuration, \(\mathbf{R}_c\). Thus, in the arbitrary coordinate system, the field and pressure of the configuration are equal: \(B_{\alpha_0}(\mathbf{R} - \mathbf{R}_c), P_{\alpha_0}(\mathbf{R} - \mathbf{R}_c)\), for \(|\mathbf{R} - \mathbf{R}_c| \leq r_0\).

We restrict currents to within a spherical magnetic surface \(|\mathbf{R} - \mathbf{R}_c| = r_0\). The radial and toroidal components of the magnetic field turn to zero at the surface, and thus \(j_1(\alpha_0 r_0) = \beta_0 \alpha_0 r_0\). For a given \(\beta_0\) this equation relates the configuration size, \(r_0\), to the extent of magnetic field twisting, \(\alpha_0\), needed to close the configuration within this size. The plasma pressure, \(P\), also turns to zero at the external boundary.

The meridional and equatorial planes (top) and radial dependence of the field and pressure for \(\beta_0 = 0.02\) (bottom left) are shown in Figure 5. The shown magnetic field lines are also the cross sections of magnetic surfaces.

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Figure 5. Top: spheromak configuration for \( \beta_0 = 0.02 \): meridional (left) and equatorial (right) planes. Magnetic field direction is marked with arrows; the off-plane component of the magnetic field is normalized per \( B_0 \) (see Equation (26)) and shown by color. Local values of plasma parameter \( \beta(r) = \mu_0 P(r)/B^2(r) \) are shown, with orange curves corresponding to levels \( \beta = 0.04, 0.08, 0.12, \) and 0.16 as marked explicitly. Bottom: radial dependence of thermal pressure, \( \mu_0 P(r)/B_0^2 \) (red curve), and magnetic pressure, \( B^2(r)/B_0^2 \) (blue curve), in the equatorial cut \( z = 0 \), for \( \beta_0 = 0.02 \) (left) and for \( \beta_0 = -2.87 \times 10^{-2} \) (right).

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