Final Report of the Team Working on the LWS TR&T Focused Science Topic: "Physics-based methods to predict connectivity of SEP sources to points in the inner heliosphere, tested by location, timing, and longitudinal separation of SEPs"

Prepared by Dr. D. Lario (david.larioloyo@nasa.gov)

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I. INTRODUCTION

In our first FST Team meeting back in January 2015, we generated the attached document entitled "**Integrated Four-Year Research Plan**". In that document, we described the tasks to be performed within our FST Team, potential collaborations and the framework for developing our activities. According to the NN14ZDA001N-LWS AO, we set a main Scientific Goal for our FST Team, i.e. "**identify the mechanism(s) that result in SEP events with extremely large extents in longitude**". We also proposed a series of Science Questions to be addressed throughout the duration of the project to help us reach our Scientific Goal. In Section II of the present document we summarize the consensus reached within our team to answer these questions. During the study and from the use of physics-based methods to predict the connectivity to SEPs sources, we have learned a series of lessons that are synthesized in Section III. From these lessons learned and the answers to the proposed questions, we draw a series of conclusions summarized in Section IV, where we address how well we can identify the mechanisms that result in widely-extended SEP events.

The main deliverables of our activities can be identified in the numerous articles we have published in scientific journals and presentations given at workshops and conferences. Section VII contains an exhaustive list of the publications by members of the FST team. Each group has also been encouraged to list their own publications on the LWS web site at lwstrt.gsfc.nasa.gov/research-highlights.

In our initial research plan, we also promised to provide recommendations on how to improve the predictability of the SEP longitudinal extent. In Section V we describe tools developed in the framework of our FST Team with the aim of improving our predictability of SEP intensities. They are based on either [1] the knowledge of the magnetic connectivity between spacecraft and the putative sources of large SEP events (i.e. shocks initially driven by CMEs) and [2] empirical relationships between particle intensities and the CME properties, the angular distance between magnetic connection footpoints and the site of the parent solar flares.

In Section VI we identify measurements that in the near future might improve the study of the effects of connectivity on the observation of SEP events and hence understand the SEP longitudinal extent.

The annual reports regularly sent to the NASA LWS Technical Officers included a comprehensive summary of [1] the activities performed by the FST Team during each year, [2] the progress to achieve the proposed goals, [3] our adherence to the original plan, [4] the collaborations engaged within the members of the FST team, and [5] our community involvement in the organization of sessions at scientific meetings not only to disseminate our own work but also to gain knowledge of the research done by other groups and thus promote research on this interesting topic.

The present document summarizes the main conclusions reached throughout our project and completes our activities as an FST Team.

II. CONSENSUAL RESPONSES TO THE PROPOSED SCIENCE QUESTIONS

By consensus we agreed with the following outline as answer to the science questions proposed back in January 2015:

(1) Does the extent of the CME-driven shock in the corona determine the extent of the SEP event in the heliosphere?

> The extent of the CME-driven shock can be used to describe the connection between spacecraft and the likely source of SEPs, but SEPs can extend to a broader range of longitudes [e.g., Lario et al., 2016, 2017, ApJ]

(2) Do the properties of the SEP sources (i.e., CME-driven shocks and/or flares) at the regions magnetically connected to the observer correlate with the observed SEP characteristics?

> The large-scale properties of the particle sources (such as CME speed, width) can be used to determine particle intensities (with some uncertainties). However, the detailed properties of the sources that may contribute to the SEP characteristics (such as shock strength, the presence of seed populations, effects of both shock ripples and magnetic turbulence on the particle acceleration processes at shocks) cannot be fully determined at present, so it is not possible to assess their influence on the production of SEPs. In the absence of this information, some average characteristics of SEP events can still be determined, as exemplified by the SEP prediction scheme based on CME direction, speed and the properties of the radio burst emissions discussed by Richardson et al. [2018, Space Weather], and that developed by Xie et al. [2019, JGR] based on CME speed and width and the connection angle of the observer.
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> There is also a correlation between SEP intensity and the X-ray intensity of the related flare [e.g., Fig. 11 of Richardson et al., 2017 Adv. Space Res]. On the other hand, flare intensity is not a good indicator of SEP intensity. In particular, most large (>=M class) flares are not associated with SEP events, often related to the lack of CMEs. For example, only 14% of the 398 M and X class flares in June, 2010 to January, 2014 were clearly associated with 25 MeV proton events [Richardson et al., 2016 presented at the SDO Workshop].
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> Other properties of SEP events, such as ion abundances, show some longitudinal dependence such as that the longitudinal distributions of ion fluences can be represented by Gaussians with widths that are smaller with increasing energy, consistent with lower energy ions experiencing more cross-field diffusion or being accelerated over a larger portion of the parent CME-drive shock or for longer times as shock expands [e.g., Cohen et al. 2017, ApJ]. However, no clear longitudinal dependence was found in terms of the charge-to-mass (Q/M) ratio of the ions. The link between ion abundances and specific properties of the SEP sources is still unsettled. In part this is because composition measurements from the STEREO spacecraft are not available at the high energies (comparable to those measured by the SIS

instrument on ACE) which are important for diagnosing the early stages of particle acceleration. In addition, the STEREO spacecraft were too widely separated from Earth when activity increased in solar cycle 24 to make comprehensive multi-point SEP composition measurements in all but a small sample of the largest events.

Uncertainties in the identification of the regions that a given spacecraft is magnetically connected (see Section III below) add ambiguity of the precise determination of the SEP sources responsible for the acceleration of the SEPs observed by the spacecraft.

(3) Why are delays observed between the parent solar phenomena and SEP event onsets? Are they related to delays in the observer becoming magnetically connected to the expanding CME-driven shocks?

There are several reasons:

a) Within the uncertainties in estimating the magnetic connection of the observer with the corona (see Section III), models of coronal shock fronts based on EUV and white-light observations can infer that there is a delay before the shock establishes connection with the observing spacecraft. However, particles can be detected even in the absence of connection to the shock.

b) Particle propagation may be influenced near the Sun by coronal structures, in the inner heliosphere by solar wind structures (e.g., ICMEs, CIRs, the heliospheric current sheet) or by self-amplified turbulence near the shock. An accurate representation of these transport processes (which however are likely to vary from event to event) should be considered in order to correctly estimate the SEP release times from observed SEP onsets.

c) Delays in the estimated release time of electrons and protons into interplanetary space have been previously observed but it is still unclear whether they are due to different injections or coronal transport effects (or both) [e.g., Kallenrode 1992, JGR; Richardson et al. 2014, Solar Phys.].

d) A proper treatment of pre-event background intensities is necessary to accurately detect event onsets and hence estimate SEP release times.

e) Different techniques (e.g., velocity dispersion analysis, time shift analysis, estimating onset times by eye vs. statistical techniques) have been evaluated/used within our FST team to estimate particle release times near the Sun, but they do not always provide consistent results for the same event. It is insufficient to perform one analysis and claim that an accurate particle release time has been determined.

(4) What are the roles played by the transport of magnetic field lines in the heliosphere and SEP cross-field diffusion in the longitudinal extent of the SEP events?

Cross-field diffusion is necessary to explain SEP events observed by extremely poorly connected spacecraft. SEP transport processes in the corona also play a significant role in the longitudinal spread of SEPs [e.g., Zhang et al. 2017, ApJ; Zhao et al. 2018, ApJ]. Global three-dimensional MHD simulations of the solar corona and solar wind including turbulence transport suggest that field lines may undergo large-scale expansion, but also concentration in regions where slab diffusion is suppressed. Whereas large-scale expansion could help to explain the wide longitudinal and latitudinal spread of energetic particles, suppression of field-line diffusion can concentrate field lines, resulting in alternating regions of enhanced and depressed energetic particle fluxes that resemble the “flux drop-outs” found in SEP events [e.g., Tooprakai et al. 2016, ApJ]. These simulations have not yet been applied to actual SEP events.

(5) What is the effect of the coronal magnetic field configuration on the injection of SEPs over a broad range of longitudes?

It depends. Non-radial expansion of coronal fields may play a role in the distribution of SEPs to distant longitudinal regions [e.g., Klein et al. 2008, A&A]. Additionally, cross-field diffusion is enhanced around the heliospheric current sheet (HCS) [e.g., Chhiber et al. 2017 ApJ; Zhao et al. 2018 ApJ]. Therefore, solar cycle variation in the particle diffusion coefficients and the wrapping of the HCS might affect the spread of SEPs [Zhao et al. 2018, ApJ]. This effect may occur both in the solar corona and in the solar wind.

Recent studies performed by researchers outside the FST team also suggest that coronal magnetic field topology has an influence on the spreading of SEPs, such as pseudostreamers [Panasenco et al. 2017, AGU] and S-web field topologies [Higginson et al. 2018, ApJ] that may contribute to the longitudinal distribution of SEPs injected from narrow and impulsive sources.

(6) How do pre-existing solar wind structures (e.g., ICMEs, multiple shocks, CIRs, HCS) and interplanetary magnetic field geometries affect the characteristics of the SEP events observed at different longitudes?

The magnetic connection between an observing spacecraft and SEP sources may be influenced by the presence of intervening structures, including structures that are present near or at the spacecraft. Hence, assumptions about the IMF geometry (such as a Parker spiral field) used to infer connection to an SEP source may be invalid, and the true field geometry may be unknown. The particle onset delay, arrival direction, anisotropies and peak intensities are affected by intervening structures [e.g., Richardson & Cane 1996, JGR; Bain et al. 2014, ApJ; Lario & Karelitz 2014, JGR; and references therein]. ENLIL simulations of multi-compound events [e.g., Bain et al. 2015, ApJ; Luhmann et al. 2018, Space Weather] show the complexity of the interplanetary medium in these events that can result in asymmetric SEP distributions, and provide some insight into the magnetic connections with SEP sources, in particular interplanetary shocks.

(7) How do the turbulent topology of the interplanetary magnetic field and the exchange of field line connectivity between the Sun and the observer influence the SEP fluxes observed at different longitudes?

Recent 3D MHD models of the heliosphere allow turbulence to be incorporated in different regimes from the corona to the inner solar wind [Usmanov et al. 2016, 2018]. In these models, turbulence parameters are computed throughout the inner heliosphere for a wide range of conditions specified by magnetograms, and variously tilted dipoles mimic the solar magnetic field during the solar activity cycle [Chhiber et al. 2017, ApJ; Zhao et al. 2018, ApJ]. Due to turbulence, stochastic field line spreading and interchange connectivity occurs, which may explain SEP flux dropouts and the observation of SEPs at distant heliospheric locations [e.g., Tooprakai et al. 2016, ApJ].

III. LESSONS LEARNED IN THE STUDY OF SEP CONNECTIVITY

Throughout the project we have faced problems and difficulties that have taught us lessons that are summarized here in the hope that they will be useful for further studies of this topic:

- Clean, isolated, simple, longitudinally-extended, SEP events are needed to accurately determine the conditions and mechanisms leading to the spread of SEP events in the heliosphere. However, such events are rare. The largest and widespread SEP events more often occur at times of multiple events and disturbed/complex interplanetary conditions, often associated with the presence of major active regions. Hence, many of these events are not suitable for study. In addition, connectivity and the conditions for particle spread in events at times of high activity may be different from those in isolated events.
- The Parker spiral field is clearly the major influence on connectivity, leading to the well-established bias towards larger SEP events originating on the western hemisphere. Determining how deviations from spiral geometry, for example due to particular coronal configurations and/or intervening interplanetary structures, are identified and modeled remains a challenge.
- There is currently no way to know the correct magnetic connectivity between a spacecraft and a particle source in the corona because the inferred coronal magnetic field is model and magnetogram dependent, and a priori, it is not obvious which model/magnetogram gives the correct result for a given event (this may not be the model that includes the most physics and is therefore expected to be most accurate). However, observations can be used to exclude those models that predict connections to incorrect regions based on, for example, the concordance between the magnetic field polarities observed in-situ and the region where the field line originates.
- Caution should be exercised when using idealized geometrical shapes to describe large-scale shock structures and connection to them. This is not only because the actual shape of the shock front as observed in EUV and white-light images might differ from these idealized geometrical shapes, but also because radio observations of coronal shocks indicate that shock-accelerated electron beams originate at multiple locations along the shock front, suggesting that shocks are not uniform and multiple ripples may form throughout their fronts [e.g., Morosan et al. 2019, Nature Astronomy].
- Combining MHD and PFSS models of the background solar corona makes it possible to estimate some of the properties of shocks in the corona (spatial extent, speed and Mach number evolution) that are controlled not only by the CME size and speed but also by the background medium. However, the shock properties do not always agree with expectations based on the production/release of the observed SEPs. Caution should be exercised when applying statistical averaged model-dependent properties of coronal shocks and their relation to SEP production. The use of such models should be carefully considered when multiple CMEs occur (so that a shock may not be propagating through a pristine background coronal field) or when describing conditions in the disturbed region downstream of a shock.
- Even for an apparently clear SEP onset, using different methods to estimate the onset time, particles in different energy ranges, different analysis methods with different assumptions, and different researchers applying the same techniques, can produce variations in the

estimated release time. A claimed definitive release time obtained from a single analysis should be viewed with caution.

- Special care should be taken when computing SEP release times from weak and slowly-rising SEP onsets, in particular where these are the most poorly-connected observations of an SEP event that are critical to inferring how particles are spread in longitude.
- The extent of the observed EUV wave in the corona is not always an indication of the longitudinal extent of the associated SEP event in interplanetary space.
- Observations from three approximately equally-separated S/C (e.g., STEREO A and B, and at Earth) around the Sun are not sufficient to [1] delimit the actual extent of an SEP event, [2] determine its longitudinal intensity profile, and [3] constrain the processes that spread SEPs. With three S/C, it is only possible to fit the intensity to a simple function such as a Gaussian in longitude. Observations from additional spacecraft are required to challenge such simple fits and determine more precisely where the SEP peak is, whether there are longitudinal asymmetries and local effects at particular locations, and estimate the longitudinal dependence of onset delays.
- There is a spectrum of SEP event widths. There is no such a thing as narrow or wide SEP event.
- The long-standing practice of using the flare as the solar event location is a reasonable choice, even if the CME is not exactly above the flare. Much of the impact of connectivity on SEP events can be accounted for by the connection angle between the spiral field line footpoint and the associated flare/solar activity.

IV. MAIN CONCLUSIONS

Our major conclusion is that the study of SEP connectivity is not straightforward. We will only be able to predict the connectivity between spacecraft in the inner heliosphere and the sources of energetic particles when the mechanisms that play a role in the arrival of SEPs at a given location in the heliosphere are completely identified and understood. Particle acceleration and transport are the mechanisms that determine whether an SEP can reach a given heliospheric location. However, there are multiple factors that control these mechanisms that remain obscure to our observing capabilities and vary from event to event (e.g., presence of seed populations, turbulence properties, coronal magnetic field configuration, interplanetary magnetic field properties, shock structure at both large and small scale, effects of intervening structures on the transport of particles and the location of the particle sources). Each of these factors cannot be disregarded since they may have a real influence on the eventual observation of SEPs at a given heliospheric location. There is a real risk of misinterpreting observations when assuming idealized scenarios or when only one factor is taken into account.

Therefore, there are several elements involved in the generation and detection of large-extent SEP events but currently we cannot completely characterize them in detail. We can put limits on their individual contributions but their combination is necessary to explain the wide variety of SEP events.

The next two sections summarize the ingredients that we consider necessary to improve the study of the connectivity to SEP sources, as well as recommendations that can be used to improve current tools to predict the longitudinal extent of SEP events.

V. TOOLS TO IMPROVE PREDICTABILITY OF THE SEP LONGITUDINAL EXTENT

From the point of view of an Earth-based forecaster, and with the currently available tools, the question to answer is: “Do the characteristics of an observed CME allow us to predict the occurrence of a SEP event at Earth?” Implicitly, this question addresses the main question we proposed within our FST Team about the predictability of the SEP longitudinal extent, since the parent solar eruption might occur at any longitude with respect to Earth.

Within the framework of the FST Team, we have addressed this issue by first analyzing whether our methods to estimate the magnetic field connectivity between a spacecraft and the shock observed in EUV and white-light (WL) coronagraph images differentiate those CMEs for which SEPs are detected. Starting from the list of >25 MeV proton events observed by either STEREO-A, STEREO-B and/or SOHO collected by Richardson et al. [2014; Solar Phys.], a fit to the large-scale structure of the parent shocks seen in EUV and WL images was performed. Then we analyzed whether the connectivity of each spacecraft via a Parker spiral magnetic field line to the fitted shock determined the observation of SEPs by such spacecraft. For 235 cases when the analysis predicted that the spacecraft was connected to the shock, then SEPs were actually observed in 75% of these cases. Conversely, when no connection to the shock was predicted, then no SEPs were observed in 81% of these 150 cases. The overall accuracy is 77%, and the frequency bias is 0.84 (a perfect score is 1), indicating that this method slightly underforecasts SEP events. This is consistent with the transport of SEPs beyond the regions that appear to be connected to shocks being a factor to consider in the arrival of SEPs at poorly connected spacecraft as discussed above.

The method used to determine the connectivity between a spacecraft and the shock requires a 3D fit to be made to the large-scale structure of the shock. Such a fit requires the observation of the shock from multiple vantage points, which was only possible when the two spacecraft of the STEREO mission were operative and conveniently separated in space. The observation of CMEs from a single point (e.g., L1) prevents us from obtaining a precise measurement of the 3D structure of the shock and hence assessing whether spacecraft are connected to the shock.

It is also important to distinguish the properties of the CME (speed, width and direction) from those of the shock initially driven by the CME. The shock may expand over a larger region than the CME. Under the assumption that the shock is the main agent responsible for both acceleration and injection of energetic particles over extended regions of the heliosphere, it is important to characterize the shock properties over all its front rather than the properties of the CME that might give us a limited extent for the source of particles.

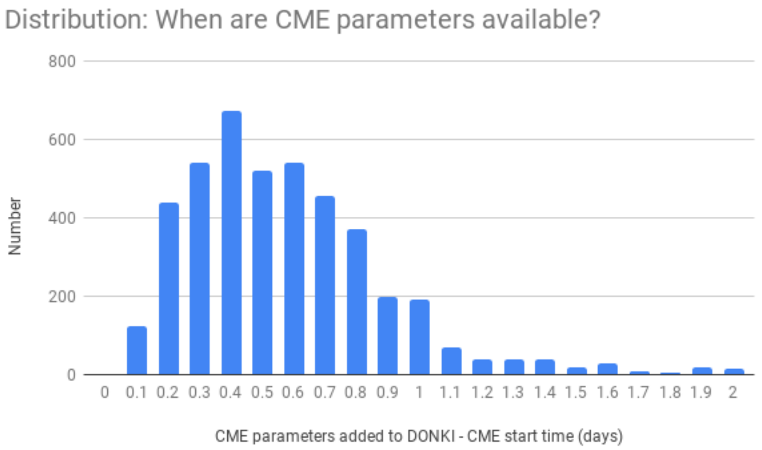
Within the framework of our FST Team, an empirical relationship between the speed and width of the parent CME together with the longitudinal distance between the site of the parent solar eruption and the magnetic footpoint connection of a given spacecraft was developed by Xie et al. [2019, JGR]. In particular, it was found that the best correlation exists between the SEP peak intensity I_0 and the proxy CME kinetic energy, $v^2\kappa^2\omega_{FO}$, where v is the speed of the shock driven by the CME and $\kappa^2\omega_{FO}$ is proportional to the true CME shock speed and flux-rope CME widths. Xie et al. [2019] applied a Gaussian fit to obtain the SEP intensity I_0, and a forward-modeling fit to determine the true shock speed and true CME width. Based on correlations between Gaussian peak intensity I_0 and the CME kinetic energy and correlations between SEP width σ and connection angles CA, they developed a formula to predict the SEP intensity observed by each spacecraft as a function of shock speed, CME width, and CA, given by:

$$I(\phi) = I_0 exp[-CA^2/2\sigma^2], \text{ where } I_0 = 10^{-0.27+1.09v^2\kappa^2\omega_{FO}}$$

$$\sigma = \begin{cases} 8.4 + 0.21CA, & \text{if } CA \geq 0 \\ 7.9 - 0.28CA, & \text{if } CA < 0 \end{cases}$$

where the CME shock speed v and CME half width ω_{FO} are in units of 10^3 km/s and 10^2 degree, respectively, whereas κ is the aspect ratio of the flux-rope CME. By including the true shock speed and true CME widths, Xie et al. [2019] reduced the root-mean-square errors on the predicted SEP intensity by ~41% for protons compared to the formula proposed by Richardson et al. [2014, Solar Phys.]. The use of this formula as a predictive tool is being worked out and will be tested and validated with SEP events observed over the new solar cycle.

Similarly, within the framework of our FST Team, the empirical SEP intensity prediction tool “SEPSTER” (SEP prediction based on STEReo observations) was developed [Richardson et al., 2018; Space Weather]. The inputs used in this tool include the parent CME characteristics (speed, width and direction) and the observation of radio bursts. This prediction scheme allows us to estimate the peak 14-24 MeV proton intensity at Earth or any other point at 1 AU. SEPSTER is one of six models chosen by the Space Radiation Group at the Johnson Space Flight Center to develop a prototype SEP prediction scoreboard for the Lunar Outpost and future Artemis missions to the Moon and Mars in conjunction with the Community Coordinated Modeling Center (CCMC). The initial model has been delivered to CCMC and uses real time-updating CME observations from the CCMC DONKI database together with the solar wind speed from an upstream (L1) spacecraft to calculate the Parker spiral field line connection to the Sun. Predictions for energy ranges other than 14-24 MeV are also made by using typical ratios between the intensities in these energy ranges based on observations of a sample of SEP events.



Ideally, these methods require the acquisition of CME observations in near real-time and from multiple viewpoints (such as are currently available from the STEREO spacecraft and SOHO at L1). However, at present, it can take several hours for CCMC to receive and analyze sufficient observations to be able to determine the CME parameters and place them in DONKI. This delay results from the time needed in obtaining enough frames (at least two) downloaded from the spacecraft and then use them to measure the CME. The figure above shows the distribution of how many days after the CME start time (first coronagraph observation time) the CME parameters were added into the CCMC's DONKI database. The estimate is that CME parameters are available on average within 0.4 days (10 hours), particularly for CMEs with speeds above 1000 km/s. In terms of using CME parameters for SEP prediction, and thus improve the feasibility of the SEP prediction methods. the delay in obtaining real-time coronagraph observations from multiple viewpoints should be minimal and their analysis should be rapidly done.

Another project within our FST team was the characterization of the magnetic connectivity to CMEs as simulated by the WSA-ENLIL+Cone model. CME-driven discontinuity/shock properties were derived along the observer's magnetic field lines and compared to SEP observations for over a dozen multi-spacecraft SEP events [Bain et al., 2016; Luhamnn et al. 2017; Luhmann et al., 2018; Guo et al., 2018]. These simulations provide a tool to interpret major SEP events involving multiple CMEs in the context of a realistic heliospheric model and to determine how much of what is observed depends on non-local magnetic connections to shock sources. The WSA-ENLIL simulations can also be used to directly drive energetic particle models such SEPMOD [Luhmann et al., 2007, 2010] and EPREM [Schwadron et al., 2010], to further compare with observations.

VI. REQUIRED MEASUREMENTS TO IMPROVE THE STUDY OF THE EFFECT OF CONNECTIVITY ON SEP EVENTS

As a team, we have identified several observations and measurements that may help us to improve the study of the connectivity between observations and SEP sources.

- Vector magnetograms, including, to the extent possible, backside and over-the-poles magnetograms. This information will be essential to obtain faithful representations of the coronal magnetic field configuration used in models of SEP transport and estimation of field connectivities. Further development of coronal models to use these magnetograms, and validation of their accuracy would be desirable, since at present, we cannot determine if these models provide an accurate representation of the coronal magnetic field configuration all around the Sun.
- More distributed in-situ measurements of SEPs, solar wind and magnetic field, in particular in the inner heliosphere, since observations from three locations are not enough to definitively define the extent of a SEP event and how the SEPs are spread in longitude and how to characterize the structures present in the solar wind. Energetic particle measurements should be clean of background and contamination enabling accurate determination of event onsets. Measurements of particle anisotropy and composition are needed to infer connectivity to the particle source and transport parameters, and properly determine SEP release times and their association with the properties of the SEP sources.
- Low-corona imaging of the formation of shocks during the early-evolution of CMEs and detailed observations of active regions and solar flares, including in near-real time. This

imaging should include multiwavelength observations as well as low-corona ultraviolet and white-light (coronagraphs). A vantage point for this type of observations related to SEP events affecting Earth would be a spacecraft at the Sun-Earth Lagrangian L4 point working in combination with near-Earth observations.

- Ground- and space-based radio observations that are made available to the community in near-real time for SEP prediction purposes, to help estimate the times of the particle release in the corona and the formation of coronal shocks.
- Models of the corona and interplanetary medium that will allow field connectivities to be inferred in the appropriate context (for example, in the presence of intervening structures) and improve SEP transport simulations.

VII. COMMUNICATIONS AND PUBLICATIONS

The team has been very productive in terms of presentations at conferences and workshops. Below is a list of articles published in refereed science journals by the FST team members. In addition, on the LWS web site at https://lwstrt.gsfc.nasa.gov/research-highlights, each group has added their own publications identified by the corresponding grant number.

2015

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2016

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