Modeling Heliophysics Phenomena with MS-FLUKSS: Connecting the Sun to the LISM

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Key Challenges

1. Flows of partially ionized plasma are frequently characterized by the presence of both thermal and nonthermal populations of ions and neutral atoms. This occurs, e.g., in the outer heliosphere – the part of interstellar space beyond the solar system whose properties are determined by the solar wind (SW) interaction with the local interstellar medium (LISM).

The Sun is at the origin, the LISM flow is from the right to the left. Their interaction creates a heliospheric termination shock, a heliopause, and a bow wave that may include a sub-shock inside its structure. The LISM is partially ionized and the mean free path of charge exchange between H atoms and H+ ions is such that this process should be modeled kinetically.
2. Understanding the behavior of such flows requires that we investigate a variety of physical phenomena: charge-exchange processes between neutral and charged particles, the birth of pick-up ions (PUIs), the origin of energetic neutral atoms (ENAs), production of turbulence, instabilities and magnetic reconnection, etc. Collisions between atoms and ions in the heliospheric plasma are so rare that they should be modeled kinetically. PUIs, born when LISM neutral atoms experience charge-exchange with SW ions, represent a hot, non-equilibrium component and also require special treatment.

From Matthew Bedford, a former BW graduate fellow: density distributions along the Voyager 1 trajectory in simulations for a single ion mixture and PUIs modeled as a separate ion fluid. The width of the heliosheath diminishes in accordance with Voyager 1 measurements.
3. The solar wind perturbs the LISM substantially: about 1000 AU upwind and 10,000 AU in the tail. This perturbation affects TeV cosmic rays and may be an explanation of their observed anisotropy.

4. Solar wind simulations from the solar surface to Earth’s orbit are important for space weather predictions, ensuring safety of personnel and electronics on board spacecraft.

5. To address these problems, we have developed a tool for self-consistent numerical solution of the MHD, gas dynamics Euler, and kinetic Boltzmann equations. Our Multi-Scale Fluid-Kinetic Simulation Suite (MS-FLUKSS) solves these equations using an adaptive-mesh refinement (AMR) technology. The grid generation and dynamic load balancing are ensured by the Chombo package.
Non-thermal (pickup) ions are created when SW ions experience charge exchange with interstellar neutral atoms. Further charge exchange of PUIs with neutral atoms creates energetic neutral atoms (ENAs) measured by IBEX.
Code parallelization

<table>
<thead>
<tr>
<th>Time (sec)</th>
<th>All MPI</th>
<th>2 threads</th>
<th>3 threads</th>
<th>6 threads</th>
<th>12 threads</th>
</tr>
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<tbody>
<tr>
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<td>167</td>
<td>170</td>
<td>181</td>
<td>208</td>
<td></td>
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</tbody>
</table>

Table 1. Performance comparison of the kinetic code with different numbers of threads per MPI task.

<table>
<thead>
<tr>
<th>Number of cores</th>
<th>Time (sec)</th>
<th>Speed up</th>
<th>Ideal</th>
</tr>
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<tbody>
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<td></td>
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<tr>
<td>40,000</td>
<td>484</td>
<td>2.07</td>
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<td>80,000</td>
<td>251</td>
<td>1.93</td>
<td>2</td>
</tr>
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<td>96,000</td>
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<tr>
<td>120,000</td>
<td>167</td>
<td>1.25</td>
<td>1.25</td>
</tr>
</tbody>
</table>

Figure 1. Strong scaling results of the kinetic code. The green line shows ideal performance. The red circles are measured time.
A 650Gb data file containing 10 billion particles (full 64-bit support is necessary) can be written as fast as 32 seconds on Lustre file system if it is striped over 100 Object Storage Targets (OSTs).

<table>
<thead>
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<tr>
<td>20,000</td>
<td>164</td>
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<td>96,000</td>
<td>177</td>
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<tr>
<td>120,000</td>
<td>167</td>
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</tbody>
</table>

Figure 2. Weak scaling results of the kinetic code.
New feature accessible to MS-FLUKSS

1. The 4$^{th}$ order of accuracy in space and time on adaptive grids

2. Adaptive mapped grids, e.g., cubed spheres.
Why it matters?

*Voyager 1 and 2 (V1 and V2), PI Edward C. Stone, crossed the heliospheric termination shock in December 2004 and in August 2007, respectively (Stone et al., 2005, 2008). After more than 40 years of historic discoveries, V2 is approaching the heliopause, while V1 in August 2012 (Stone et al., 2013) penetrated into the LISM and measures its properties directly. They acquire often puzzling information about the local properties of the SW and LISM plasma, waves, energetic particles, and magnetic field, which requires theoretical explanation. In the next few years, the heliospheric community has a unique chance to analyze and interpret Voyager measurements deriving breakthrough information about physical processes occurring more than $1.3 \times 10^{10}$ miles from the Sun. Illustrations courtesy of NASA at voyager.jpl.nasa.gov.*
Our team has proposed a quantitative explanation to the sky-spanning “ribbon” of unexpectedly intense flux of ENAs detected by the Interstellar Boundary Explorer (IBEX, PI David J. McComas). Our physical model makes it possible to constraint the direction and strength of the interstellar magnetic field (ISMF) in the near vicinity of the global heliosphere (Heerikhuisen & Pogorelov, 2011; Heerikhuisen et al, 2014, 2015, 2017; Zirnstein et al., 2014, 2015, 2016, 2017; Pogorelov et al., 2011, 2016, 2017). Heliophysics research is faced with an extraordinary opportunity to use *in situ* measurements from Voyagers and extract information about the global behavior of the heliosphere through ENA observations by IBEX.
From the Parker Solar Probe web site at JHU Applied Physics Laboratory [http://parkersolarprobe.jhuapl.edu/]: “Parker Solar Probe will swoop to within 4 million miles of the sun's surface, facing heat and radiation like no spacecraft before it. Launching in 2018, Parker Solar Probe will provide new data on solar activity and make critical contributions to our ability to forecast major space-weather events that impact life on Earth. In order to unlock the mysteries of the corona, but also to protect a society that is increasingly dependent on technology from the threats of space weather, we will send Parker Solar Probe to touch the Sun. In 2017, the mission was renamed for Eugene Parker, the S. Chandrasekhar Distinguished Service Professor Emeritus, Department of Astronomy and Astrophysics at the University of Chicago.... This is the first NASA mission that has been named for a living individual.”

Solar Wind Electrons, Alphas, and Protons (SWEAP) instrument (PI Justin Kasper) onboard SPP, to be launched in the summer of 2018, will directly measure the properties of the plasma in the solar atmosphere. In particular, the time-dependent distribution functions will be measured, which requires the development of sophisticated numerical methods to interpret them.

Each consecutive trajectory of PSP will take it closer to the Sun.
Recently, a great wealth of information about the directional variation (which is commonly referred to as anisotropy) in the flux of cosmic rays arriving at Earth in the TeV to PeV energy range has been obtained by a number of air shower experiments. Among those that have achieved excellent data quality with large event statistics are Tibet (Amenomori, et al. 2006, 2010); Milagro (Abdo et al. 2008, 2009); Super-Kamiokande (Guilian et al. 2007); IceCube/EAS-Top (Abbasi et al. 2010, 2011, 2012), and ARGO-YGB (Di Sciascio et al. 2012). The observational results are quite surprising and, to some extent, confusing. Zhang et al. (2014), Zhang & Pogorelov (2016) showed that the observed small-scale anisotropy may be due to the distortions to the LISM magnetic field by the heliosphere.

To address these issues in more detail, one needs to perform long-tail simulations in very large simulation boxes of the kind we perform using our Blue Waters resources.
Science funding


Our accomplishments supported by NSF PRAC award OCI-1615206

1. We used coronograh images from SOHO and STEREO spacecraft to simulations of CMEs starting from the lower corona of the Sun; (2)
2. We used the Wang-Sheeley-Arge coronal model driven by the Air Force Data Assimilative Photospheric Flux Transport (ADAPT) model to simulate SW properties at Earth and demonstrated advantages of our model over existing space weather prediction models;
3. We have refined our model for shocks propagating through the LISM, demonstrated good agreement with observational data, and predicted a few events to be observed at V1 in the future;
4. We have performed a time-dependent simulation of the heliosphere that produces a comet-like heliotail, and showed that the 11-year solar cycle leads to the formation of ENA lobes with properties remarkably similar to those observed by IBEX;
5. We have analyzed the heliotail flow and quantity distribution in the heliospheric bow wave for different LISM conditions in a computational box extended to $12,000 \times 10,000 \times 8,000$ astronomical units cubed, and showed that the observed multi-TeV cosmic ray anisotropy may be explained by the LISM magnetic field distortion by the heliosphere;
6. We have used simulations on adaptive meshes to further understand MHD instabilities and magnetic reconnection at the heliopause;
7. We have reproduced properties of pickup ions at New Horizons.

Our last year’s results are published in 6 papers (one more paper is in press and three are in preparation) and reported at over 10 scientific meetings. Our research was highlighted by the American Astronomical Society (https://aasnova.org/2018/02/09/probing-the-structure-of-our-solar-systems-edge/) and other web resources, e.g., https://phys.org/news/2018-04-supercomputer-simulations-heliospheric-interface.html.
Data-driven solar wind models: Research approach.

To attack the outlined problem efficiently, we propose an approach that is based on synergy of time dependent, 3D, numerical simulations, and observational data analysis. Characteristically-consistent boundary conditions are essential.

Synchonic vector magnetograms and horizontal velocity data.

We use SDO/HMI vector magnetograms with 720 s cadence to get 2 components of the magnetic field vector. DAVE4VM method (Schuck, 2008; Liu et al., 2013) is applied to compute the horizontal velocity data in the vicinity of active regions.

Away from the active regions, the surface boundary conditions – the longitudinal and latitudinal flow velocities, and the radial and longitudinal magnetic field components – are produced in near real time by assimilating vector magnetic field data from SDO/HMI into our surface flux transport code, the Advective Flux Transport (AFT) code (Hathaway & Rightmire, 2010, 2011). This approach can eventually be extended to active regions as well.
Results from the Adaptive Flux Code

Figure 1: Boundary conditions for 03/15/2015 at 00:00:00. Upper left panel: longitudinal flow velocity; upper right panel: latitudinal flow velocity; bottom left panel: radial magnetic field; and bottom right panel: longitudinal magnetic field. The flow velocities are dominated by the convective flows with a typical range of ±1500 m/s. The active region quenching is indicated by the fuzzy white patches.
Results obtained with DAVE4VM

Although we do not have magnetic field observations of the Sun’s far side, we do have EUV images from STEREO. Such images can be used to provide fairly precise estimates of the total unsigned flux in an active region on the far side. If a new active region emerges, or an old active region increases in size, new flux (with balanced polarities) is added at the observed location on the far side.
Data-constrained Model for Coronal Mass Ejections Using Graduated Cylindrical Shell Method (Singh et al., 2018)

(Above) Solar eruption observed on 7 March 2011 by the Atmospheric Imaging Assembly (AIA) in 13.1 nm wavelength.

(Right) Simulated velocity and magnetic field lines 1 min (top panel) and 1 hr (bottom panel) after the eruption.
Animations of the SW temperature and magnetic field lines as the CME propagates towards Earth.
Figure 10. Comparison of height vs. time graphs between LASCO/C3 observations and simulation results.
WSA/ADAPT (Air Force Data Assimilative Photospheric Flux Transport) model provides Br and V; we further derive density and temperature at 21.5 Rs using my Ulysses formulae for 2003-2004 and 2007, or Heather Elliott's OMNI formulae for 2012. [Simulations of Tae Kim.]
A new, data-driven model of the SW-LISM interaction (Kim et al., 2016)

Constructing the boundary conditions: Top: a diagram showing the temporal variation of the latitudinal extents of the PCHs (light blue) and OMNI data (yellow) at 1 au. Also shown are the heliographic latitudes of Earth (blue) and Voyager 1 (red). Bottom: average HCS tilt shown as a function of time (courtesy of WSO).
(Left panel) Comparison of our simulations with the SW measurements along the *Ulysses* trajectory. (Bottom panels) Comparison with Voyager 2 and New Horizons observations.

From Kim et al. (2016).
Model solar wind radial velocity, number density, and temperature are compared with NH/SWAP observations (Elliott et al. 2016) in the left column. Model interstellar pickup proton density and temperature are marked by open circles and compared with NH/SWAP observations (McComas et al. 2017). Turbulence parameters such as $Z^2$ (total turbulent energy density in turbulent magnetic and velocity fluctuations), $\sigma_c$ (cross helicity), and $\lambda$ (correlation length) are shown in the right column.
The heliopause – the boundary between the heliosphere and LISM – is unstable to KH and RT instabilities. Occasional magnetic reconnection is also possible.

The polarity of heliospheric magnetic field (HMF) changes every solar cycle at the maximum of solar activity. With a lot of simplification, we can say that the solar magnetic dipole flips every 11 years.
Heliospheric Boundary Layer in Front of the Heliopause

Fig. 5.— The distribution of plasma density (left panel) along the V1 trajectory and its comparison with the plasma waves events detected by the spacecraft beyond the heliopause, and (right panel) in the meridional plane.

Fig. 6.— Voyager 1 measurements of plasma oscillation frequency and electron density derived from it.
TeV Cosmic Rays Anisotropy: Longer Tail is Better

10000 AU Tail

4400 AU Tail

Model fit

Tibet ASy measurements
Our newest results are reproducing the BV-boundary with high accuracy.

The heliosphere clearly affects the flux of 1-10 TeV cosmic rays. This feature has been overlooked by astrophysicists for years. It appears that the heliotail and the B-V plane are prominently seen on the all-sky maps.
Why Blue Waters?

To analyze the stability of the heliopause and magnetic reconnection in turbulent plasma, we should perform simulations with the local resolution 5 – 6 orders of magnitude smaller than the size of our typical computational region.

Heliotail simulations additionally require very large computational regions, while Monte Carlo modeling produces very large data sets (each ~ 2-5 Tb) in time-dependent MHD-kinetic simulations.
Broader impacts

The development of codes that embrace “coupling complexity” via the self-consistent incorporation of multiple physical scales and multiple physical processes in models is viewed as a pivotal development in the different plasma physics areas for the current decade.

Blue Waters support

We greatly acknowledge support from all people on the Blue Waters team, especially Greg Bauer and Andriy Kot. The help desk is superb!
Future work with our new PRAC allocation

1. We will perform further analysis of the heliopause instability and magnetic reconnection in the turbulent plasma in its vicinity. The results will be compared with Voyager 1 and 2 measurements.
2. We will continue kinetic simulations of PUIs and ENAs, and use them to interpret IBEX observations.
3. We will improve on the time-dependent, data-driven and data-motivated modeling of the solar wind for the SPP mission.
4. We will finalize our long-heliotail calculations and use them to constraint the LISM properties through fitting the observed TeV cosmic ray anisotropy.