Blue Waters Symposium Sunriver, OR, 11 – 13 May, 2015

Modeling Solar Wind Flow with a Multi-Scale Fluid-Kinetic Simulation Suite

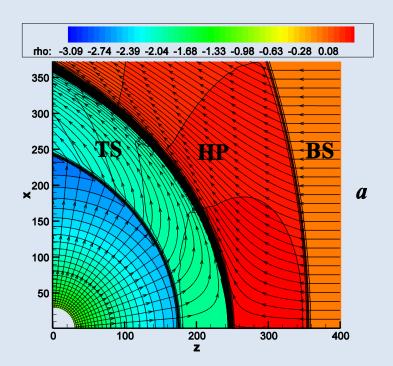
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In collaboration with M. C. Bedford, R. Fermo, T. K. Kim, I. A. Kryukov, G.P. Zank, and the Chombo team led by Phillip Colella at LBNL

Key Challenges

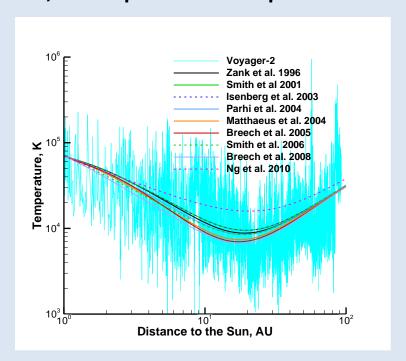
1. Flows of partially ionized plasma are frequently characterized by the presence of both thermal and nonthermal populations of ions and neutral atoms. This occurs, e.g., in the outer heliosphere – the part of interstellar space beyond the solar system whose properties are determined by the solar wind (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 (there are maybe 3 times more H atoms than H+ ions, hence charge exchange becomes of importance.

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 Kryukov et al. (2012): turbulence produced by nonthermal ions heats up the solar wind, which otherwise would have cooled down with heliocentric distance adiabatically.

- 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. 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.

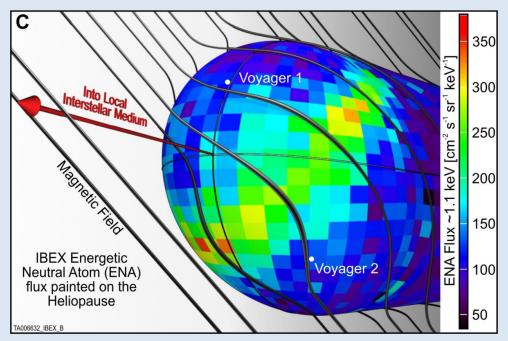
Why it matters?





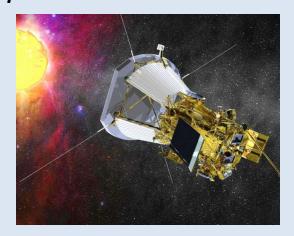
Voyager 1 and 2 (V1 and V2), PI Edward C. Stone, crossed the heliospheric termination shock in December 2004 and in August 2007, respectively (Stone et al., 2005, 2008). After more than 37 years of historic discoveries, V2 is approaching the heliopause, while V1 in August 2012 (Stone et al., 2013) penetrated 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 1.2×10^{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; Zirnstein et al., 2014, 2015; Pogorelov et al., 2011) . For the next 5–10 years, 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 McComas et al. (2009)

From the SPP official web site http://solarprobe.gsfc.nasa.gov/: "Solar Probe Plus will be an extraordinary and historic mission, exploring what is arguably the last region of the solar system to be visited by a spacecraft, the Sun's outer atmosphere or corona as it extends out into space. Solar Probe Plus will repeatedly sample the near-Sun environment, revolutionizing our knowledge and understanding of coronal heating and of the origin and evolution of the solar wind and answering critical questions in heliophysics that have been ranked as top priorities for decades. Moreover, by making direct, in-situ measurements of the region where some of the most hazardous solar energetic particles are energized, Solar Probe Plus will make a fundamental contribution to our ability to characterize and forecast the radiation environment in which future space explorers will work and live."



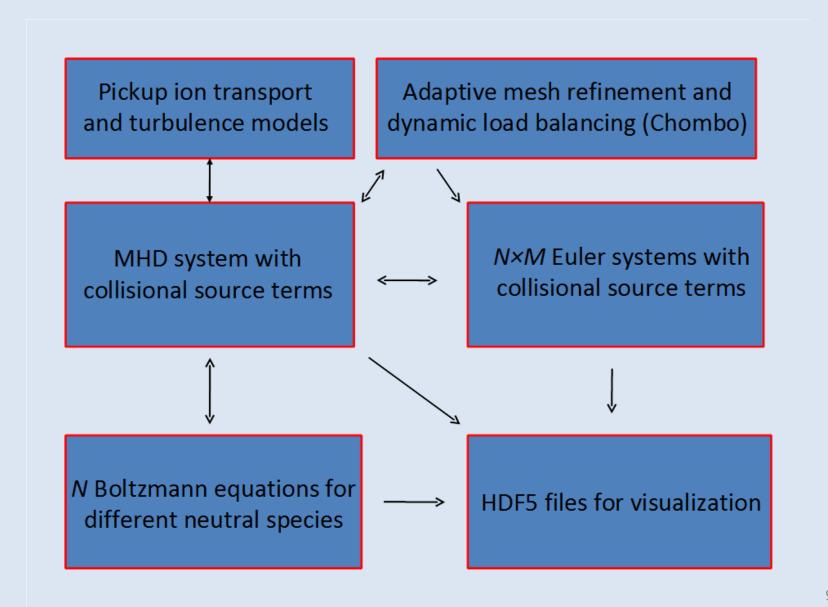
Artist's view of SPP from https://www.cfa.harvard.edu/sweap/

Solar Wind Electrons, Alphas, and Protons (SWEAP) instrument (PI Justin Kasper) onboard SPP, to be launched in 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.

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) 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 a very large simulation box $6,000 \times 4,000 \times 4,000$ AU, of the kind we perform using our Blue Waters resources.

The Structure of the Multi-Scale Fluid-Kinetic Simulations Suite



Code parallelization

	All MPI	2 threads	3 threads	6 threads	12 threads
Time (sec)	180	167	170	181	208

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

Number of	Time	Speed up	Ideal
cores	(sec)		
20,000	1003		
40,000	484	2.07	2
80,000	251	1.93	2
96,000	209	1.20	1.2
120,000	167	1.25	1.25

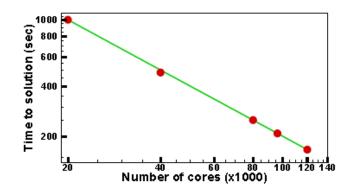


Figure 1. Strong scaling results of the kinetic code. The green line shows ideal performance. The red circles are measured time.

Parallelization (continued)

Number of	Time
cores	(sec)
20,000	164
40,000	159
80,000	168
96,000	177
120,000	167

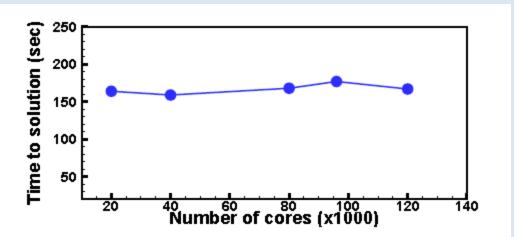


Figure 2. Weak scaling results of the kinetic code.

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).

Science funding

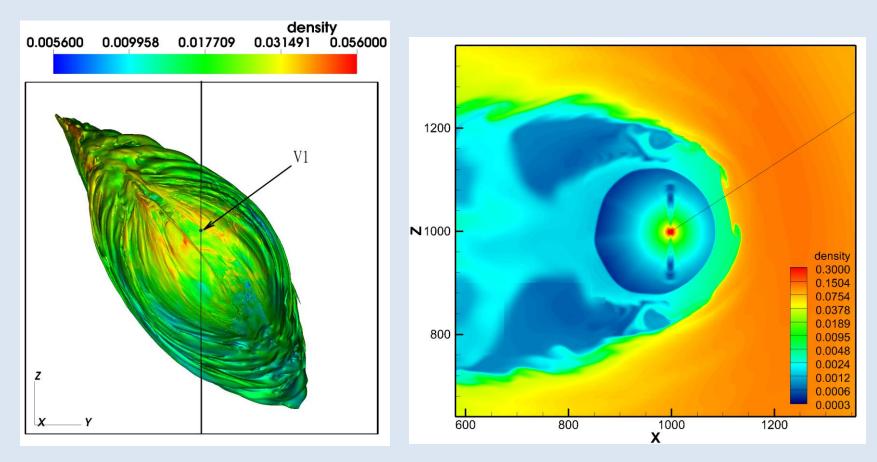
- 1. Pogorelov, N. (Principal), "F/NSF/Solar WInd with a Time-dependent, MHD, Interplanetary Scintillation Tomography," Sponsored by NSF, Federal, \$343,400.00. (July 1, 2014 June 30, 2017).
- 2. Pogorelov, N. (Principal), "Multi-Scale Investigation of the Energetic Particle Behavior in the Vicinity of the Heliopause," Sponsored by NASA, Federal, \$1,050,000.00. (May 30, 2014 May 29, 2017).
- 3. Pogorelov, N. (Principal), "Analysis of Heliospheric Transient Events at Earth Orbit from Multiple Spacecraft Observations," Sponsored by NASA, Federal, \$406,395.00. (April 1, 2014 March 31, 2017).
- 4. Pogorelov, N. (Principal), "Modeling Heliophysics and Astrophysics Phenomena with a Multi-Scale Fluid-Kinetic Simulation Suite," Sponsored by NSF, Federal, \$31,945.00. (July 1, 2012 June 30, 2016).
- 5. Pogorelov, N. (Principal), "Heliosheath Flow and Energetic Neutral Atom Fluxes in the Time-dependent Heliosphere," Sponsored by NASA, Federal, \$445,531.00. (October 26, 2011 October 25, 2015).
- 6. Pogorelov, N. (Principal), "Collaborative Research: A Model of Partially Ionized Plasma Flows with Kinetic Treatment of Neutral Atoms and Nonthermal Ions," Sponsored by DOE, Federal, \$270,000.00. (October 1, 2012 September 30, 2015).
- 7. Pogorelov, N. (Principal), Bedford, M. C., "Blue Waters Fellowship 2014-2015 (PhD student Bedford)," Sponsored by NSF/University of Illinois, Federal, \$50,000.00. (August 1, 2014 July 31, 2015).

Our accomplishments

Two questions related to Voyager 1 observations:

- (1) Why no substantial change in the magnetic field direction was initially observed?
- (2) Why did the heliocentric distance of the HP in the V1 direction turn out to be so small (121 AU)?
- (1) One of our models reproduces the magnetic field direction beyond the heliopause. A puzzle: the best fit to V1 observations may differ from the best fit to the IBEX ribbon.
- (2) We have demonstrated that a Rayleigh-Taylor-type instability of the heliopause caused by charge exchange between ions and neutral atoms (Liewer et al., 1996; Zank et al., 1996; Florinski et al., 2004; Borovikov et al., 2008; Borovikov & Pogorelov, 2014; Pogorelov et al., 2015) might be a possible explanation of Voyager measurements. Another possibility is magnetic reconnection, which we will explore during the 3rd year of our PRAC project.

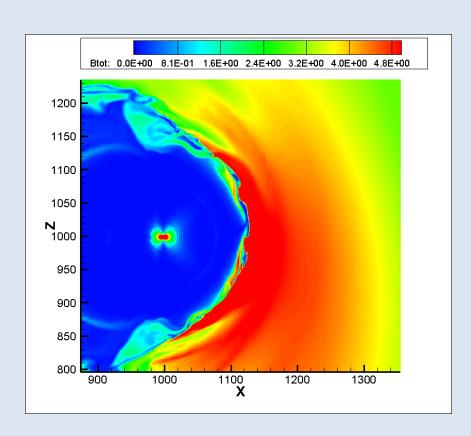
Instability of the HP: a mixture of the RT and KH instability

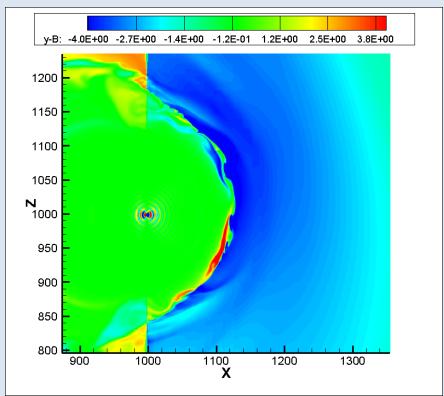


(Left) The frontal view of the HP and (right) the plasma density distribution in the meridional plane: solar cycle (Borovikov & Pogorelov, 2014).

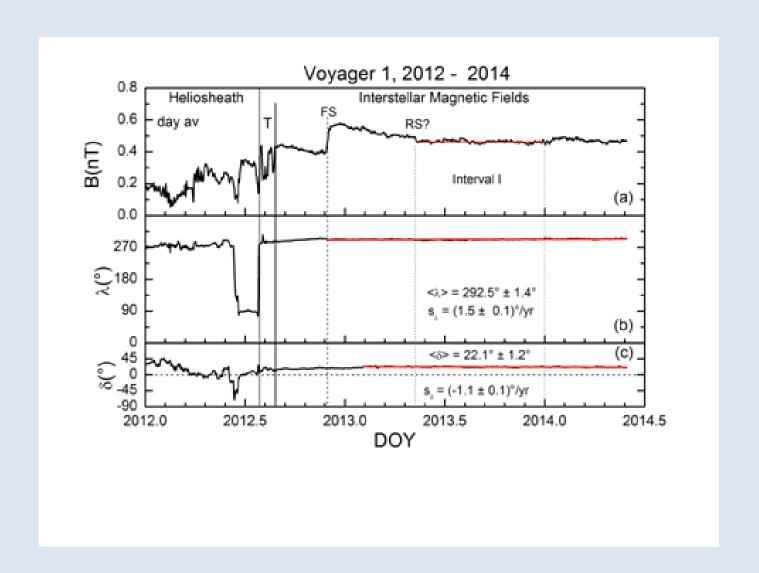
The topology of instability (and of the SW-LISM mixing) is quite different, especially at V1, from earlier axially symmetric simulations.

Instability simulation with the new LISM quantities from McComas et al. (2015)

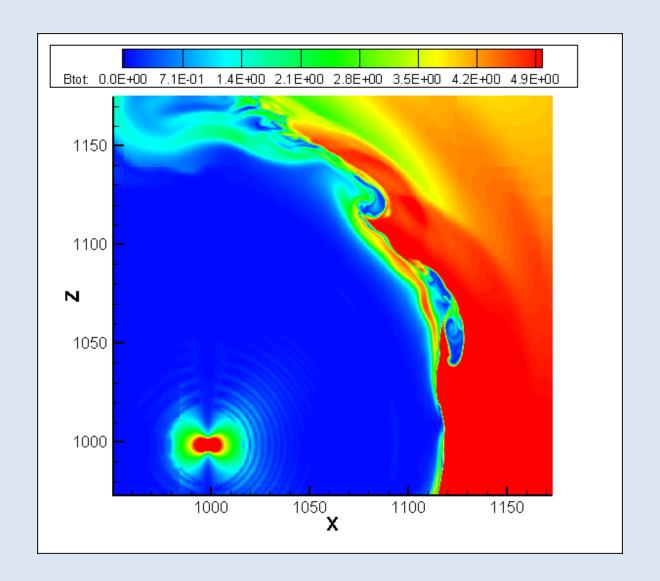




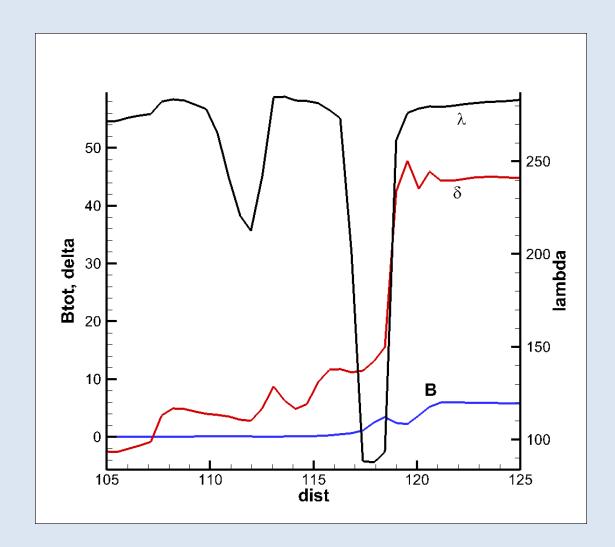
Time evolution of |B| and B_{ϕ} : the RT instability of the heliopause is accompanied by tearing mode instabilities, which may be the signatures of magnetic reconnection – the subject to be addressed by us with AMR in turbulent plasma.



Voyager measurements of the magnetic field strength, B, and its elevation and azimuthal angles from Burlaga & Ness (2014).



A snapshot of |B|

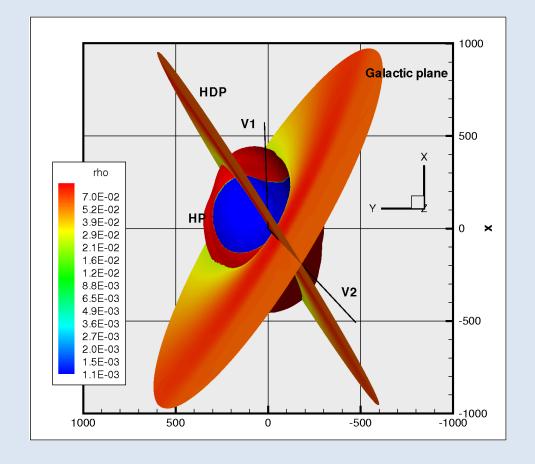


There is an impression that the magnetic field sector crossings by Voyager 1 close to the heliopause were so infrequent that they possibly should not be attributed to the HCS crossings, but rather to the sectors created by nonmonotonicity in the angle between the Sun's magnetic and rotation axes.

The distribution of B, δ , and λ in the solution of Borovikov & Pogorelov (2014)

The heliopause colored by the sign of B_R , the hydrogen deflection plane, the Galactic plane, and the trajectories of the V1 and V2 spacecraft

Pogorelov, Heerikhuisen, Zank (2008)



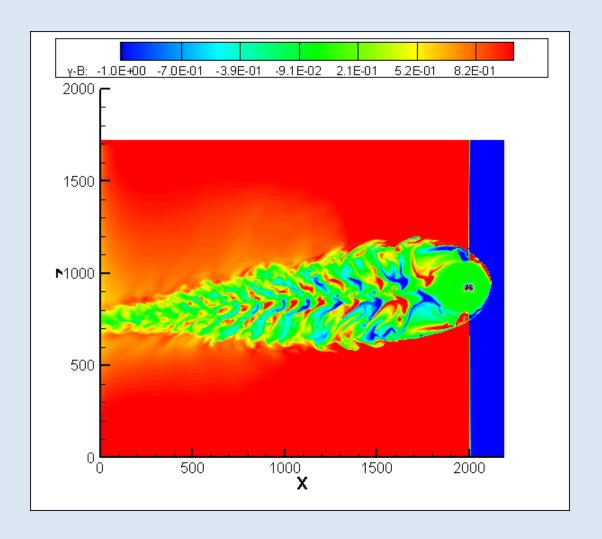
The HP is not symmetric with respect to the BV-plane!

H-atom deflection almost entirely in the BV-plane!

BV-plane parallel to the HDP, B_{∞} at 30° to V_{∞} (B_{∞} = 3 μ G), $n_{H\infty}$ = 0.15 cm⁻³

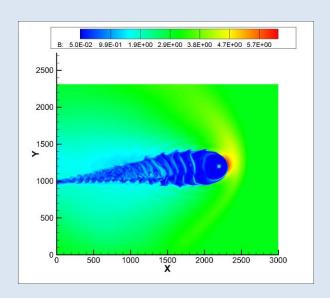
The LISM parameters are chosen to fit the IBEX ribbon data (more details in the talk of Jacob Heerikhuisen tomorrow).

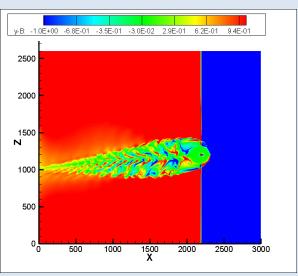
The position of the heliotail may give more information on the ISMF direction through fitting the observed small-scale TeV cosmic ray anisotropy

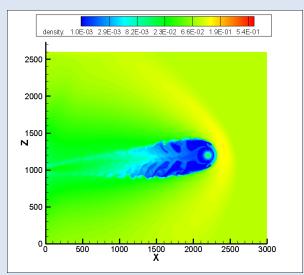


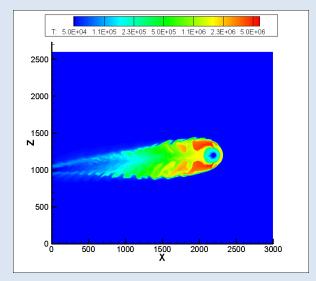
On the left: the distribution of the toroidal component of the heliospheric magnetic field in the meridional plane defined by the Sun's rotation axis (vertical in the figure) and the LISM velocity vector. The patches of opposite magnetic field polarity seen in the tail are due to the change in the Sun's dipole polarity every 11 years.

The heliotail with the LISM properties from McComas et al. (2015)









Clockwise: the distributions of the magnetic field strength, its toroidal component, plasma density, and temperature in the meridional plane.

We have performed a series of simulations that allow us to constraint the LISM properties using TeV cosmic ray anisotropy.

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 ~ 1 Tb).

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 Gengbin Zheng. Gengbin spends a lot of his time with us addressing issues related to the most efficient implementation of MS-FLUKSS on Blue Waters. We have even identified something which looks like a Fortran compiler bug a few weeks ago. The help desk is superb!

Future work

- 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 datamotivated 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.