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Modeling Heliophysics and Astrophysics Phenomena with a Multi-Scale Fluid-Kinetic Simulation Suite

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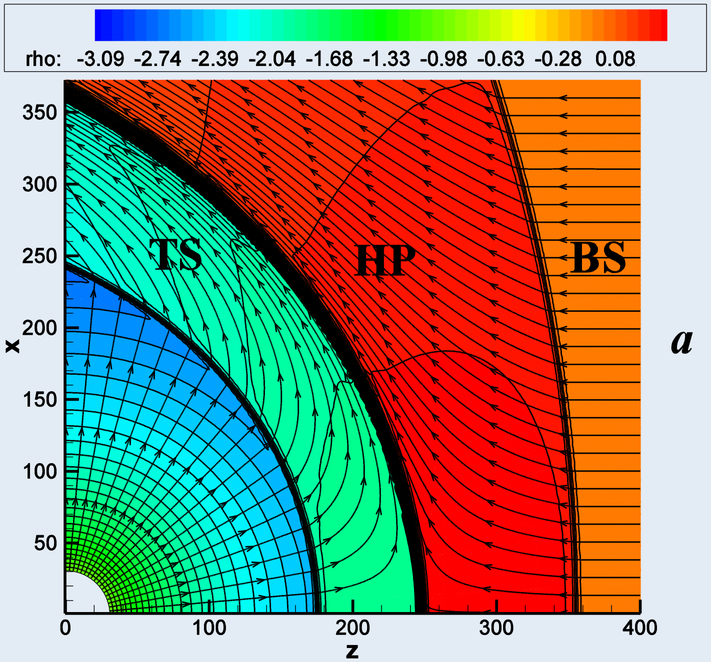
Key Challenges

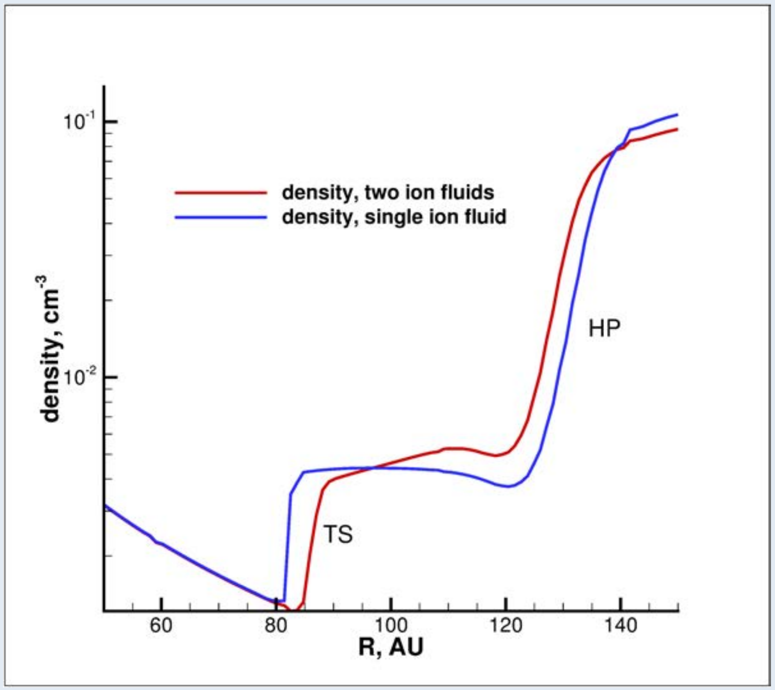
1. **Flows of partially ionized plasma are frequently characterized by the presence of both thermal and nonthermal populations of ions and neutral atoms. This occurs, e. g., in the outer heliosphere – the part of interstellar space beyond the solar system whose properties are determined by the solar 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.



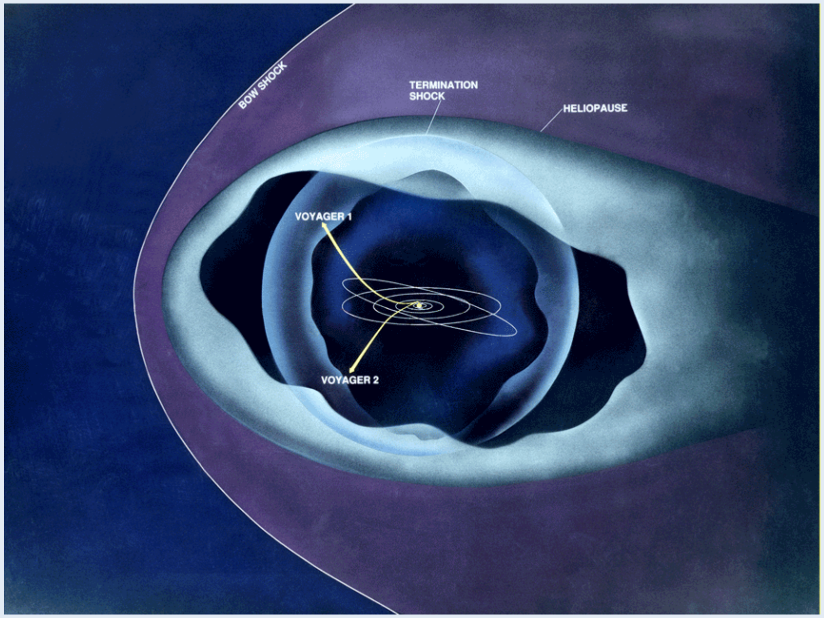
From Bedford et al. (2016): density distributions along the Voyager 1 trajectory in simulations for a single ion mixture and PUIs modeled as a separate ion fluid. The width of the heliosheath diminishes in accordance with Voyager 1 measurements.

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.**

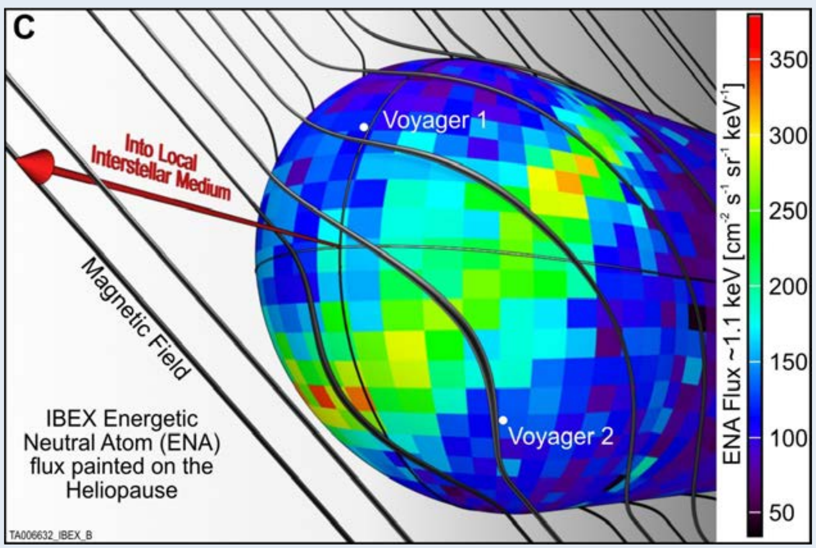
5. **To address these problems, we have developed a tool for self-consistent numerical solution of the MHD, gas dynamics Euler, and kinetic Boltzmann equations. Our Multi-Scale Fluid-Kinetic Simulation Suite (MS-FLUKSS) solves these equations using an adaptive-mesh refinement (AMR) technology. The grid generation and dynamic load balancing are ensured by the Chombo package.**

Why it matters?

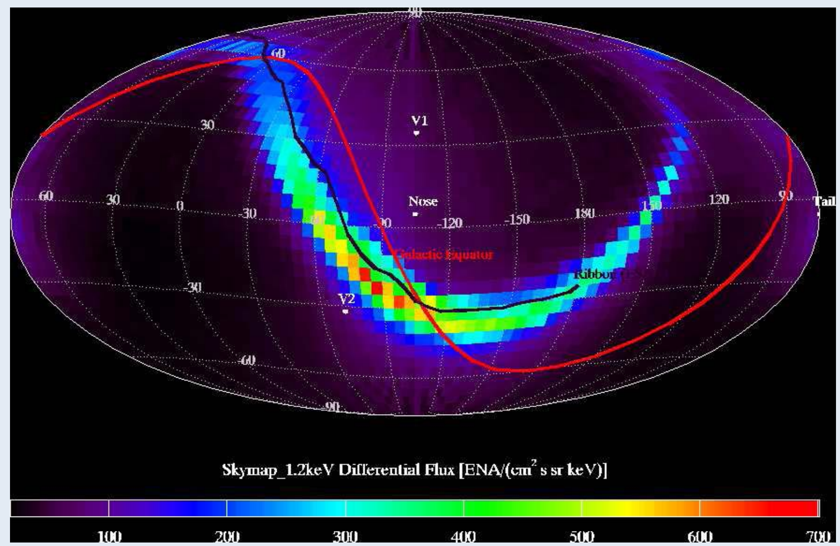


Voyager 1 **and** ***2 (V1*** **and** ***V2),*** **PI Edward C. Stone*****,*** **crossed the heliospheric termination shock in December 2004 and in August 2007, respectively (Stone et al., 2005, 2008). After more than 37 years of historic discoveries, V2 is approaching the heliopause, while V1 in August 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, 2016; Pogorelov et al., 2011, 2016) . 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.

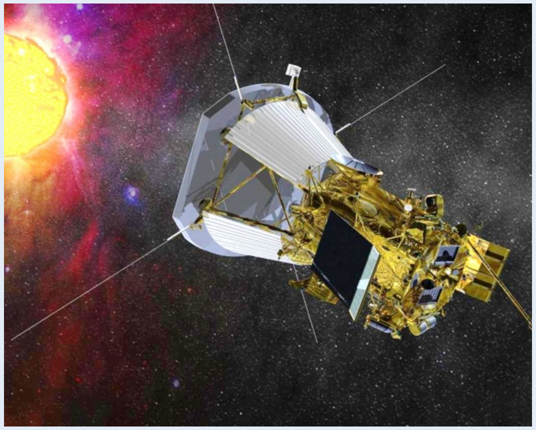


From McComas et al. (2009)



Simulated ENA flux

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."

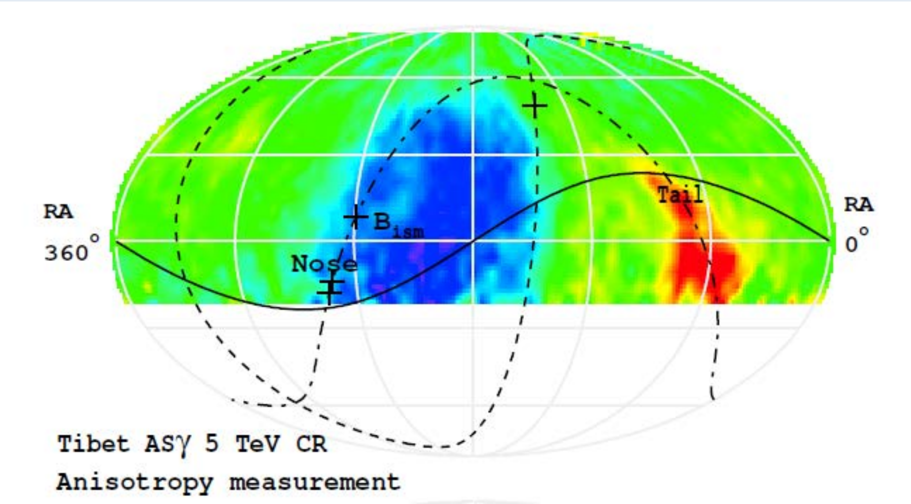


Artist's view of SPP from https://www.cfa.harvard.edu/sweap/

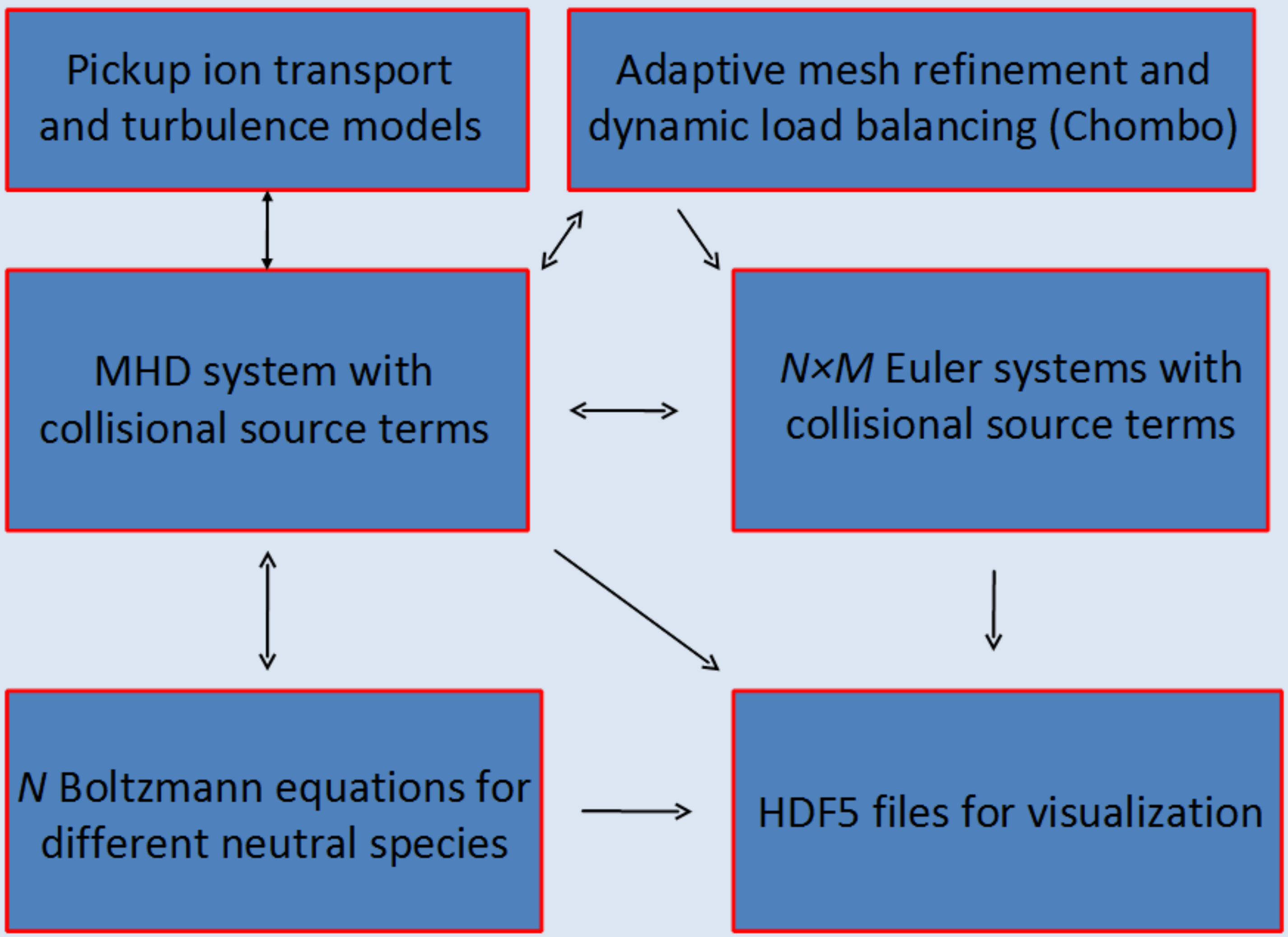
Solar Wind Electrons, Alphas, and Protons (SWEAP) instrument (PI Justin Kasper) onboard SPP, to be launched in 2018, will directly measure the properties of the plasma in the solar atmosphere. In particular, the time-dependent distribution functions will be measured, which requires the development of 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), 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 a very large simulation box 20,000 × 5,000 × 5,000 AU, of the kind we perform using our Blue Waters resources.



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



Code parallelization

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

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

Number of cores	Time (sec)	Speed up	Ideal
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

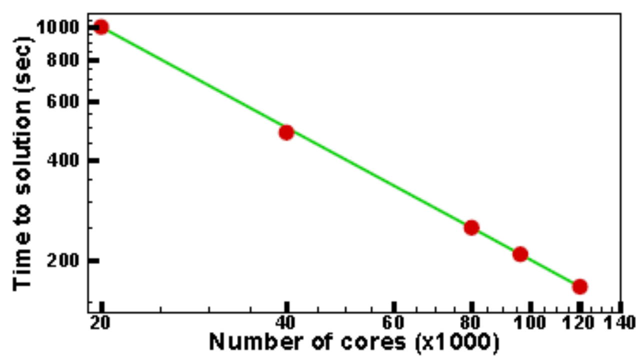


Figure 1. Strong scaling results of the kinetic code. The green line shows ideal performance. The red circles are measured time.

Parallelization (continued)

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

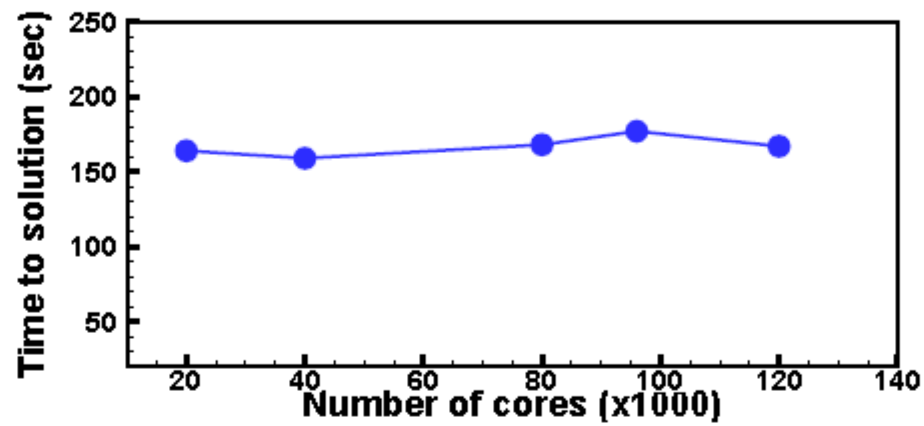


Figure 2. Weak scaling results of the kinetic code.

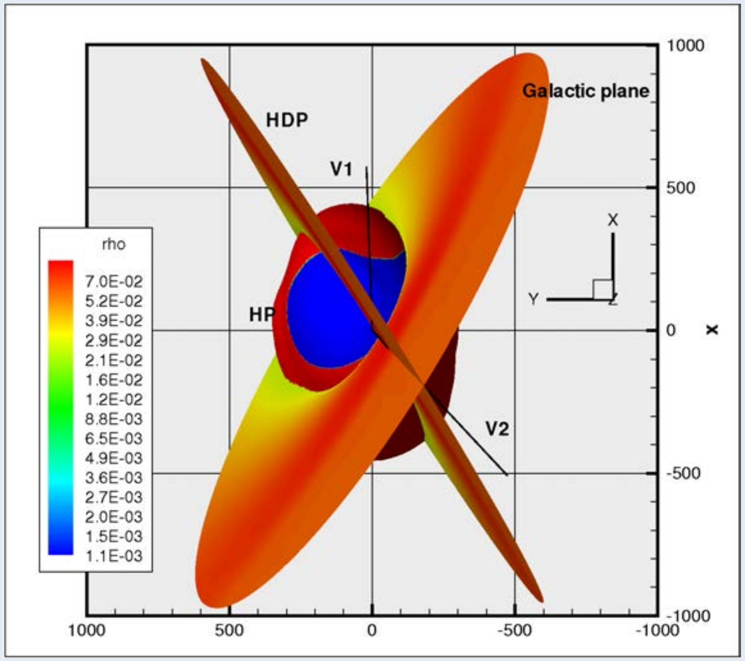
A 650Gb data file containing 10 billion particles (full 64-bit support is necessary) can be written as fast as 32 seconds on Lustre file system if it is striped over 100 Object Storage Targets (OSTs).

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), "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, 2016).
6. Heerikhuisen, J. (Principal), "REU Site: Solar and Heliospheric Physics at UAH and MSFC,'' Sponsored by NSF, Federal, $621,922.00. (June 1, 2015 – May 31, 2020).
7. Heerikhuisen, J. (Principal), "Pick-up Ions and Energetic Neutral Atoms: Implications for the Termination Shock," Sponsored by NASA, Federal, $461,264.00 (May 1, 2016 – April, 30, 2019).

Total science funding: $3,184,926.

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



Our models are data-driven:

1. **Remote and in situ solar wind data;**
2. **Voyager observations of plasma, magnetic field, and cosmic rays in the heliosphere and beyond;**
3. **Ly α backscattered emission (SOHO) gives us the orientation of the hydrogen defection plane and Ly α absorption profiles in directions toward nearby stars (HST);**
4. **The LISM temperature and velocity derived from Ulysses and IBEX measurements are in agreement now;**
5. **IBEX ENA data;**
6. **Neutral H densities at the heliospheric termination shock derived from Ulysses PUI measurements;**
7. **Multi-TeV cosmic ray anisotropy.**

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Our accomplishments

(1) we have performed data-driven SW flow simulations starting from the solar surface;

(2) we have calculated SW propagation from the Earth orbit to Pluto along the New Horizons spacecraft trajectory and further to the heliopause and demonstrated good agreement with observational data;

(3) we have explained the existence of extended regions of the SW sunward flow near the heliopause and spontaneous transition to turbulence;

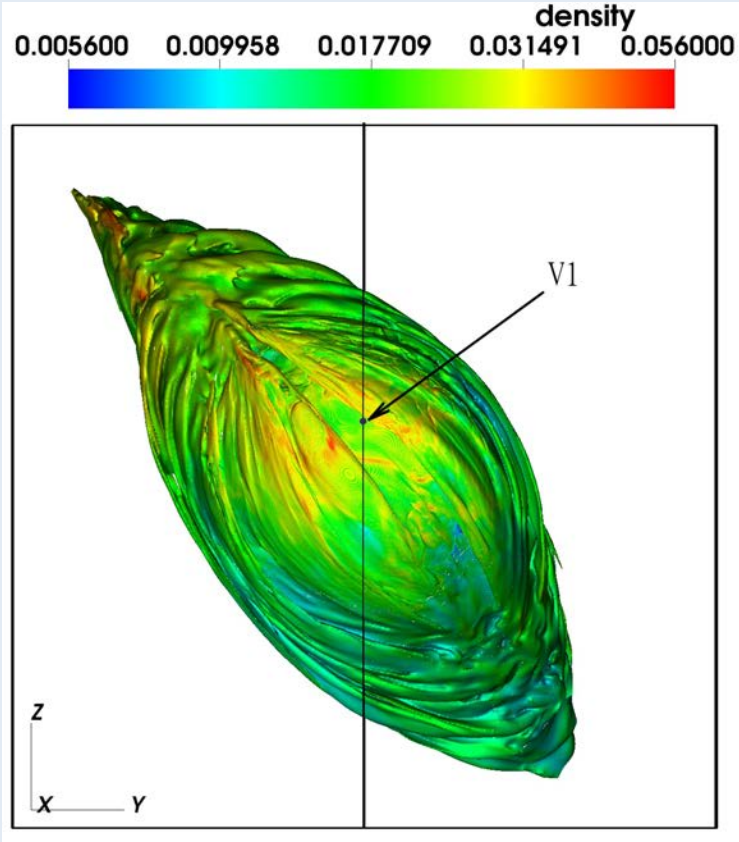
(4) we have performed high-resolution simulations of the heliopause instability and identified the areas of possible magnetic reconnection near the heliopause crossed by Voyager trajectories, which allowed us put forward a possible explanation of V1 observations that showed a few consecutive increases and decreases in the galactic and anomalous cosmic ray flux intensities;

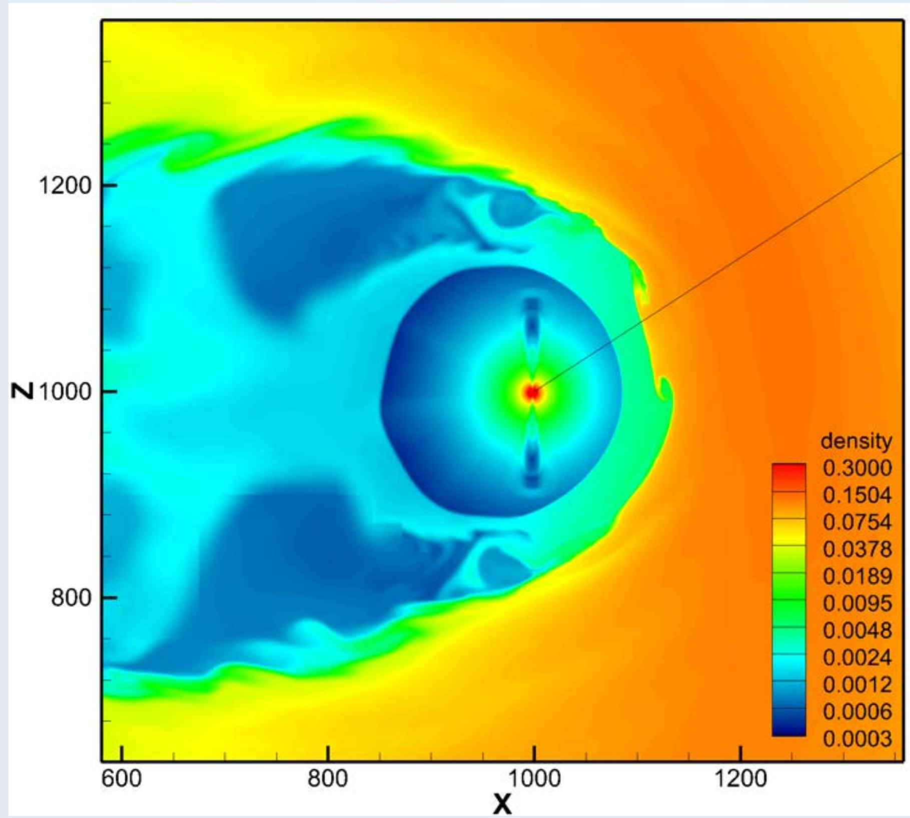
(5) we have analyzed the heliotail flow and quantity distribution in the heliospheric bow wave for different LISM conditions and showed that the observed multi-TeV cosmic ray anisotropy may be explained by the LISM magnetic field distortion by the heliosphere;

(6) we have investigated the effect of non-thermal ions on time-dependent plasma distributions in the SW and LISM.

(7) The results of the third year are published in 10 papers and reported at over 20 (10 invited) scientific meetings.

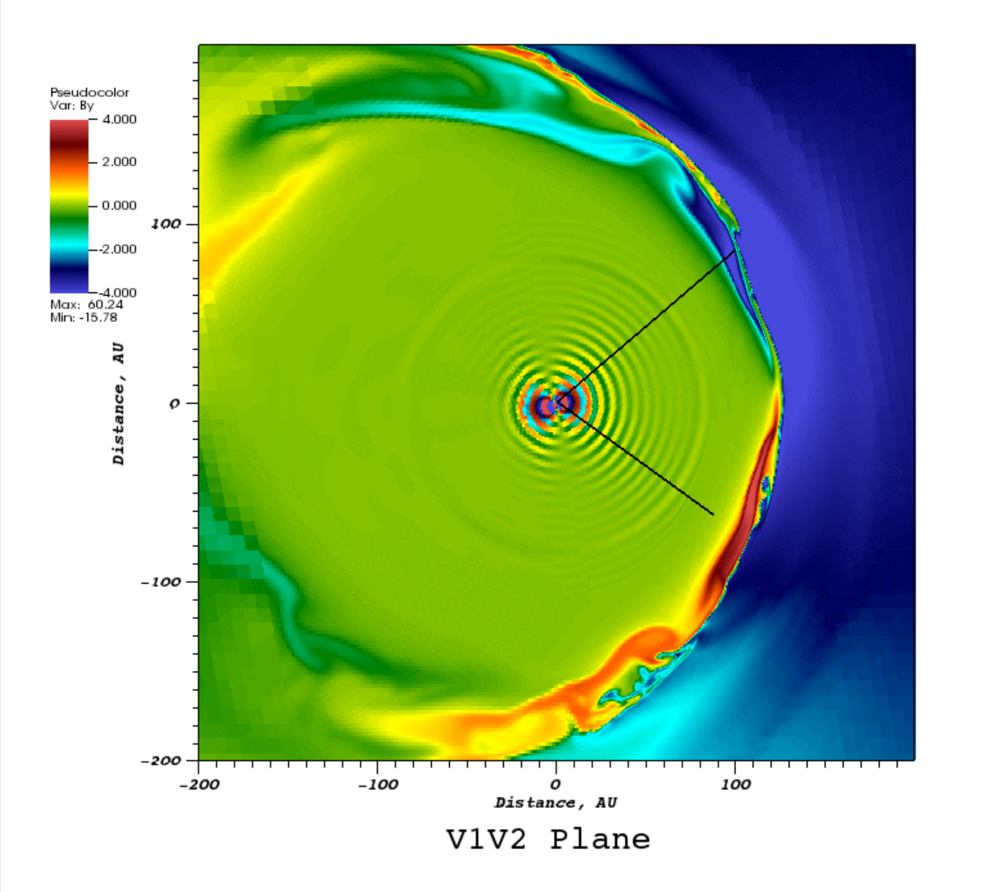
Instability of the HP: a mixture of the RT and KH instability



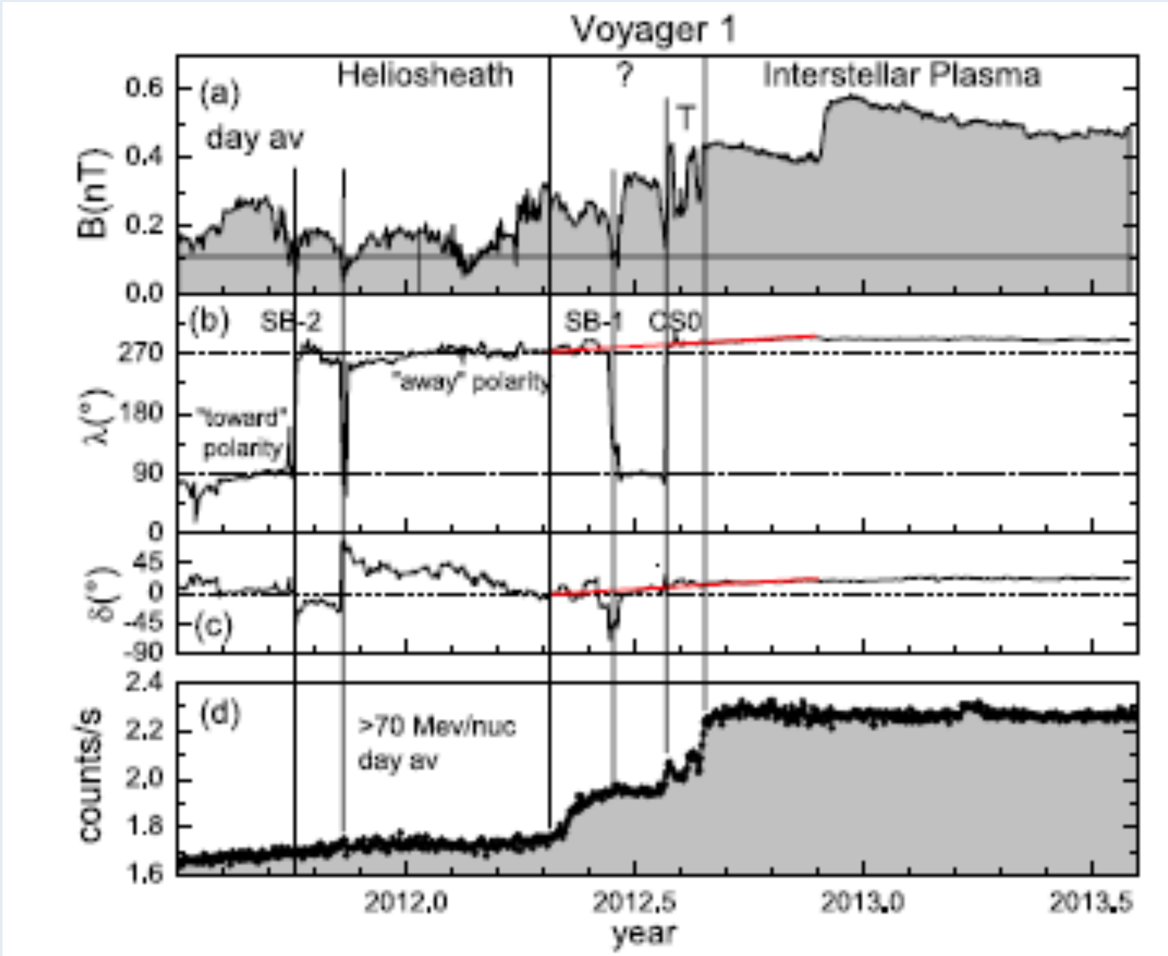


(*Left*) The frontal view of the HP and *(right*) the plasma density distribution in the meridional plane: solar cycle (Borovikov & Pogorelov, 2014).

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



Animation of the y-component of the magnetic filed vector demonstrates the heliopause instability and magnetic reconnection on its surface. Both processes are affected by turbulence – the subject of our current research.



Voyager 1 measurements of the magnetic field strength, B, its elevation and azimuthal angles, and the galactic cosmic ray flux (from Burlaga & Ness, 2014).

INTERSTELLAR WAKE OF SOLAR WIND

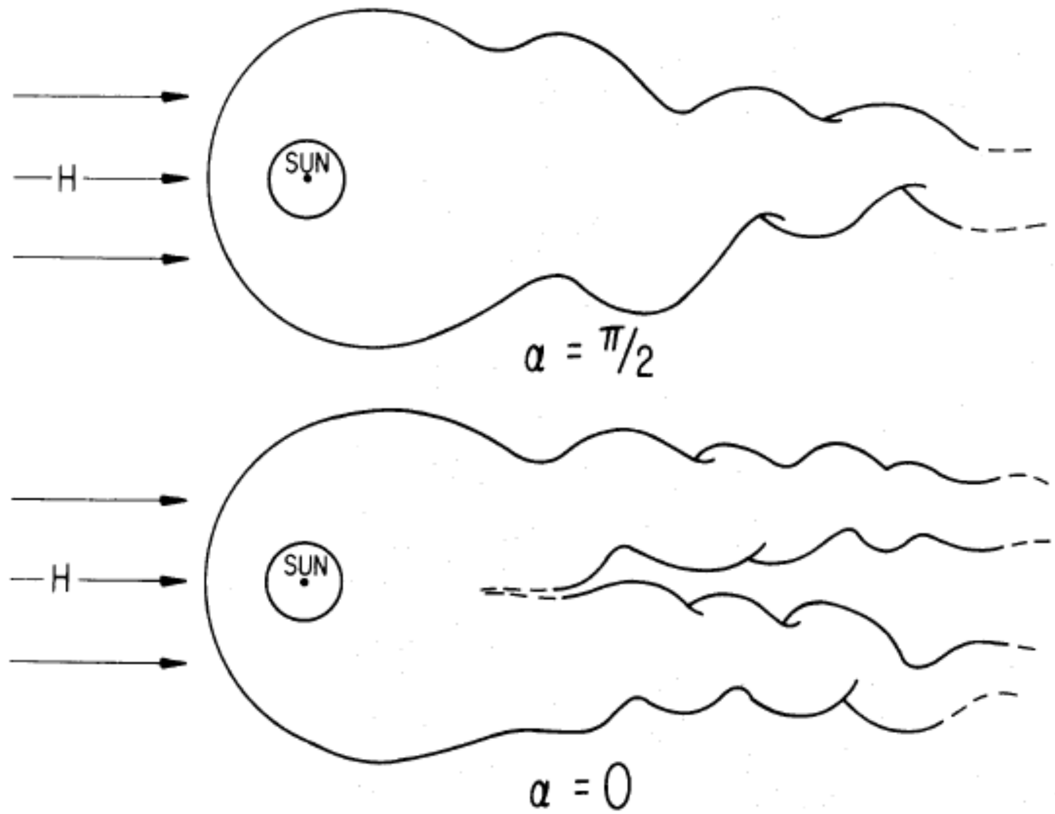
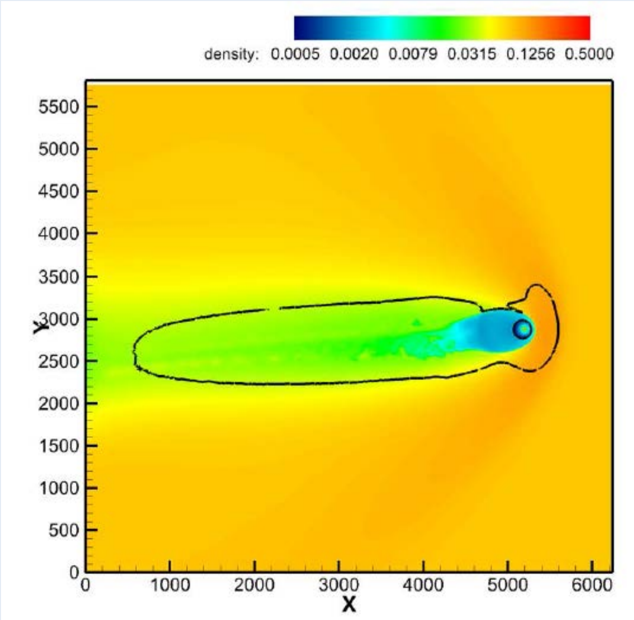
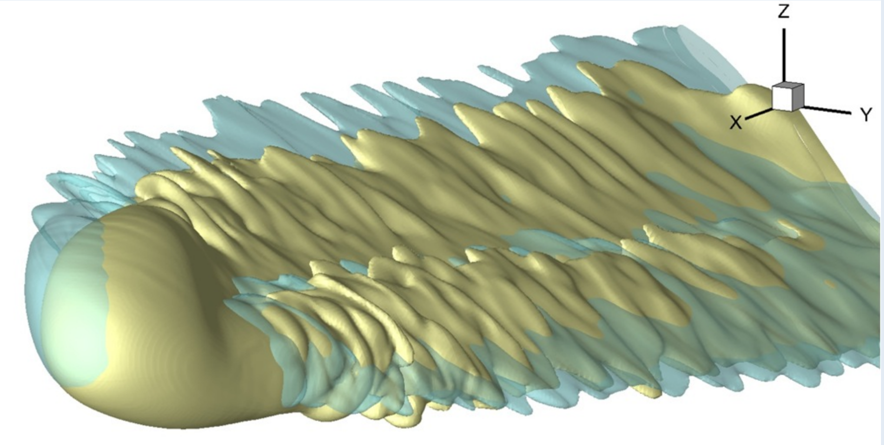


FIG. 7.—The buckling of the solar wind wake

From Yu (1974)

5000 AU heliotail with the unipolar IMF and kinetic treatment of H atoms (Pogorelov et al., 2013; 2015)

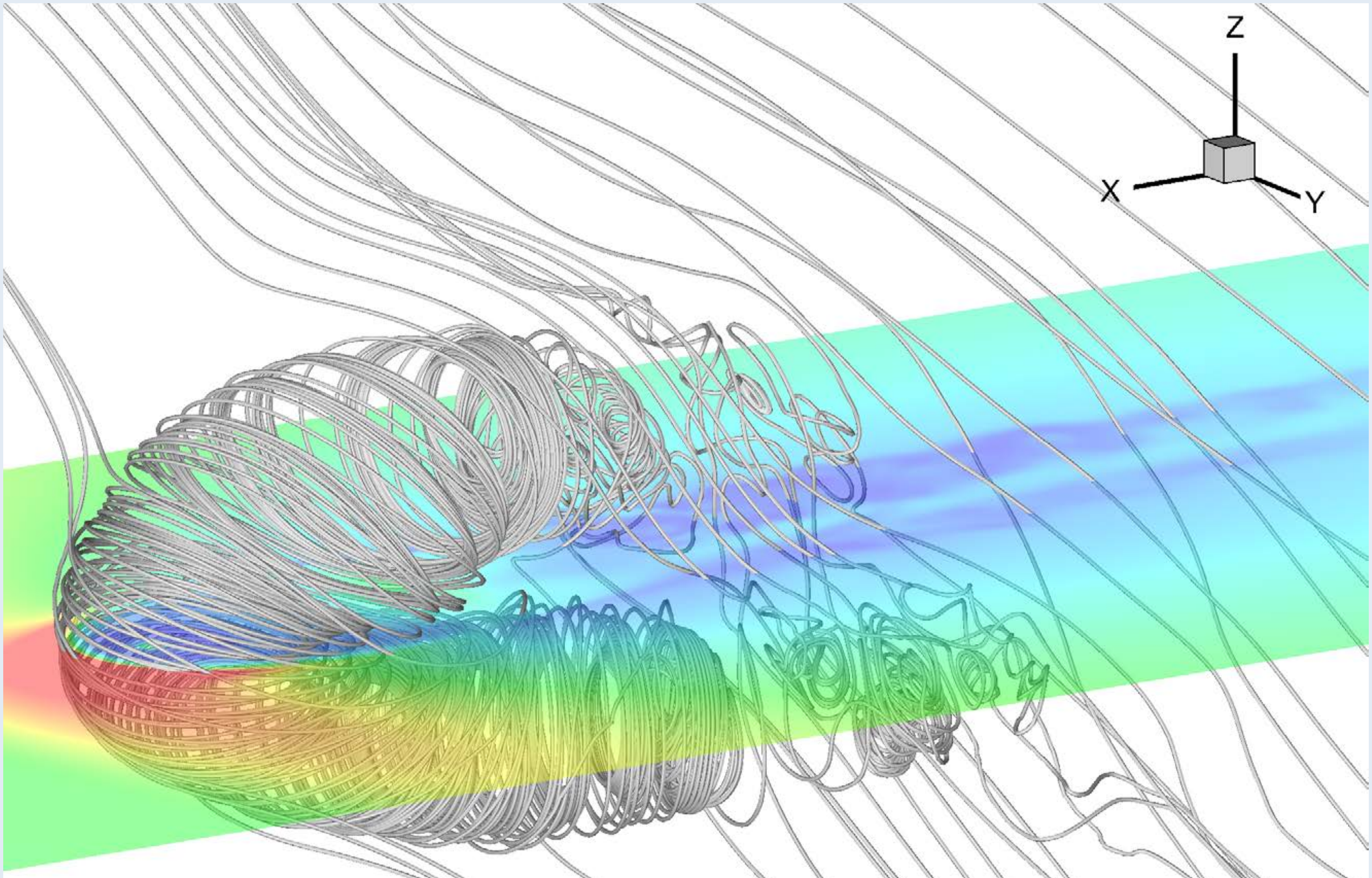




Plasma density in the solar equatorial plane. The black line if defined be the condition M_f=1.

Pogorelov et al. (2013): the HP for B_∞ = 3 μG (yellow) and B_∞ = 4 μG (blue): no two-lobe structure in agreement with Izmodenov & Alexashov (2015).

HMF and ISMF lines: the regular Parker field is destroyed in the tail



According to Yu (1974) and Opher et al. (2015), the SW will form a two-lobe structure collimated by the Parker spiral field.

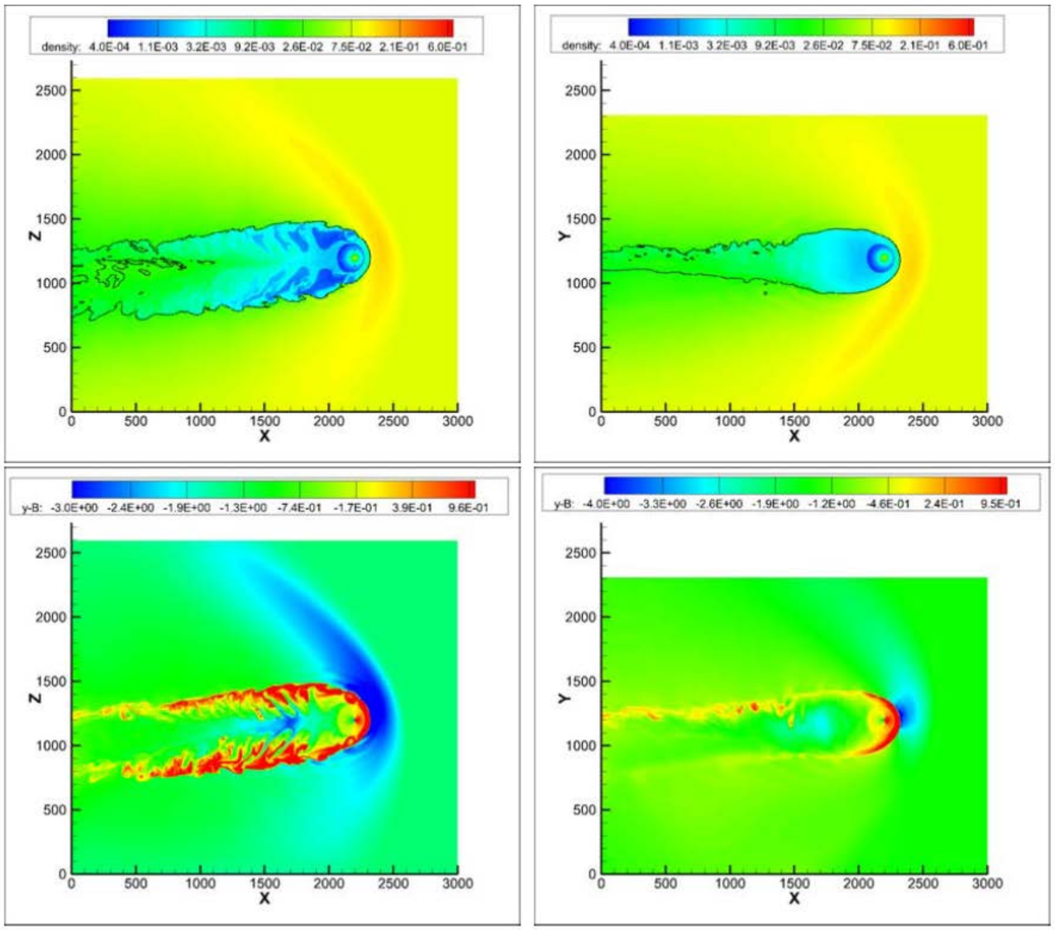
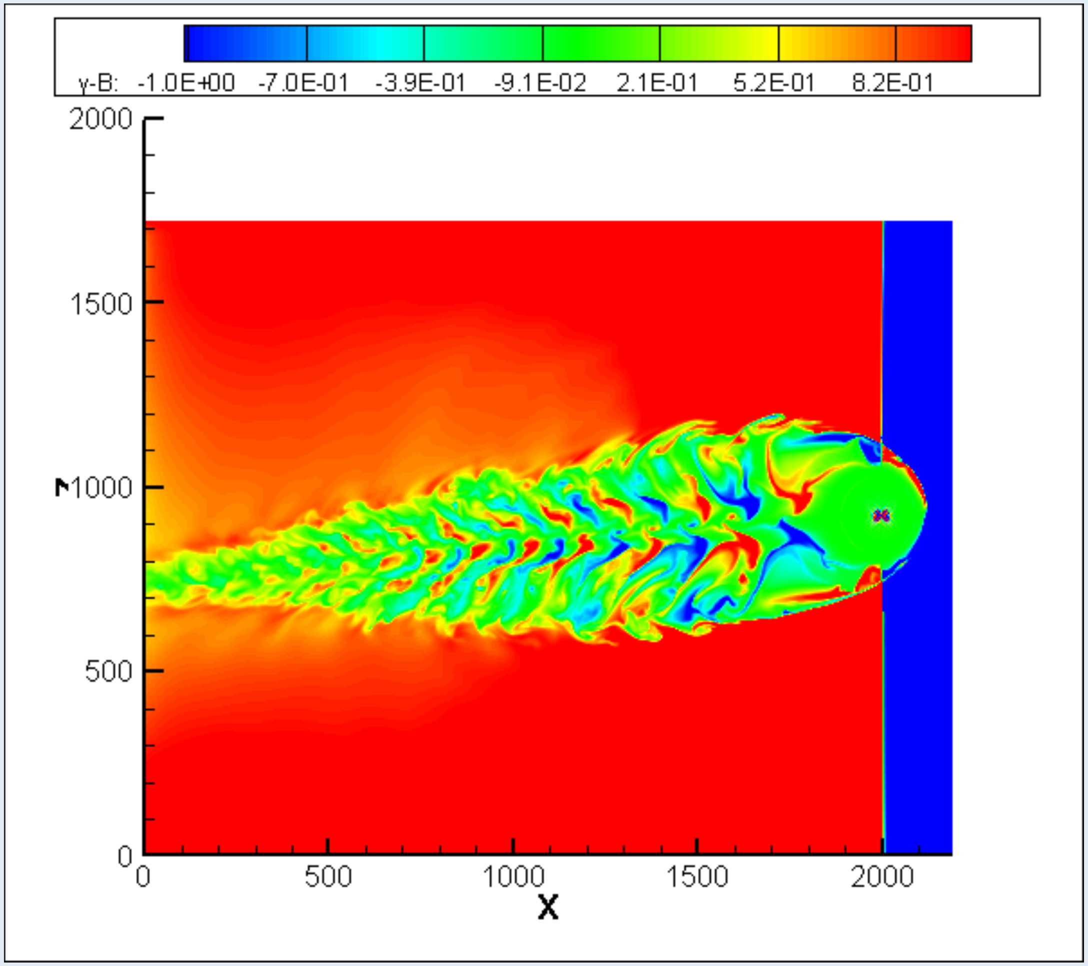


Figure 3. Meridional (left panels) and equatorial (right panels) cross-cuts of the heliosphere showing the plasma density (top panels) and the y-component of the magnetic field vector (bottom panels) in the SW–LISM simulation where the HMF is assumed to be unipolar during the solar cycle.

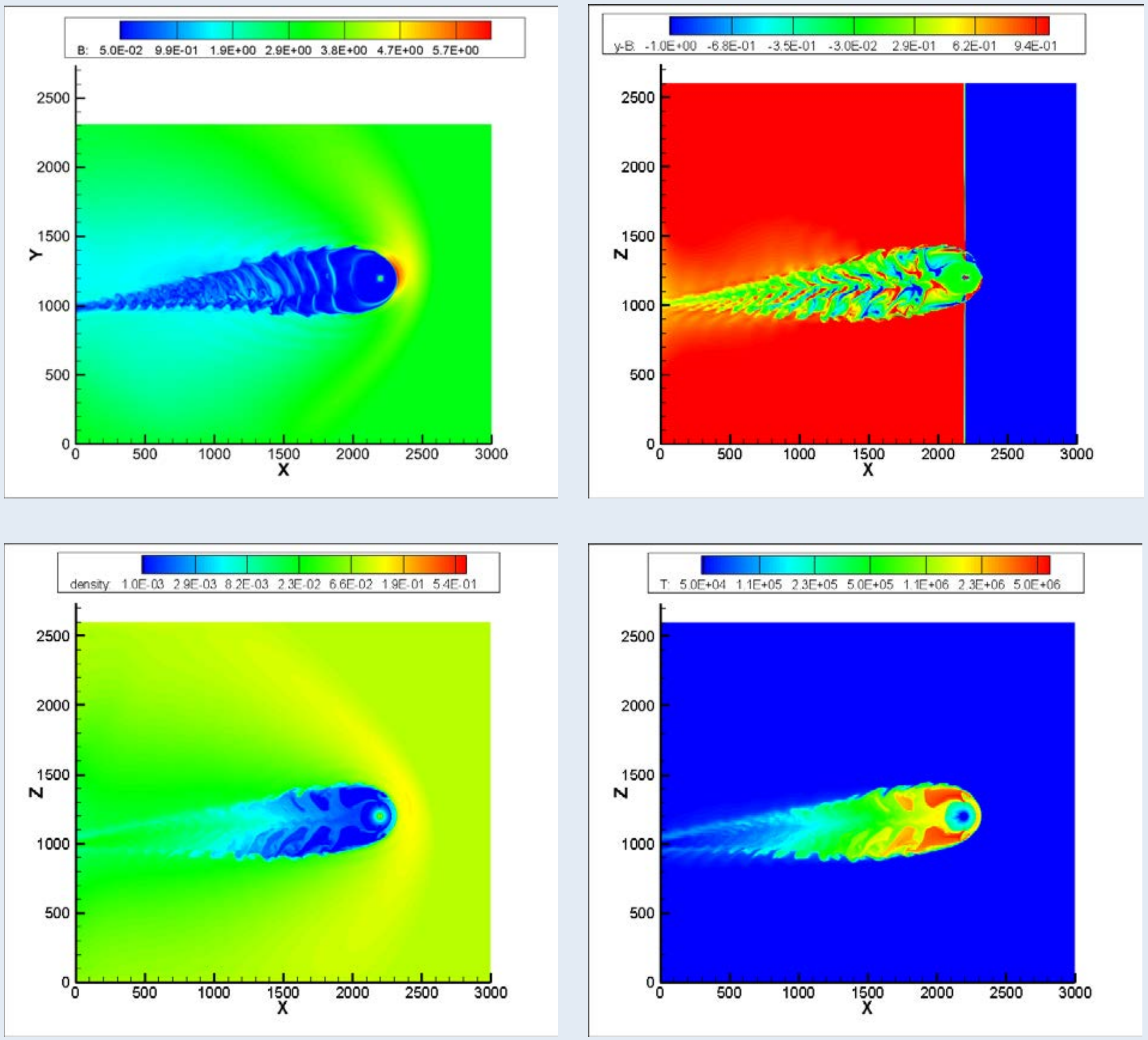
These scenario does not reveal itself even in the assumption of unipolar HMF if solar cycle effects are taken into account (Pogorelov et al., 2016).

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.

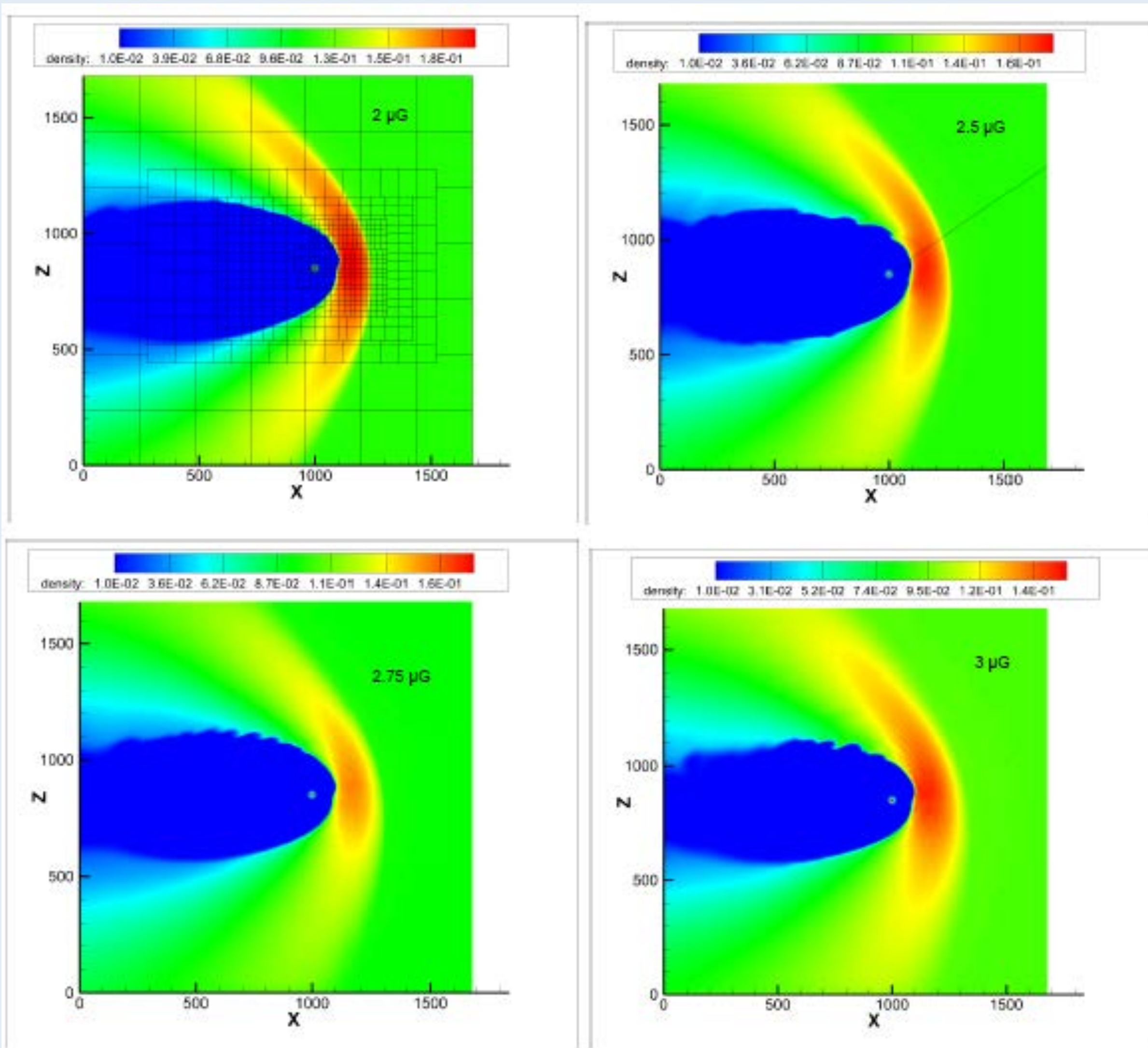
The heliotail with the LISM properties from McComas et al. (2015)



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.

Density distribution in the meridional plane as function of the LISM properties

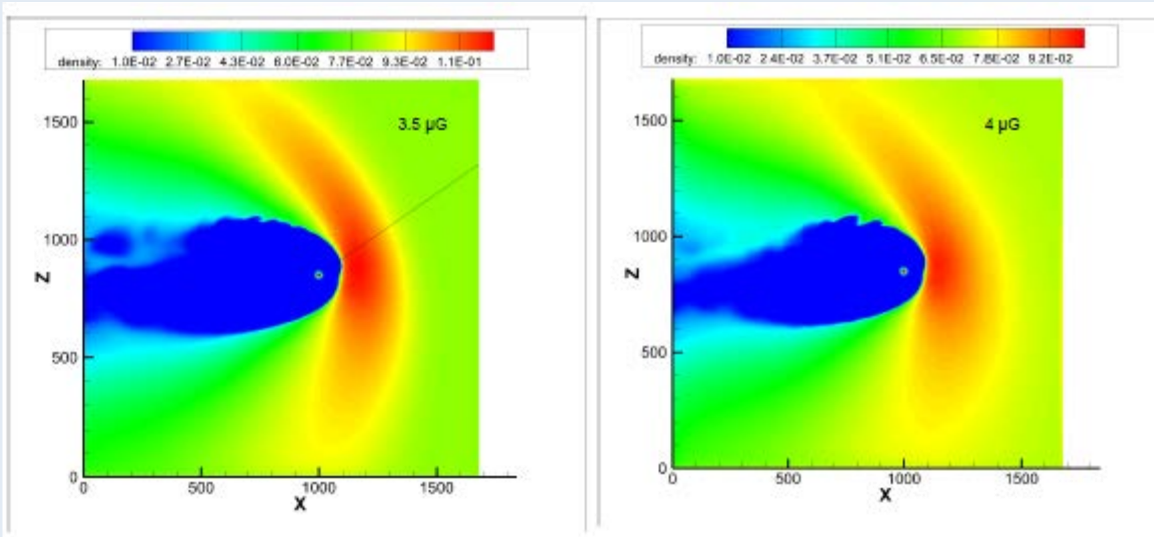


On the left: the distributions of the plasma density in the meridional plane of our MHD plasma / kinetic neutral atoms simulations of the SW--LISM interaction.

The meridional plane is formed by the Sun's rotation axis (the z-axis) and the plasma velocity vector in the unperturbed LISM. The SW parameters are taken from the OMNI data, while the LISM properties represent the best fit to the IBEX ribbon while preserving reasonable agreement with the neutral H density at the heliospheric termination shock (TS), the hydrogen deflection plane orientation in space, and the heliocentric distance to the heliopause.

The LISM He velocity and temperature data are from McComas et al. (2015): V_{LISM} = 25.4 km/s and T_{LISM} = 8,000 K, other parameters from Zirnstein et al. (2016).

In the SW at 1 AU, n_p = 5.924 cm^{-3}, V_p = 409 km/s, T_p = 82,336 K, and $|B_R|$ = 39 μG.



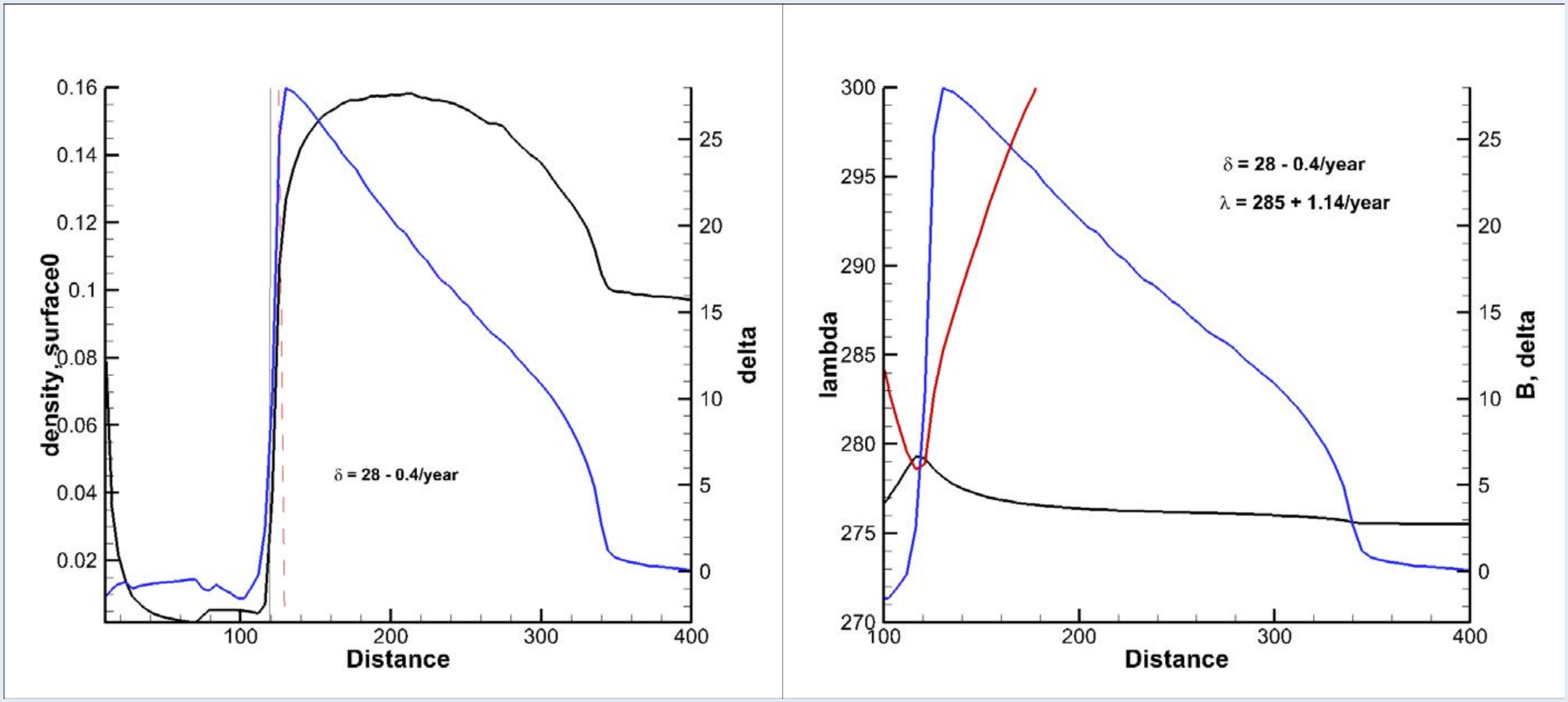
Summary:

(1) The secondary H atoms created due to charge exchange of primary interstellar atoms with solar wind protons are able to propagate far upwind of the heliopause and affect the properties of the LISM (Baranov & Malama, 1993; Zank et al., 1996; Heerikhuisen et al., 2006; Pogorelov et al., 2006; McComas et al., 2013; Zank et al., 2013), i.e., the LISM protons are decelerated and heated.

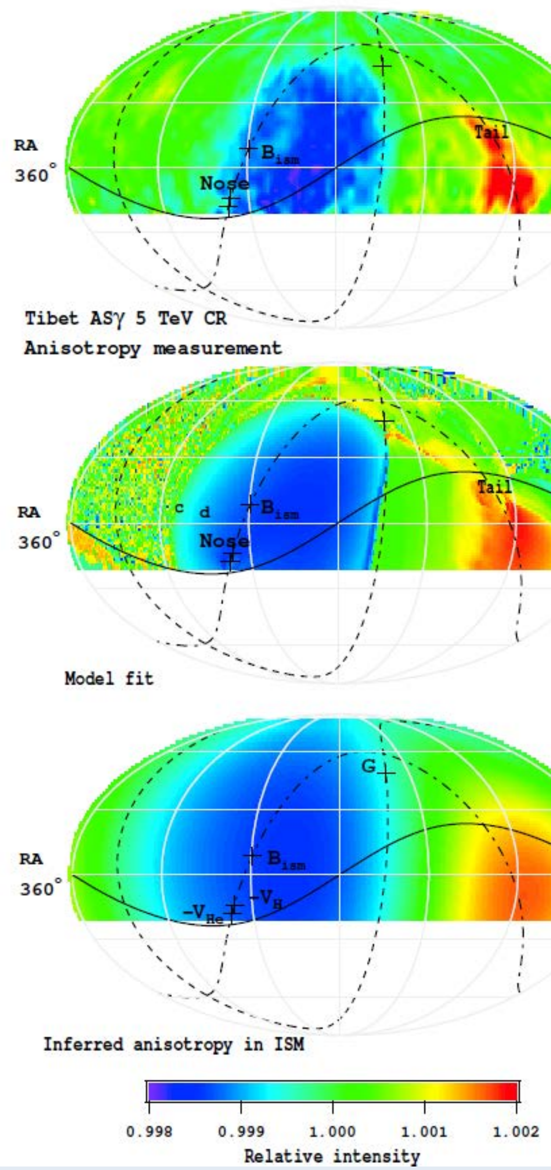
(2) The presence of the charge-exchange source term in the MHD system cannot affect the shock boundary conditions. However, the plasma parameters in front of and behind a shock are modified. As a result, the total variation of quantities in a bow wave connecting the unperturbed LISM with the heliopause may either have a shocked transition inside it or be entirely smooth.

(3) The width of the bow wave increases with the increase of the fast magnetosonic Mach number M_f calculated in the unperturbed LISM. On the other hand, the intensity of the wave (the maximum of plasma density inside it) decreases with M_f.

Plasma density, B, and magnetic field angles (B_{LISM} = 2.75 μG)



No jump in B across the HP, the angles beyond the HP are reproduces as well at the gradients in their distributions. The depletion layer in front of the HP is rather wide and deep (good for radio emission).



(Top) Tibet ASγ measurements of 5 TeV cosmic-ray relative flux as a function of declination and right ascension. (Middle) least χ^2 fit to Tibet measurements using Liouville mapping of anisotropy and the proposed distribution function. (Bottom) inferred map of cosmic-ray anisotropy in the pristine interstellar medium without any distortion by the heliosphere. The ”+” signs indicate the direction of interstellar magnetic field B_{ism}, the directions of interstellar neutral helium ($-V_{He}$) and hydrogen ($-V_H$) inflows, and the direction of perpendicular cosmic-ray density gradient. The dot-dashed curve is the B-V plane. The dashed curve is the plane perpendicular to the interstellar magnetic field Bism. The solid curve is the ecliptic. The sun is placed at the nose.

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!

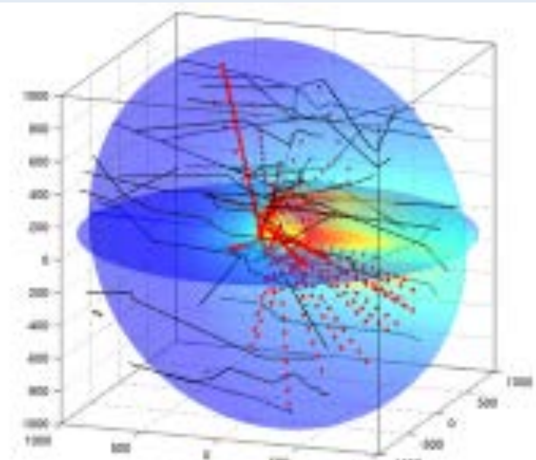
Future work with our new PRAC allocation

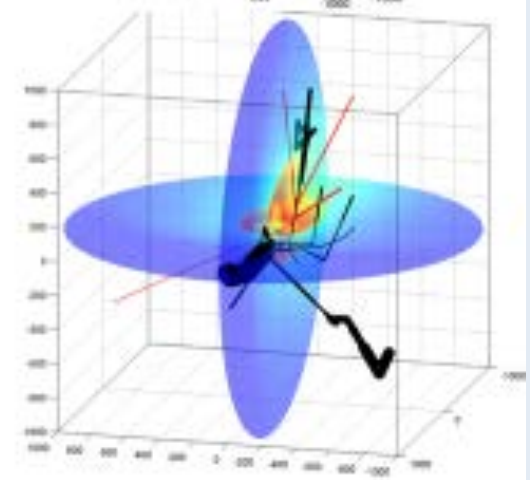
1. **We will perform further analysis of the heliopause instability and magnetic reconnection in the turbulent plasma in its vicinity. The results will be compared with *Voyager* 1 and 2 measurements.**
2. **We will continue kinetic simulations of PUIs and ENAs, and use them to interpret *IBEX* observations.**
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.**

A few words about out PAID collaboration with Bill Tang and Bei Wang at Princeton, the goal of which is to use GPUs in our kinetic simulation module.

Kinetic Simulation of neutral H

- Monte-Carlo algorithm that treats H-atoms as particles.
- Charge-exchange collisions occur based on local plasma conditions and alters particle velocities.
- Energy & Momentum changes of charge-exchange events are recorded on a grid and passed to the MHD code as source terms.
- MHD & neutrals codes iterate until a steady-state is reached.
- Include splitting of trajectories to improve charge-exchange statistics on the smaller grid cell nearer the Sun.





MS-FLUKSS optimizations on multi-core and many-core processors enabled by PAID IME program

FOCUS: *Significance of Progress Achieved (from beginning of PAID Program until present) in collaboration with PAID IME "Best Practices" Team*

I. Performance Challenges Identified

II. Original OpenMP implementation (distributed-like) changed to loop level OpenMP.

III. Explored Array-of-Structures (AoS) and Structure-of-Arrays (SoA) layouts for particle data representation (a two-fold acceleration has been obtained).

IV. First OpenACC version of the MS-FLUKSS code implemented and ported to Blue Waters GPU System. 15x speed up is obtained for one of the most time consuming kernels compared with single thread CPU.

V. Outstanding Challenges and Future Plans: scaling, optimization, and porting to MS-FLUKSS. Involve collaborative R&D with current PAID IME "Best Practices" and "Accelerator" (Wen-Mei Hwu, PI) Teams.