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Modeling Heliophysics Phenomena with Multi-Scale Fluid-Kinetic Simulation Suite

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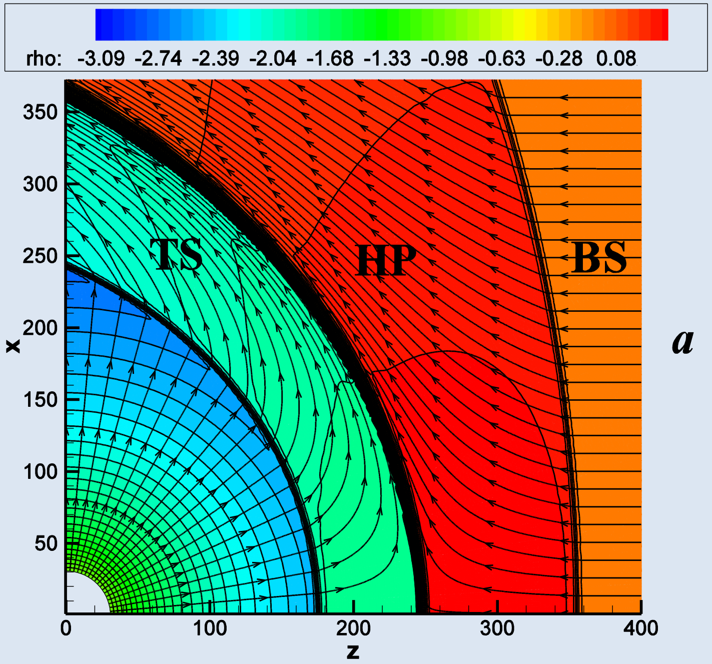
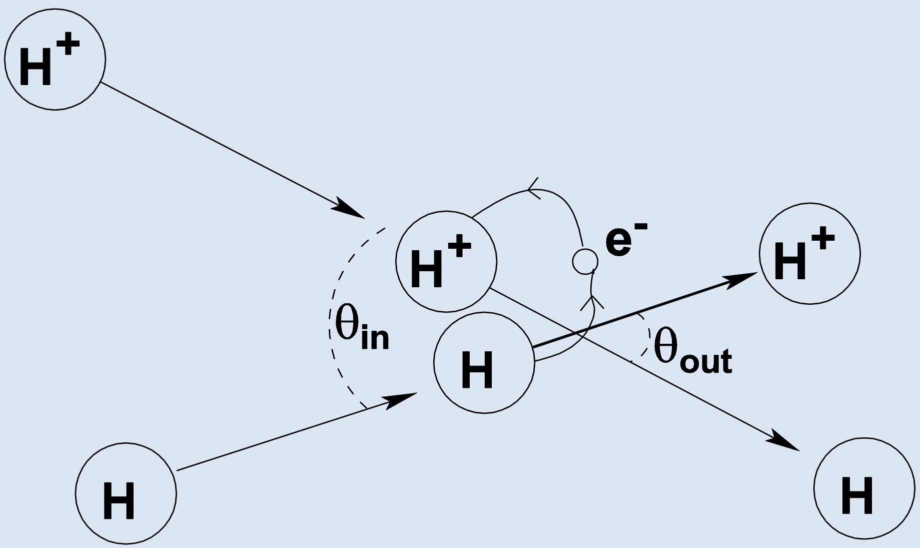
Key Challenges

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 properties of which 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.**



Any charge exchange event creates a secondary neutral atom with the properties of the parent ion and a non-thermal ion, which is picked up by the surrounding plasma. High-energy pickup ions, after another charge exchange give birth to an ENA, which will contribute to Interstellar Boundary Explorer (IBEX) measurements.

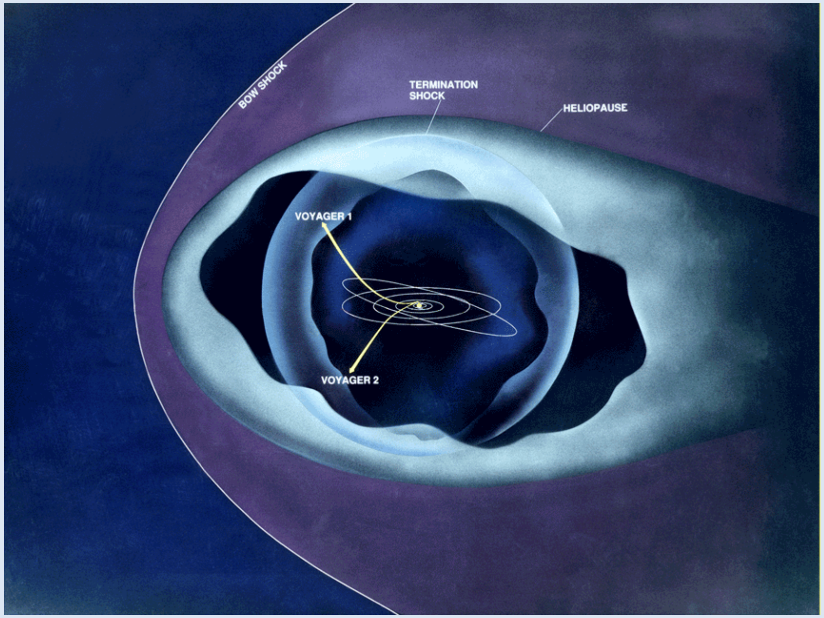
3. **Voyager 1 measures the interstellar magnetic field and plasma waves in the LISM. Observations indicate the presence of a low-density boundary layer on the outer side of the heliopause.**

4. **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.**

5. **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.**

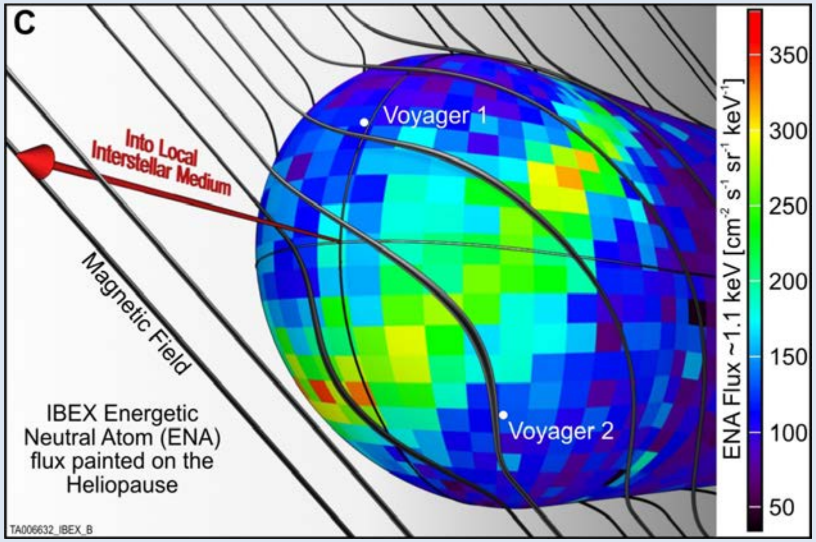
5. **To address these problems, we have developed a tool for self-consistent numerical solution of the MHD, gas dynamics Euler, and kinetic Boltzmann equations. Our Multi-Scale Fluid-Kinetic Simulation Suite (MS-FLUKSS) solves these equations using an adaptive-mesh refinement (AMR) technology. The grid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

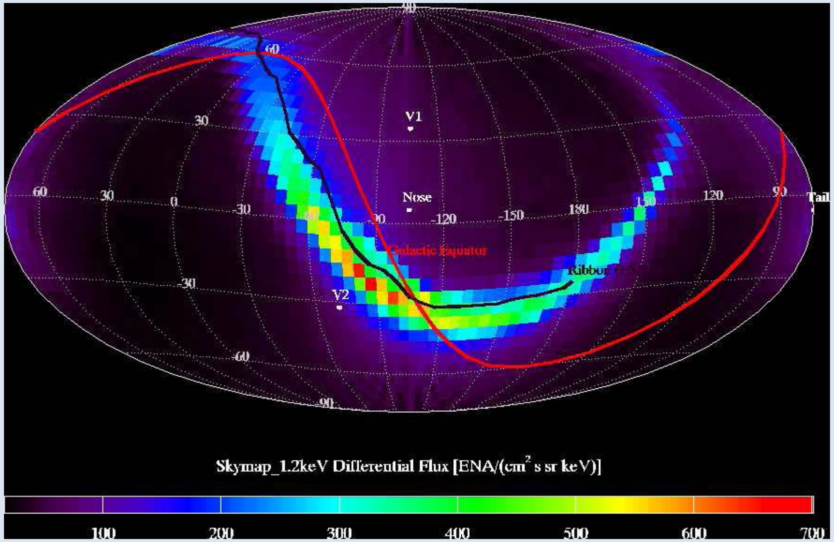
Why it matters?



***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 July 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, 2017) . 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.

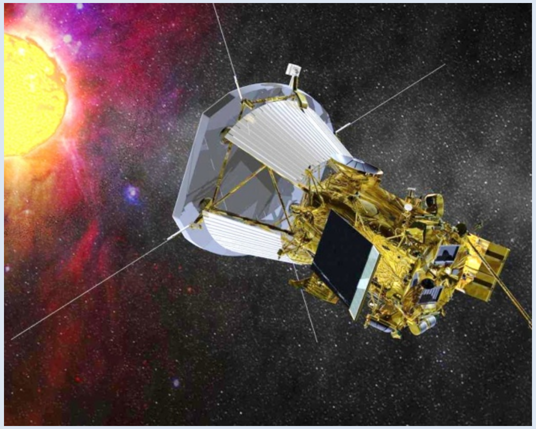




From McComas et al. (2009)

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."

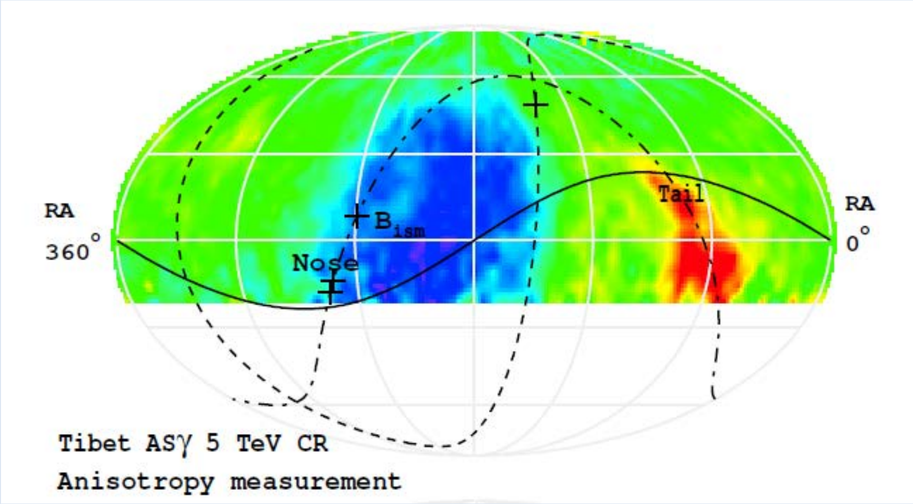


Artist's view of SPP from https://www.cfa.harvard.edu/sweap/

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.

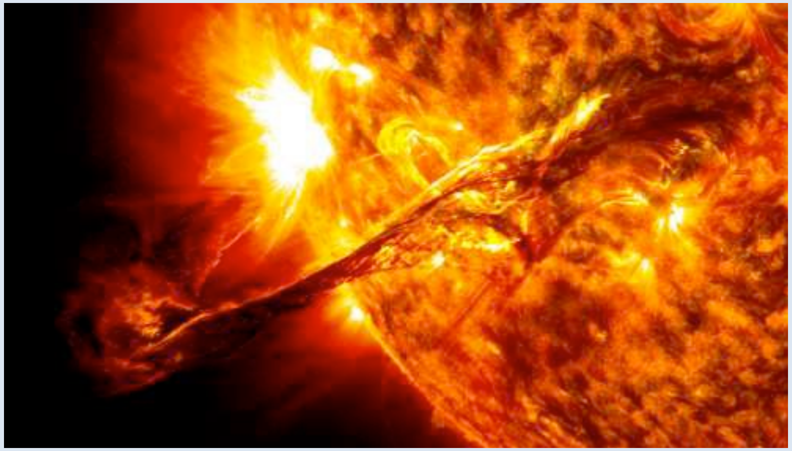
Recently, a great wealth of information about the directional variation (which is commonly referred to as anisotropy) in the flux of cosmic rays arriving at Earth in the TeV to PeV energy range has been obtained by a number of air shower experiments. Among those that have achieved excellent data quality 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.



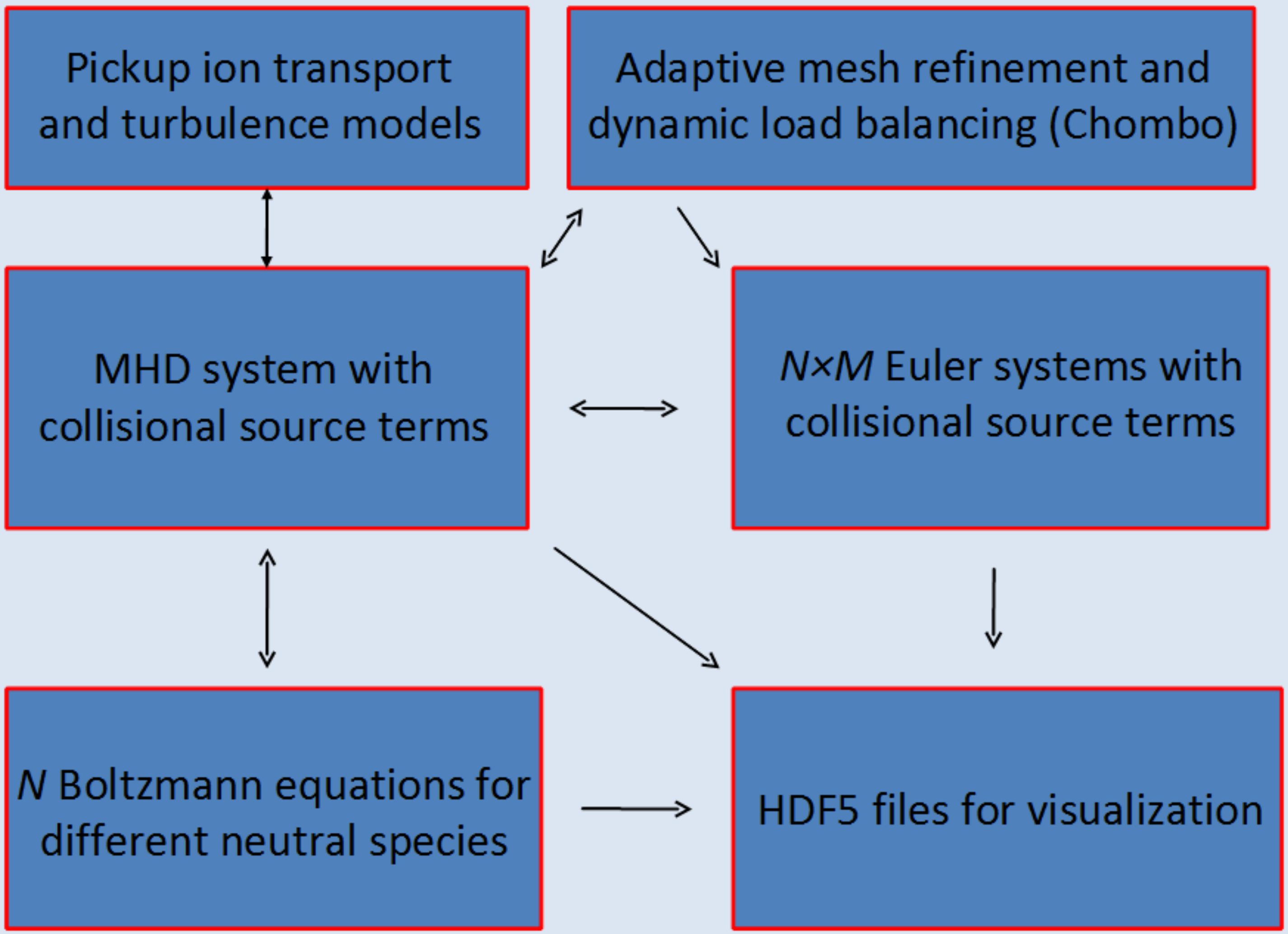
Artist's view of the New Horizons flyby past Pluto (courtesy of NASA at https://www.nasa.gov/mission_pages/newhorizons/overview/index.html).

The New Horizons mission is helping us understand worlds at the edge of our solar system by making the first reconnaissance of the dwarf planet Pluto and by venturing deeper into the distant, mysterious Kuiper Belt – a relic of solar system formation.



(*Left panel*) Geomagnetic storm in Alberta, Canada. [Photo by Zoltan Kenwell]. (*Right panel*) On August 31, 2012, the Solar Dynamics Observatory caught the sun launching streams of plasma into space at nearly 900 miles/sec. Credit: NASA/GSFC/SDO.

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 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

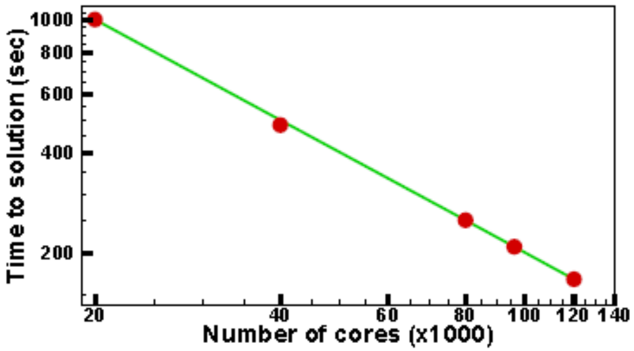


Figure 1. Strong scaling results of the kinetic code. The green line shows ideal performance. The red circles are measured time.

Parallelization (continued)

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

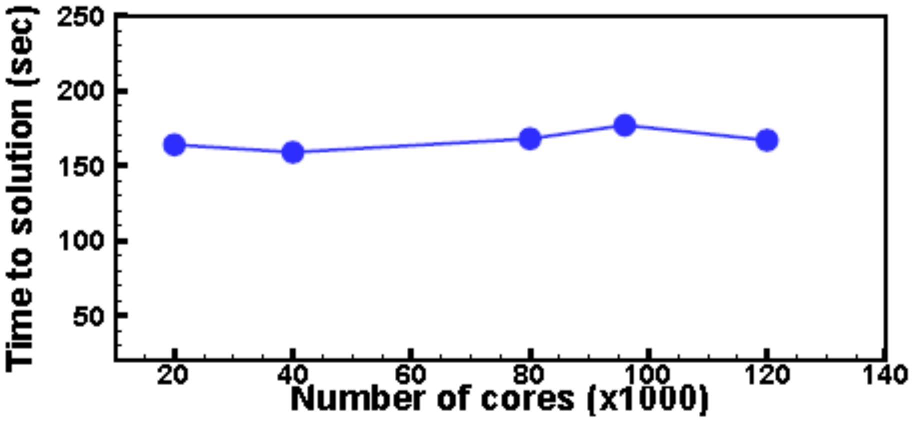


Figure 2. Weak scaling results of the kinetic code.

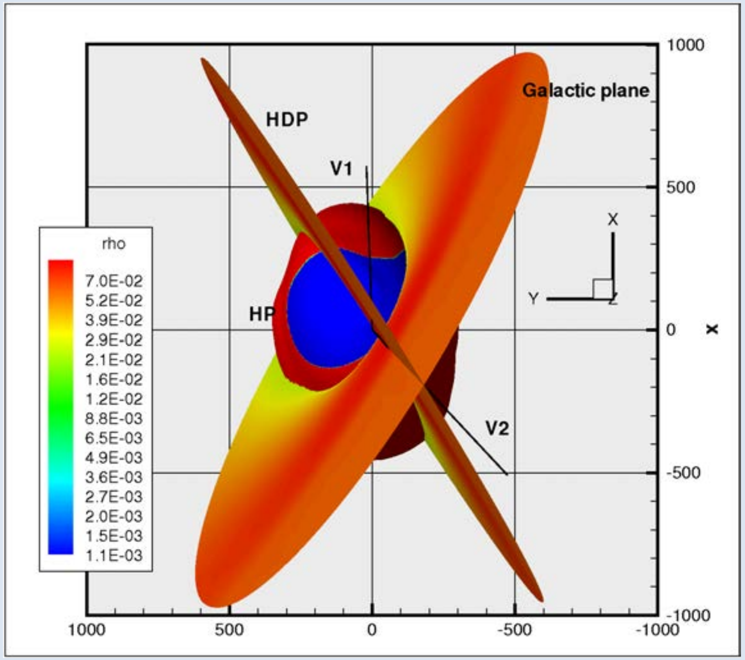
A 650Gb data file containing 10 billion particles (full 64-bit support is necessary) can be written as fast as 32 seconds on Lustre file system if it is striped over 100 Object Storage Targets (OSTs).

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, 2018).
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, 2018).
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, 2018).
4. Pogorelov, N. (Principal), "Modeling Heliophysics Phenomena with a Multi-Scale Fluid-Kinetic Simulation Suite," Sponsored by NSF, Federal, $31,945.00. (May 1, 2017 – April 30, 2018).
5. 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).
6. 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 funding is $2.9M.

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



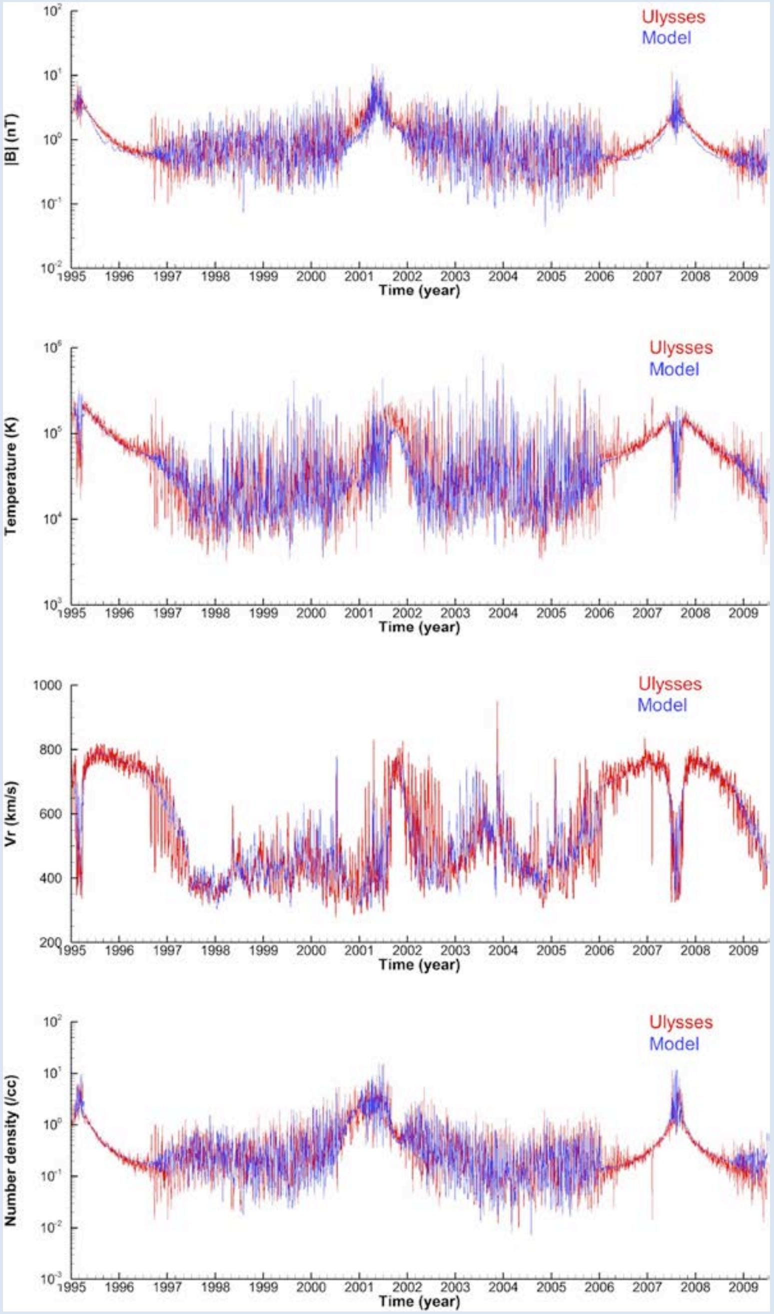
Our models are data-driven:

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.**

14

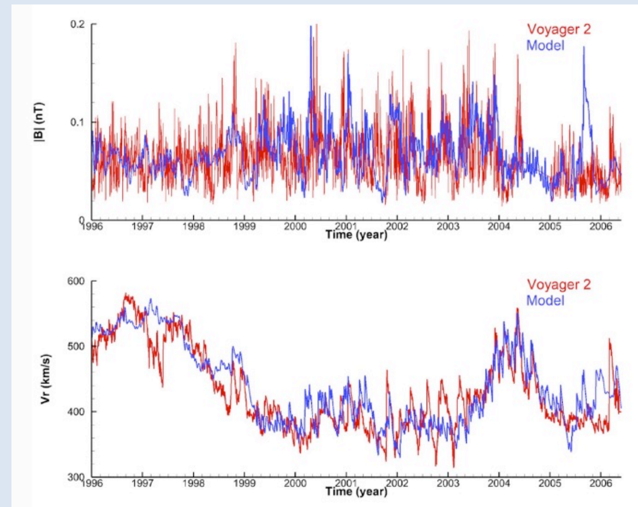
Our accomplishments

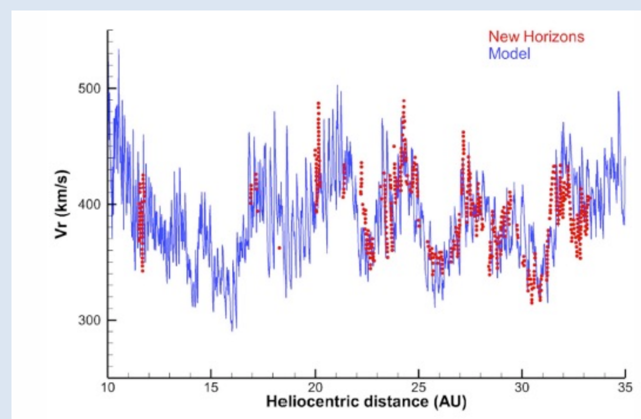
(1) we have performed data-driven SW flow simulations starting from the solar surface and used observational data to initiate coronal mass ejections;
(2) we have calculated SW propagation from the Earth orbit to Pluto along the New Horizons spacecraft trajectory, at Uranus, and further to the heliopause, and demonstrated good agreement with observational data;
(3) we have explained the existence of a thick, low-density boundary layer on the interstellar side of the heliopause;
(4) we have performed high-resolution simulations of the heliopause instability and identified the areas of possible magnetic reconnection near the heliopause;
(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 charge exchange on the bow wave that exists in front of the heliopause;
(7) the results of the first year are published in 14 papers and reported at 12 scientific meetings, 8 of them being invited talks.

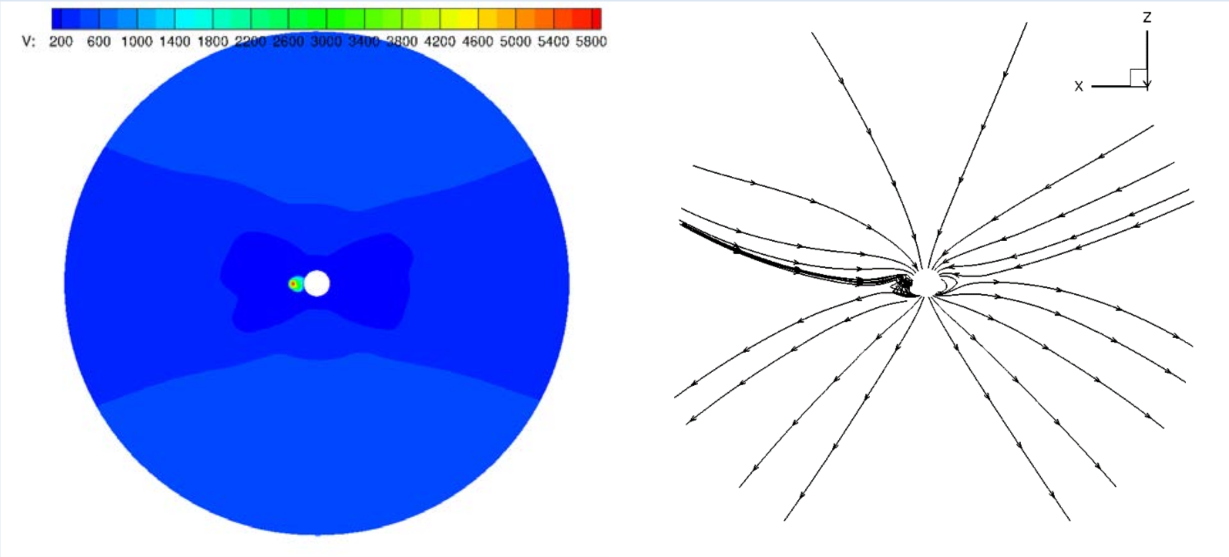


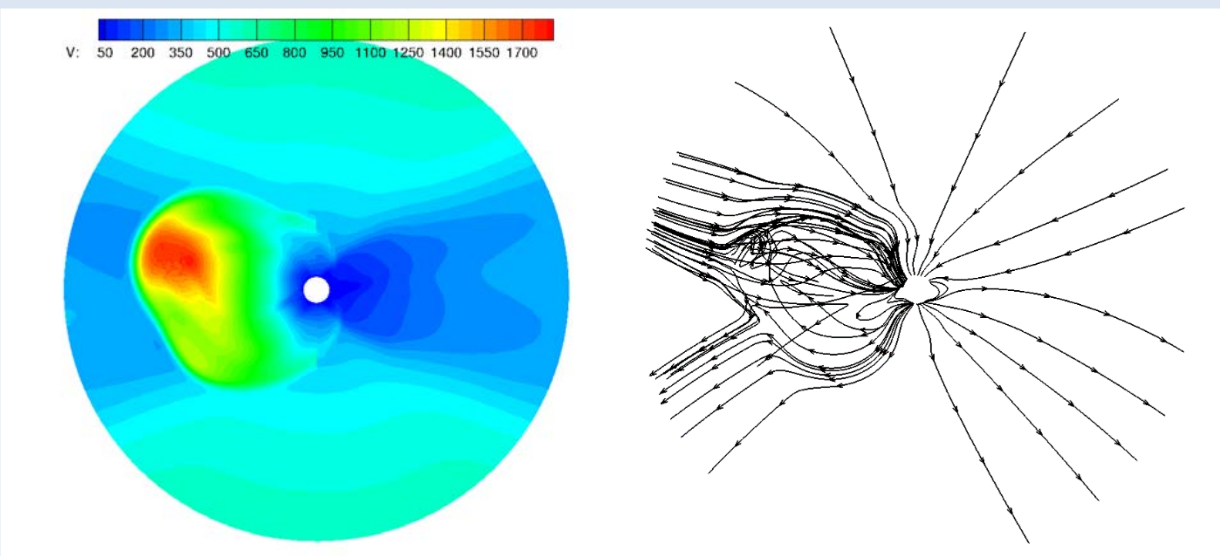
(*Left panel*) **Comparison of our simulations with the SW measurements along the *Ulysses* trajectory.**
(*Bottom panels*) **Comparison with Voyager 2 and New Horizons observations.**

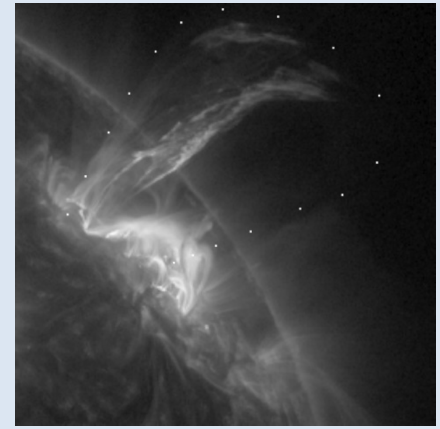
From Kim et al. (2016).





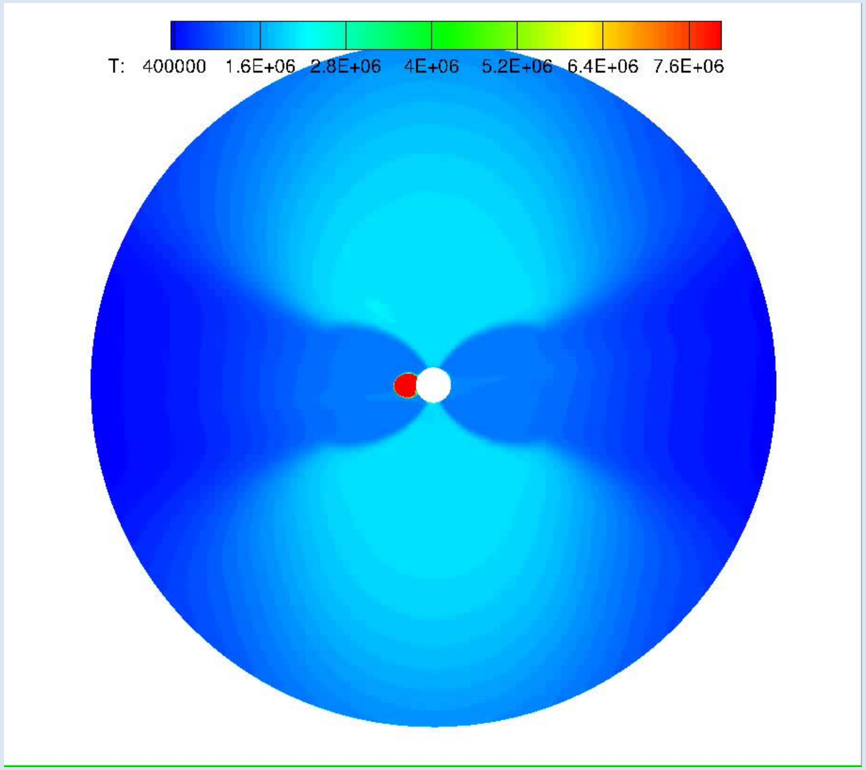


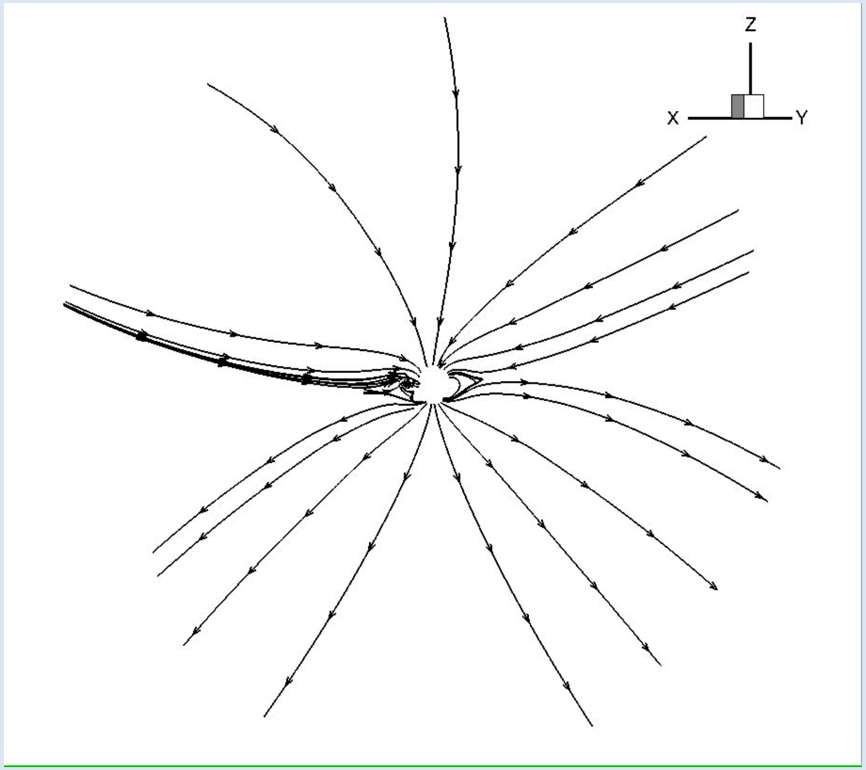




(Above) Solar eruption observed on 7 March 2011 observed by Atmospheric Imaging Assembly (AIA) in 13.1 nm wavelength.

(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.

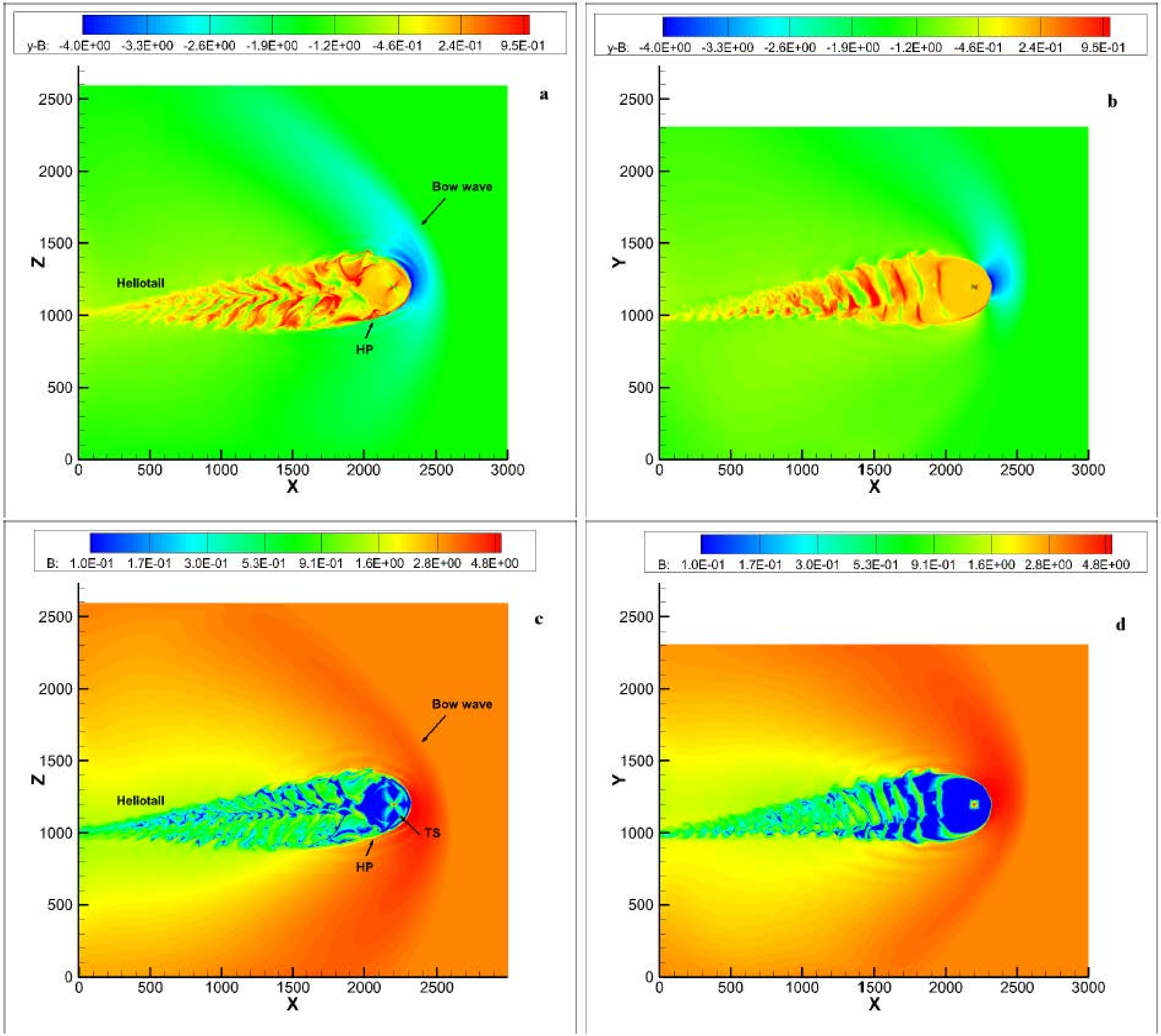


FIG. 1.— SW–LISM interaction pattern in the presence of solar cycle effects. The y-component (top panels) of the magnetic field vector and its magnitude (bottom panels) in the meridional (left panels) and equatorial (right panels) planes. Distances are given in AU and magnetic field in μG. One can see the TS, HP, and bow wave.

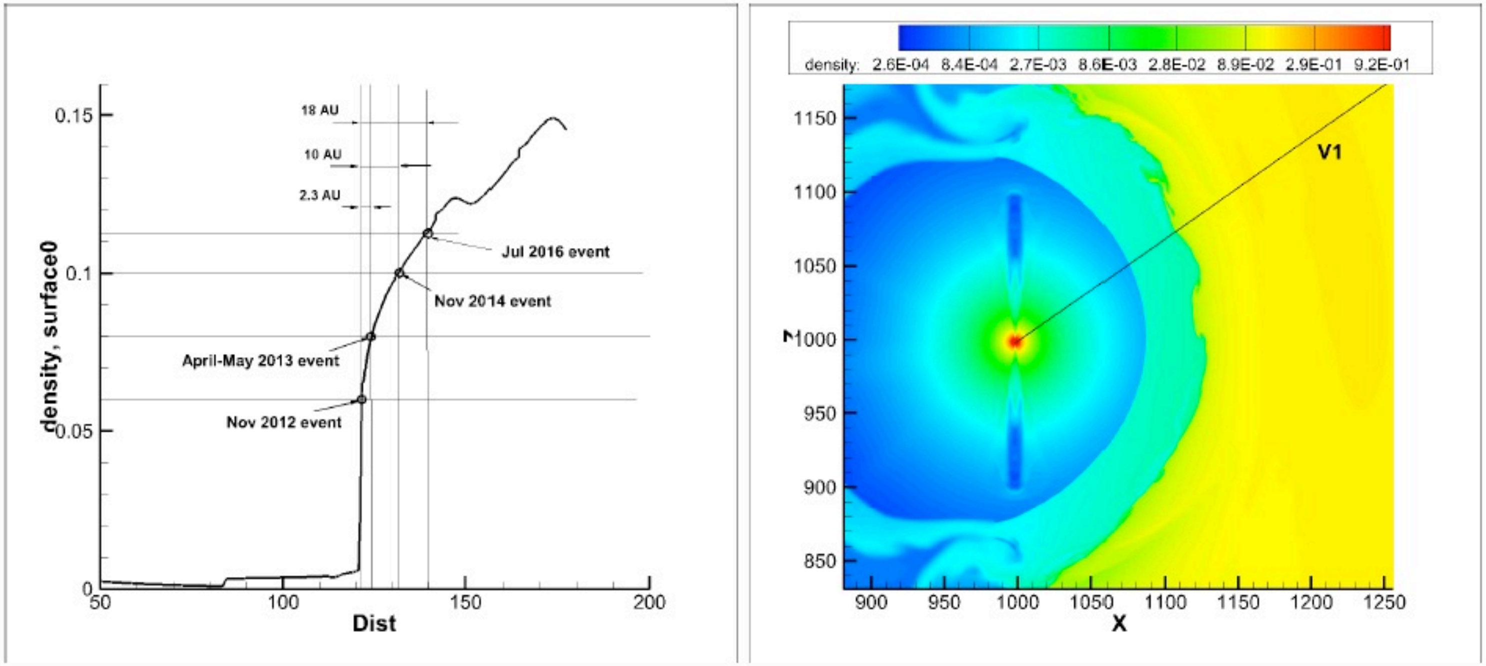


FIG. 5.— The distribution of plasma density *(left panel)* along the *V1* trajectory and its comparison with the plasma waves events detected by the spacecraft beyond the heliopause, and (*right panel*) in the meridional plane.

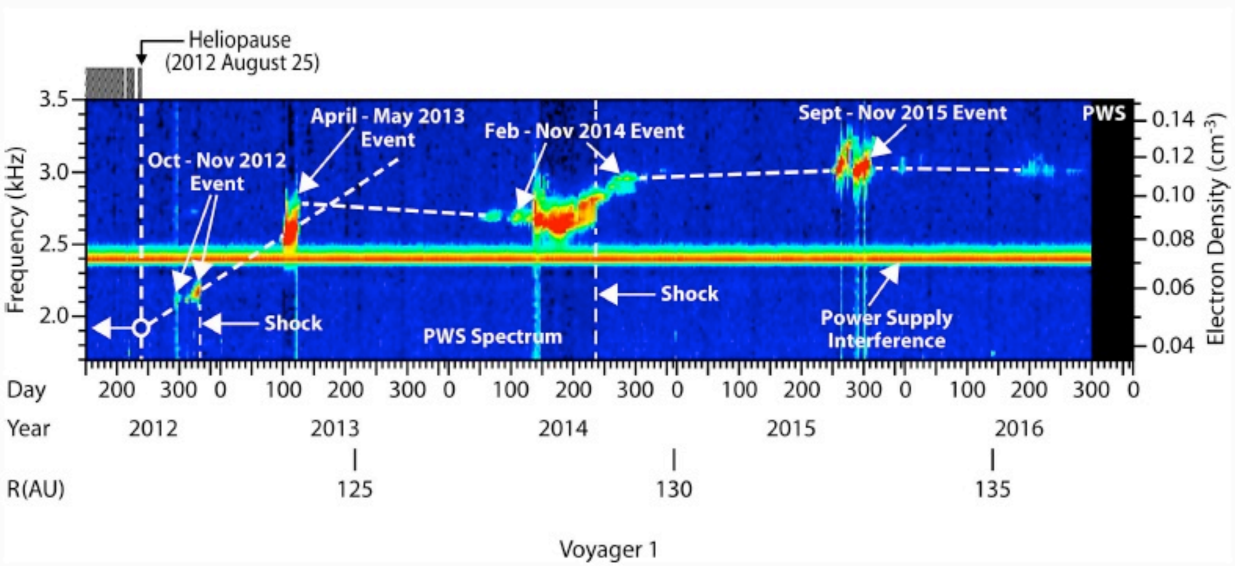
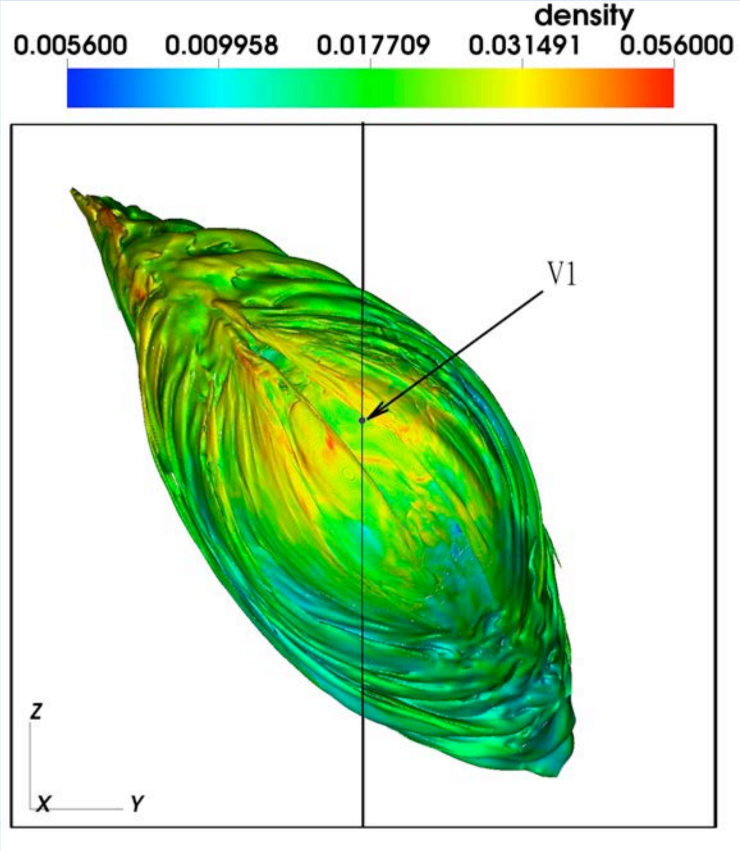
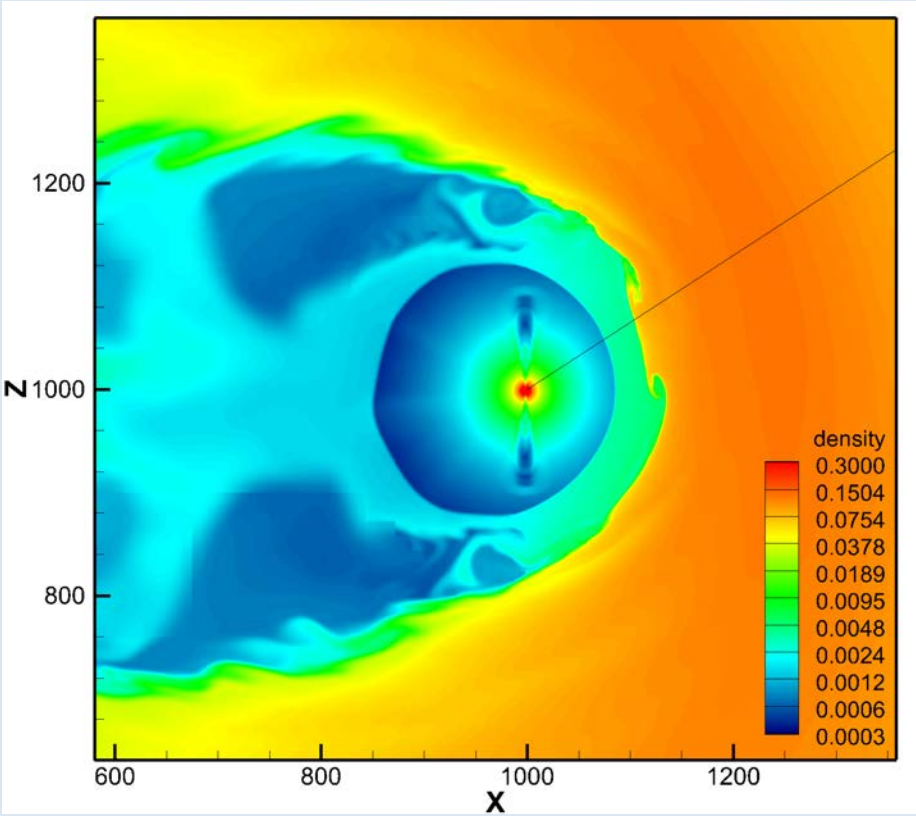


FIG. 6.— *Voyager* 1 measurements of plasma oscillation frequency and electron density derived from it.

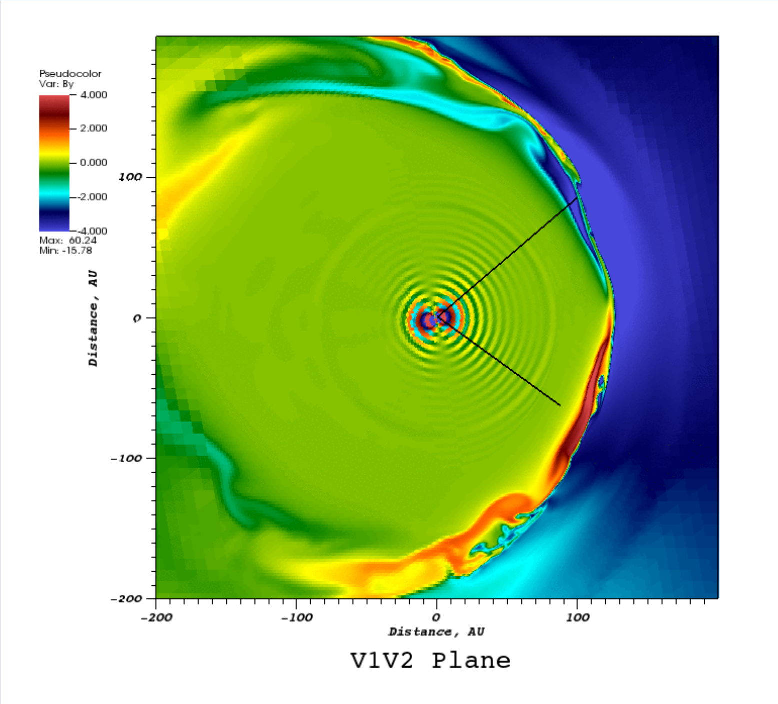
Instability of the HP: a mixture of the RT and KH instability

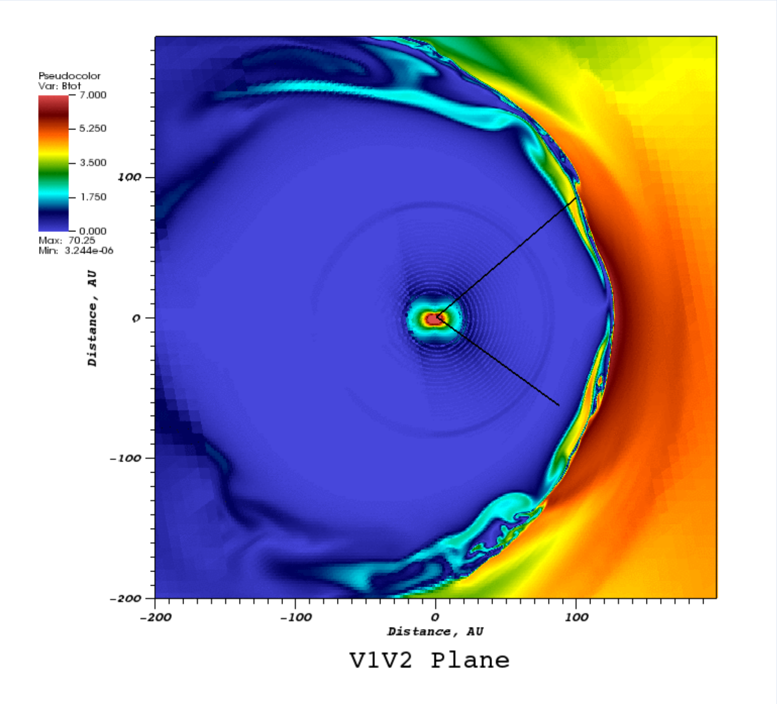




(*Left*) The frontal view of the HP and *(right*) the plasma density distribution in the meridional plane: solar cycle (Borovikov & Pogorelov, 2014).

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.

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.

Future work during the second year

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.**