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Multi-Scale, MHD-kinetic Modeling of the Solar Wind and its Interaction with the Local Interstellar Medium

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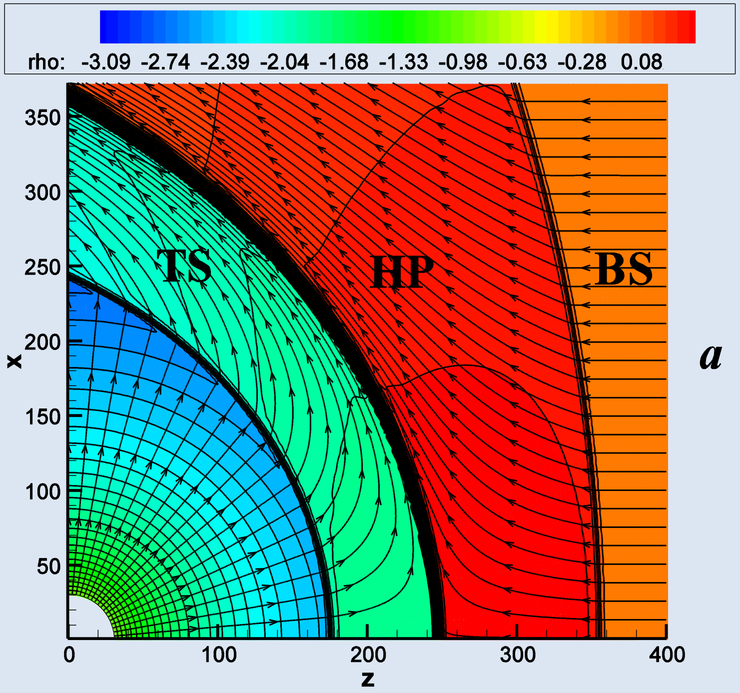
Key Challenges

Objective 1. Physical processes involving non-thermal ions. **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).**

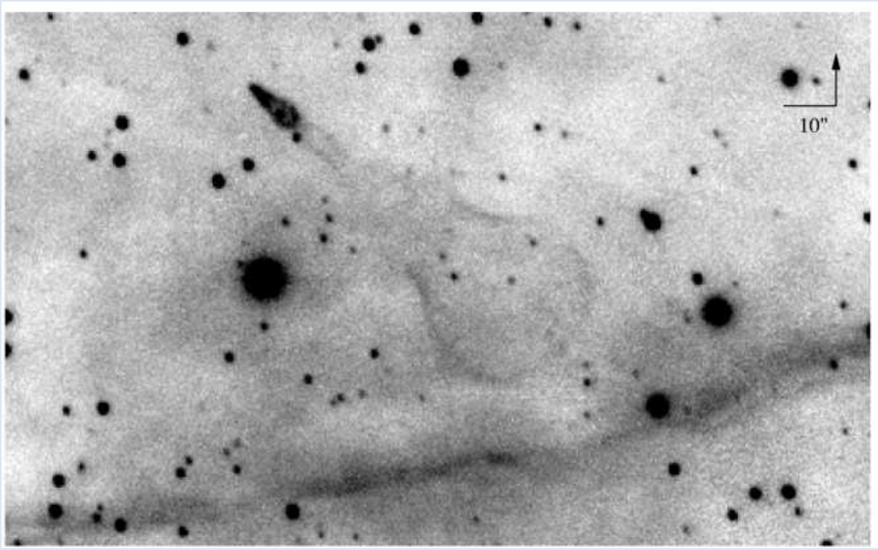


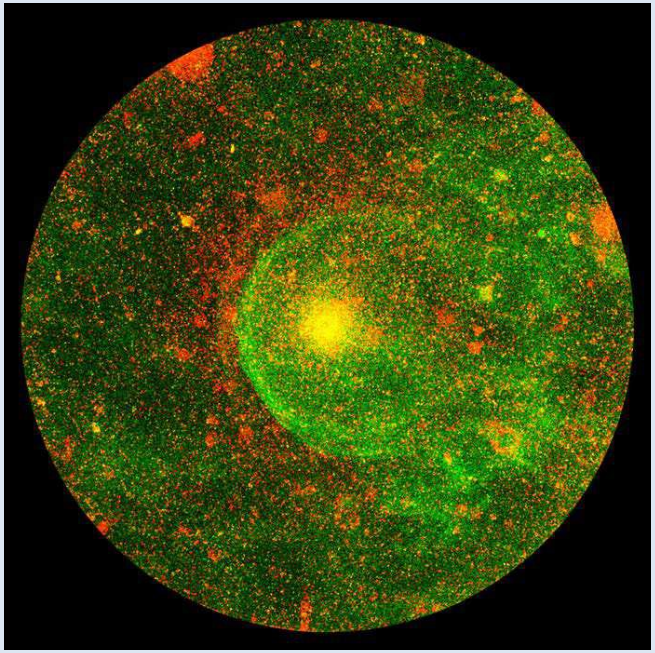
The Sun is at the origin, the LISM flow is from the right to the left. Their interaction creates a heliospheric termination shock, a heliopause, and a bow wave that may include a sub-shock inside its structure. The LISM is partially ionized and the mean free path of charge exchange between H atoms and H+ ions is such that this process should be modeled kinetically.

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 atom (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 (KINETIC) treatment.

Objective 2: Helium in the heliosphere. Approximately 40% of the dynamic pressure of the interstellar plasma is due to the presence of He^+ since their relative abundance compared to H is ~10% (e.g., Slavin & Frisch, 2008) and they have four times the mass of H. We have developed and implemented in our Multi-Scale Fluid-Kinetic Simulation Suite (MS-FLUKSS), and now testing on Frontera a new model of The SW–LISM interaction which involves He+ and protons, and neutral H and He atoms. The atoms are treated kinetically, in the same way we treated neutral H atoms in the past. New simulations renewal make it possible to perform global simulations of the SW–LISM interaction and describe the transport of He atoms towards Earth, where they are measured by the Interstellar Boundary Explorer (IBEX).

Objective 3. Perform solar wind simulations from the solar surface to Earth's orbit to improve space weather predictions, thus ensuring safety of personnel and electronics on board spacecraft.

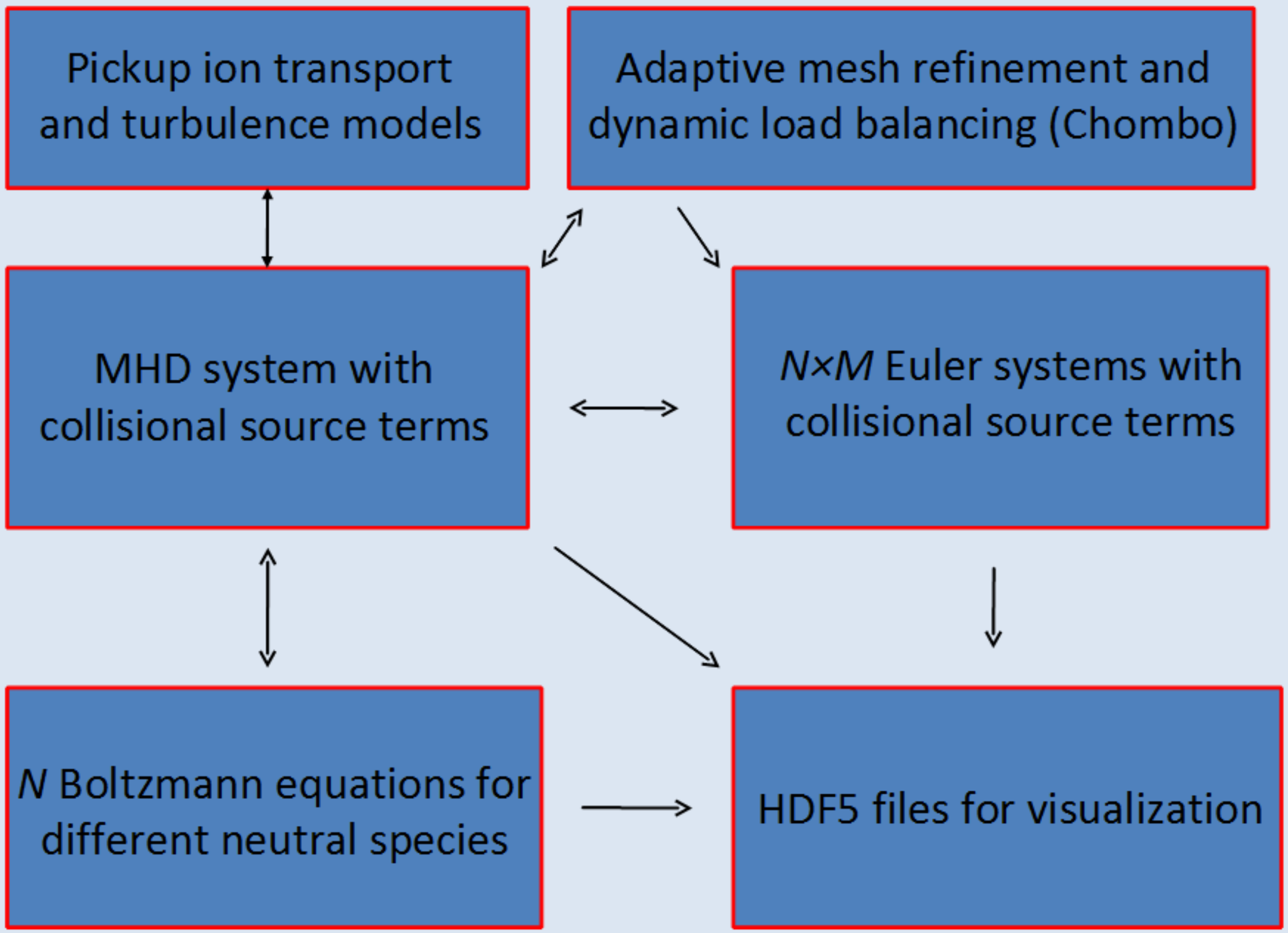




(Left panel.) The Guitar nebula (from Chatterjee & Cordes, 2002).
(Right panel.) Carbon Star IRC+10216 (from Sahai & Chronopoulos, 2010).

Clearly the interaction pattern is substantially different!
How about the heliosphere interaction with the LISM?

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



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

	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

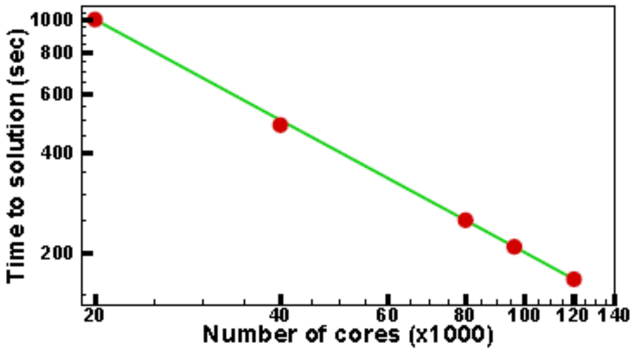


Figure 1. Strong scaling results of the kinetic code. The green line shows ideal performance. The red circles are measured time.

Parallelization (continued)

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

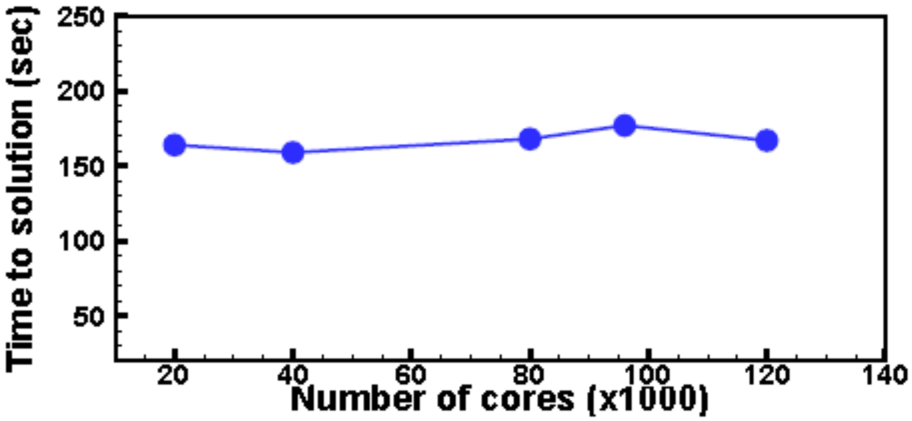
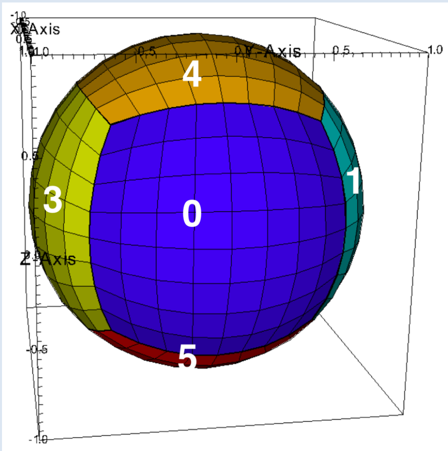


Figure 2. Weak scaling results of the kinetic code.

HelioCubed: A Next-Generation Model Using Mapped-Multiblock Grids and Heterogeneous Processors

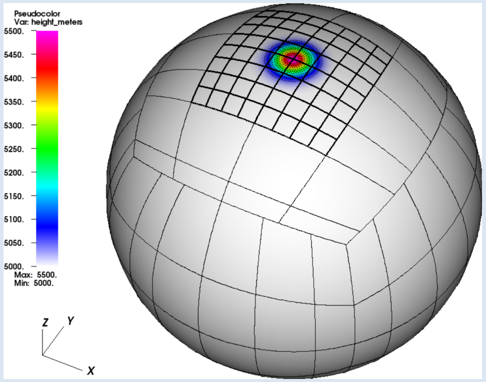


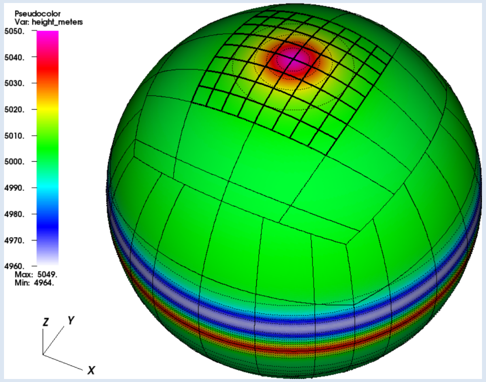
Mapped Multiblock Grids

- Representation of spherical geometry using a conforming cubed-sphere mapping of spherical shells eliminates pole singularity.
- Fourth-order accurate finite-volume method for MHD.

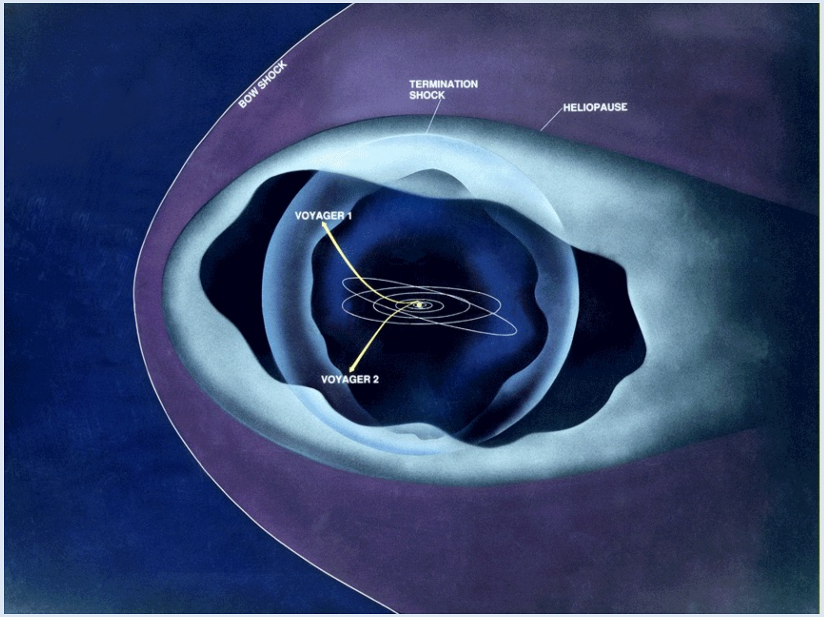
Performance Portable C++ Abstraction Library

- *Proto* library developed under DOE Exascale Computing Project support provides a highly productive programming environment for implementing such algorithms.
- Retargeted implementations of Proto provides performance portability across different architectures, including multicore and heterogeneous (e.g. GPU) systems, without any changes to user-level code.



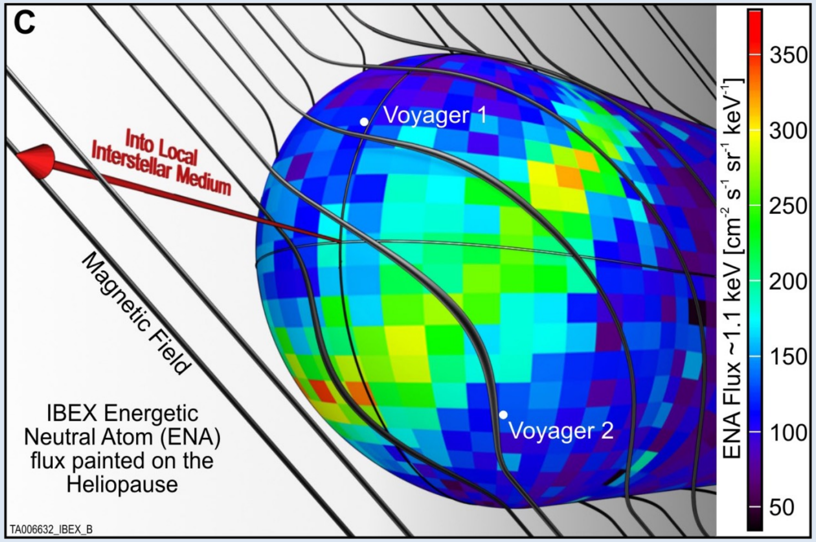


Why it matters?

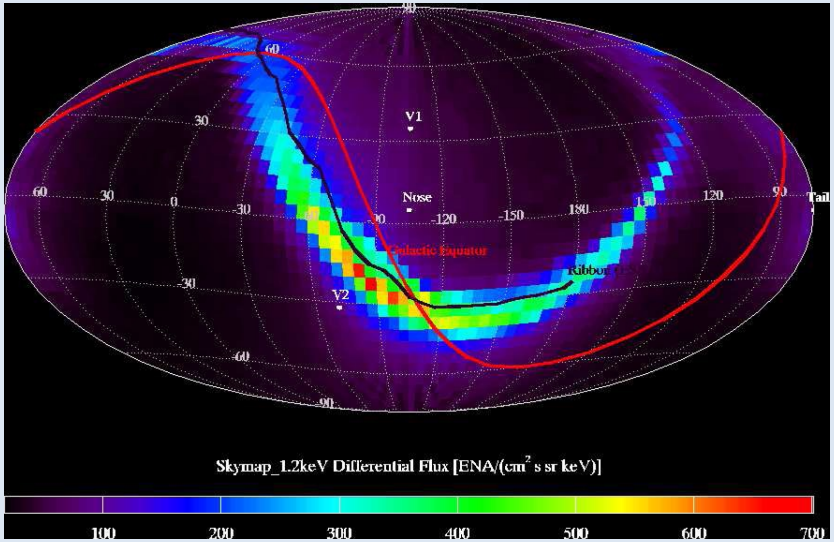


Voyager 1* and *2 ***(V1*** **and** ***V2),*** **crossed the heliospheric termination shock in December 2004 and in August 2007, respectively (Stone et al., 2005, 2008). After more than 45 years of historic discoveries, V1 and V2 crossed the heliopause and penetrated into the LISM and measures its properties 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. The heliospheric community has a unique chance to analyze and interpret Voyager measurements deriving breakthrough information about physical processes occurring more than 1.3×10^{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 constrain 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+; Pogorelov et al., 2011+) . 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.

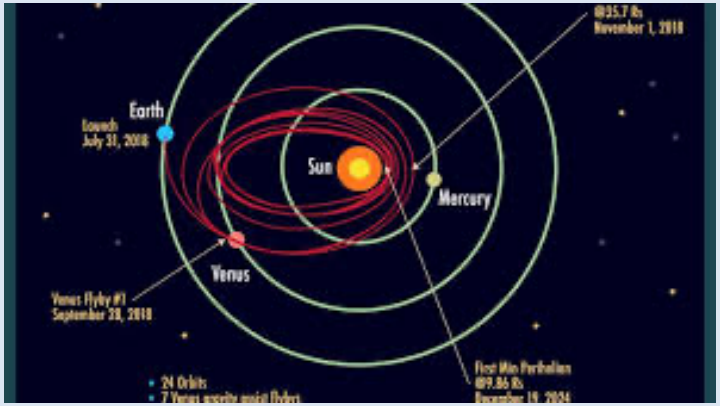


From McComas et al. (2009)



Simulated ENA flux

From the 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. This is the first NASA mission that has been named for a living individual."



Each consecutive trajectory of PSP takes it closer to the Sun.

Solar Wind Electrons, Alphas, and Protons (SWEAP) instrument (PI Justin Kasper) onboard PSP is directly measuring 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.

Science funding exceeds $6M

1. Pogorelov, N. (Principal), Helium in the Heliosphere, sponsored by NASA, $644,036 (6/26/2018 – 31/12/2022).
2. Pogorelov, N. (Principal), Space Weather with Quantified Uncertainties: Improving Space Weather Predictions with Data-Driven Models of the Solar Atmosphere and Inner Heliosphere, sponsored jointly by NSF and NASA, $3.5M (09/01/2020 – 08/31/2023).
3. Pogorelov, N. (Principal), Pickup Ions in the Outer Heliosphere and Beyond, sponsored by NASA, $746,285 (09/05/2018 – 09/04/2022).
4. Pogorelov, N.V. (Principal), NSF-BSF: Collaborative Research: Rankine-Hugoniot Conditions Relating the Gyrotropic Regions of Collisionless Shocks in Non-thermal Plasma, sponsored by NSF, $197,178 (7/1/2020 – 6/30/2023).
5. Pogorelov, N. (Principal), Turbulence as Indicator of Physical Processes at the Heliospheric Interface, sponsored by NASA, $524,773 (3/1/2019 – 2/28/2023).
6. Pogorelov, N. (Principal), Modeling Space Weather with Quantified Uncertainties, supported by the NASA FINESST program, $135,000 (09/01/2021 – 08/31/2024)
7. Pogorelov, N. (Co-I), The Solar Probe Plus Phase C/D/E Activities of the Parker Solar Probe, sponsored by the Smithsonian Astrophysics Observatory, $791,533 (04/01/2014 – 09/30/2025).
8. Pogorelov, N. (Co-I), IBEX-Interstellar Boundary Explorer Extended Mission, sponsored by Princeton University, $208,503 (4/1/2020 - 3/31/2023).

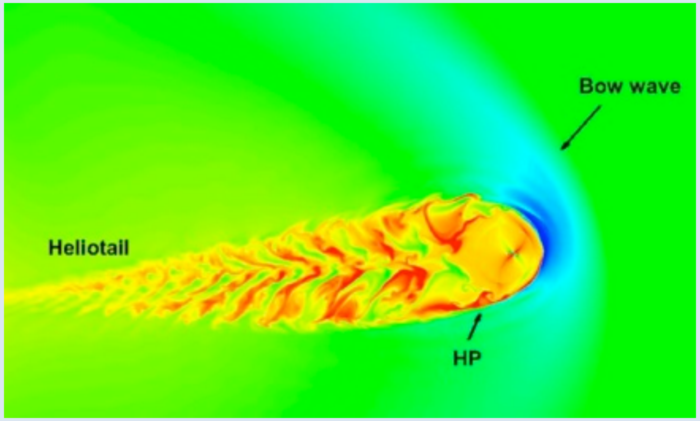
Recent accomplishments are published in 14 papers and presented in over 20 scientific presentations.

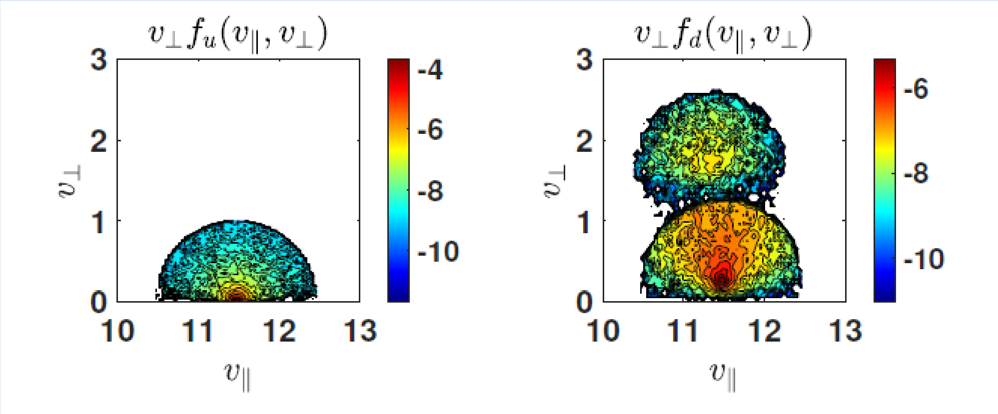
Press releases:

1. **UAH-led space weather prediction research could be critical to U.S. Space Command (June 24, 2021, https://www.uah.edu/news/news/uah-led-space-weather-prediction-research-could-be-critical-to-space-force-command).**
2. **Which Way Does the Solar Wind Blow? (June 3, 2021, https://www.tacc.utexas.edu/-/which-way-does-the-solar-wind-blow-).**
3. **Research student from Siddapur taluk receives NASA grant (November 22, 2021, https://www.thehindu.com/news/national/karnataka/research-student-from-siddapur-taluk-receives-nasa-grant/article61427733.ece).**
4. **Predicting the weather in space (November 29, 2021, https://businessalabama.com/predicting-the-weather-in-space/).**

Boundary conditions at collisionless shocks

- SW-LISM interactions performed so far have been using either highly approximate or NO boundary conditions for PUIs at the termination shock.
- Our aim is to use kinetic simulations to derive such boundary conditions and use them in global simulations.





The upstream and downstream distributions of PUI for B_d/B_u = 2.7 and θ_u = 85°. Directly transmitted and those reflected once and proceeding further downstream afterwards. 22% of PUIs are reflected, i.e., higher than due to the cross-shock potential only. The downstream perpendicular temperature of reflected PUIs is an order of magnitude lower than it was proposed in Chalov et al. (1995) and Zank et al. (2010). **From Gedalin et al. (2021).**

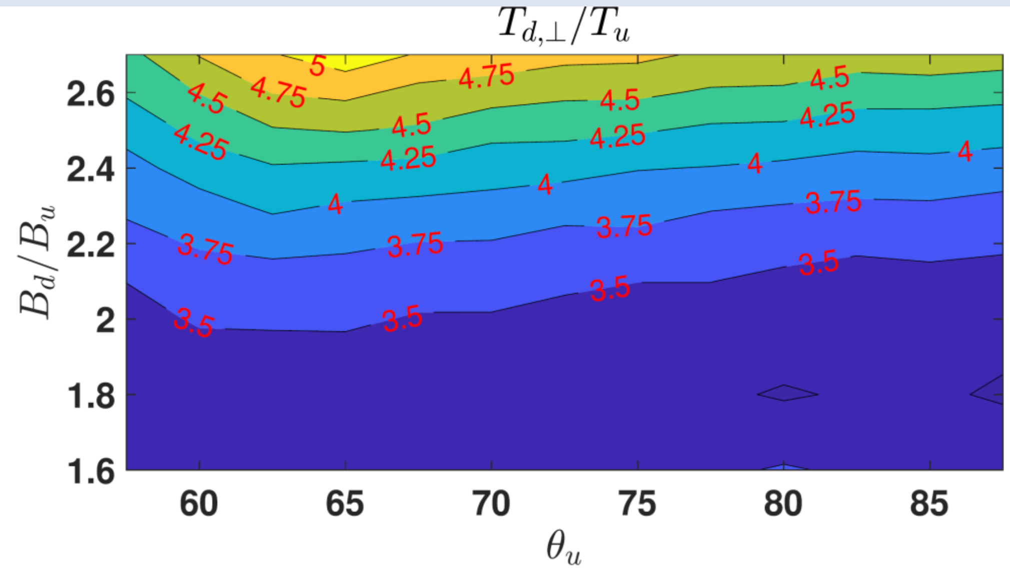


Figure 6. Perpendicular heating $T_{d,\perp}/T_u$ as a function of B_d/B_u and θ_u.

For TS parameters close to V2 measurements (Richardson et al., 2008) and the PUI fraction of ξ=20%,

$$T_{d,\mathrm{PUI}} \approx 2.9 \times 10^6\ \mathrm{K},\ \ T_{d,\mathrm{SW}} \approx 4.6 \times 10^5\ \mathrm{K},\ \ T_d = 9.6 \times 10^5\ \mathrm{K}.$$

For ξ=30%,

$$T_{d,\mathrm{PUI}} \approx 2.9 \times 10^6\ \mathrm{K},\ \ T_{d,\mathrm{SW}} \approx 1.4 \times 10^5\ \mathrm{K},\ \ T_d = 9.8 \times 10^5\ \mathrm{K}.$$

For ξ=5%,

$$T_{d,\mathrm{SW}} \approx 8 \times 10^5\ \mathrm{K}.$$

Important observation: the increase of the PUI fraction in front of a shock substantially decreases the SW temperature behind the shock, but does not affect the temperatures of the PUIs and of the mixture much.

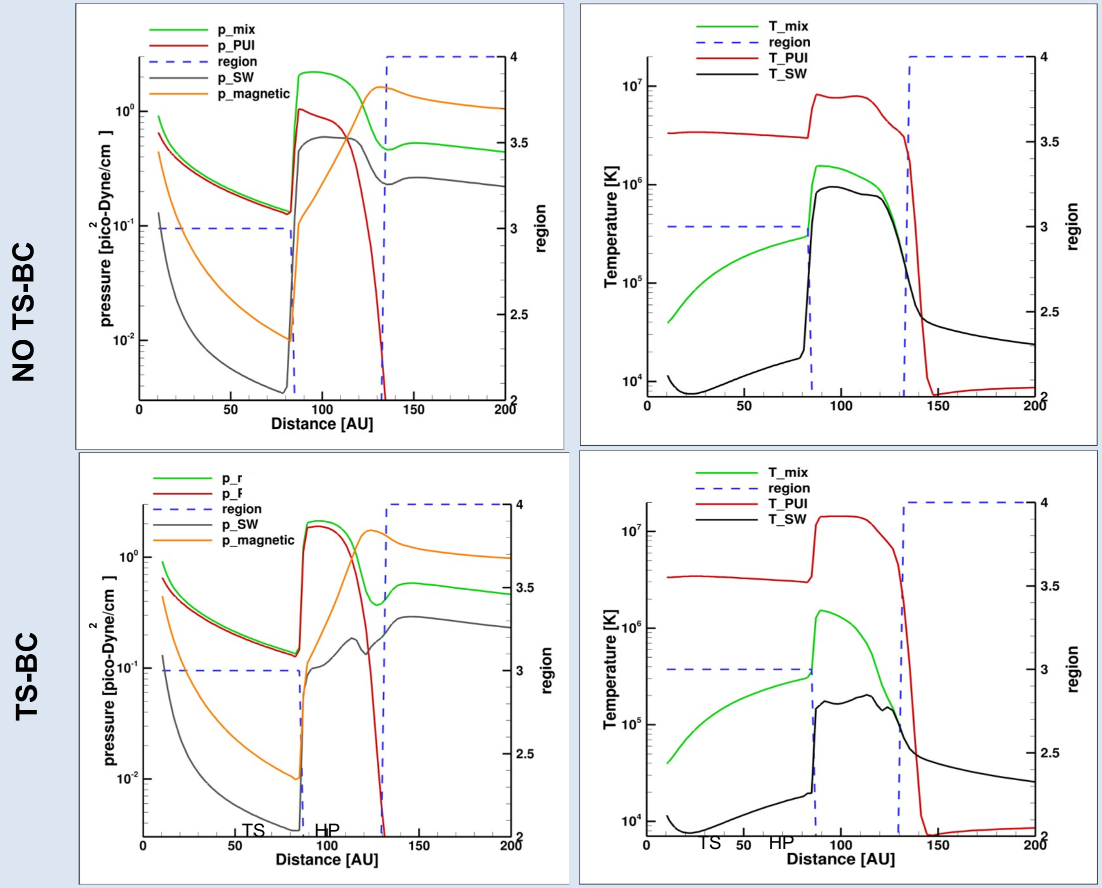
Simulation results: applying kinetically designed boundary conditions for pickup ions at the termination shock

- The MHD equations and standard Rankine-Hugoniot (RH) relations are not suitable for the description of highly anisotropic PUIs near the TS.

- The simulations are performed using boundary conditions (BC) for PUIs derived from the kinetic analysis based on test-particle (Gedalin et al 2020) and hybrid simulations (V. Roytershtein)

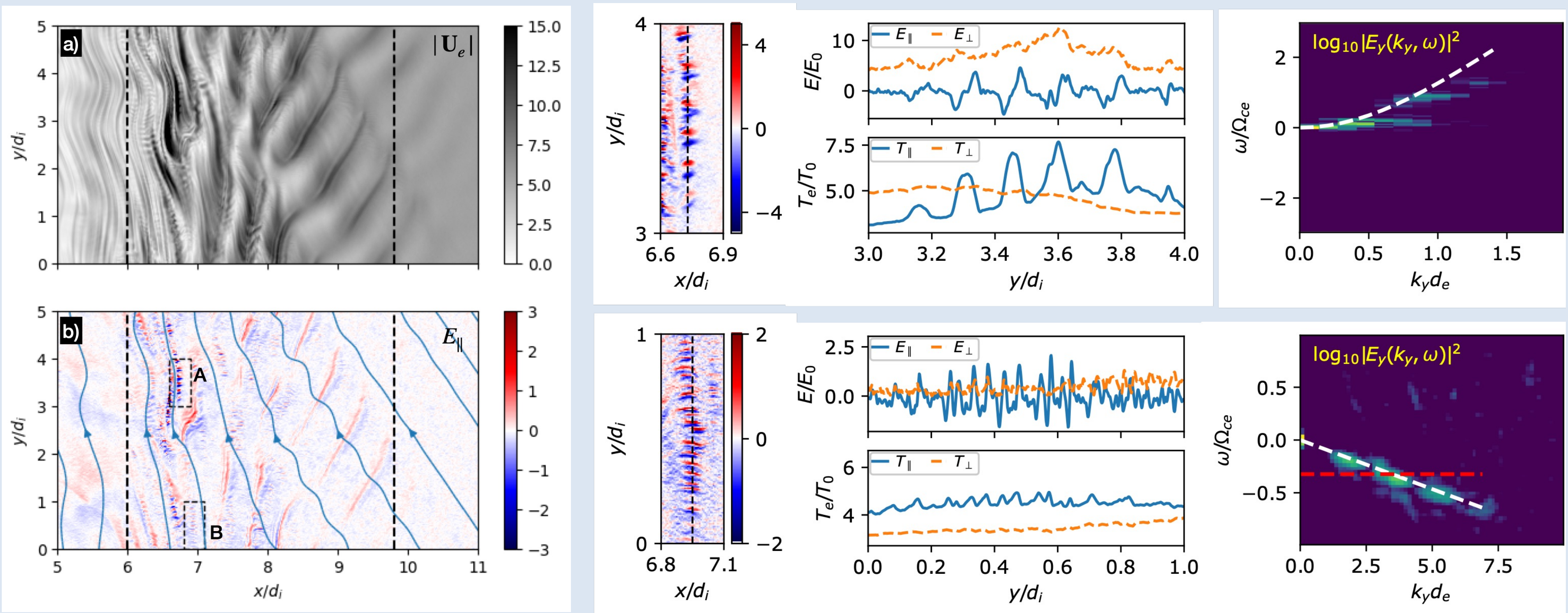
Downstream PUIs parameters at TS	NO TS-BC	TS-BC
pressure [pico-Dyne/cm^2]	1.02	1.87
Temperature [K]	8×10^{6}	14×10^{6}

- The width of IHS decreases by ~7-10 AU when the kinetic BCs for PUIs are applied.



: Distributions of the SW, PUI and mixture pressure (left) and temperature (right) vs. heliocentric distance along the V2 direction, obtained without applying the BCs (NO TS-BC) (top) and with BCs (TS-BC) (bottom).

Micro- to Macro-scale Coupling in Collisionless Shocks: Do Micro-Instabilities Play a Role in Shock Dynamics



This problem is encountered in all collisionless shocks. As a first step, we are using Frontera to analyze near-Earth shocks (IP shocks and the bow shock). Typical simulation: the VPIC code on 512-768 nodes, MPI + 4 pthreads per rank, HDF5 output, ~200 total hours of wall-time. The simulation shows instabilities developed in a transition region of a collisionless shock with $M_A = 6.5$, $\theta = 65^\circ$. The instabilities generate large fluctuations in $E_\parallel$, which affect electron energization. The right panels show zoom-in into the two boxes (A and B) + line cuts of $E_\parallel$ and electron temperature fluctuations + spectra aiding identification of the instabilities. In box A, the dominant mode is a short-wavelength whistler (called Lion Roar in magnetospheric physics). In box B, the dominant mode is an ion-acoustic fluctuation. Solitary structures (electron and ion holes) are also present.

Transport of neutral He atoms into the heliosphere allows us to determine the properties of the VLISM (Fraternale et al., 2021)

As usual, we model the SW-LISM interaction by solving the MHD equations for the ion mixture in the conservation-law form with appropriate source terms due to charge exchange, photoionization, Coulomb collisions, etc. To model the transport of He atoms into the heliosphere towards the IBEX detectors, we need to add He+ ions, which are described by

$$\partial_t n_{\mathrm{He}^+} + \nabla \cdot (\boldsymbol{u}\, n_{\mathrm{He}^+}) = S^n_{\mathrm{He}^+}, \qquad (1)$$

$$\partial_t p_{\mathrm{He}^+} + \nabla \cdot (\boldsymbol{u}\, p_{\mathrm{He}^+}) = (1-\gamma)\, p \nabla \cdot \boldsymbol{u} + S^p_{\mathrm{He}^+} + Q^C, \qquad (2)$$

where S describe the charge exchange and Q^C describes the thermal equilibration process due to Coulomb collisions between protons and He+ ions.

The transport of He and H atoms is treated kinetically by solving the Boltzmann equation with a Monte Carlo method.

Typical He + He^{+} collisions occur in the LISM in the energy range 0.1–10 eV. According to Scherer et al. (2014), the process He + $He^{+} \rightarrow He^{+}$ + He at such low energies is the dominant for He in the LISM. Therefore, we consider only these collisions.

Not only the inclusion of He atoms and He+ ions affects the solution, the new simulations allow us to determine the properties of the pristine LISM. This is done by tracking the transport of He atoms that experience no charge exchange at all before they reach the IBEX detector. However, they arrive highly anisotropic!

Transport of neutral He atoms into the heliosphere allows us to determine the properties of the VLISM (Fraternale et al., 2021)

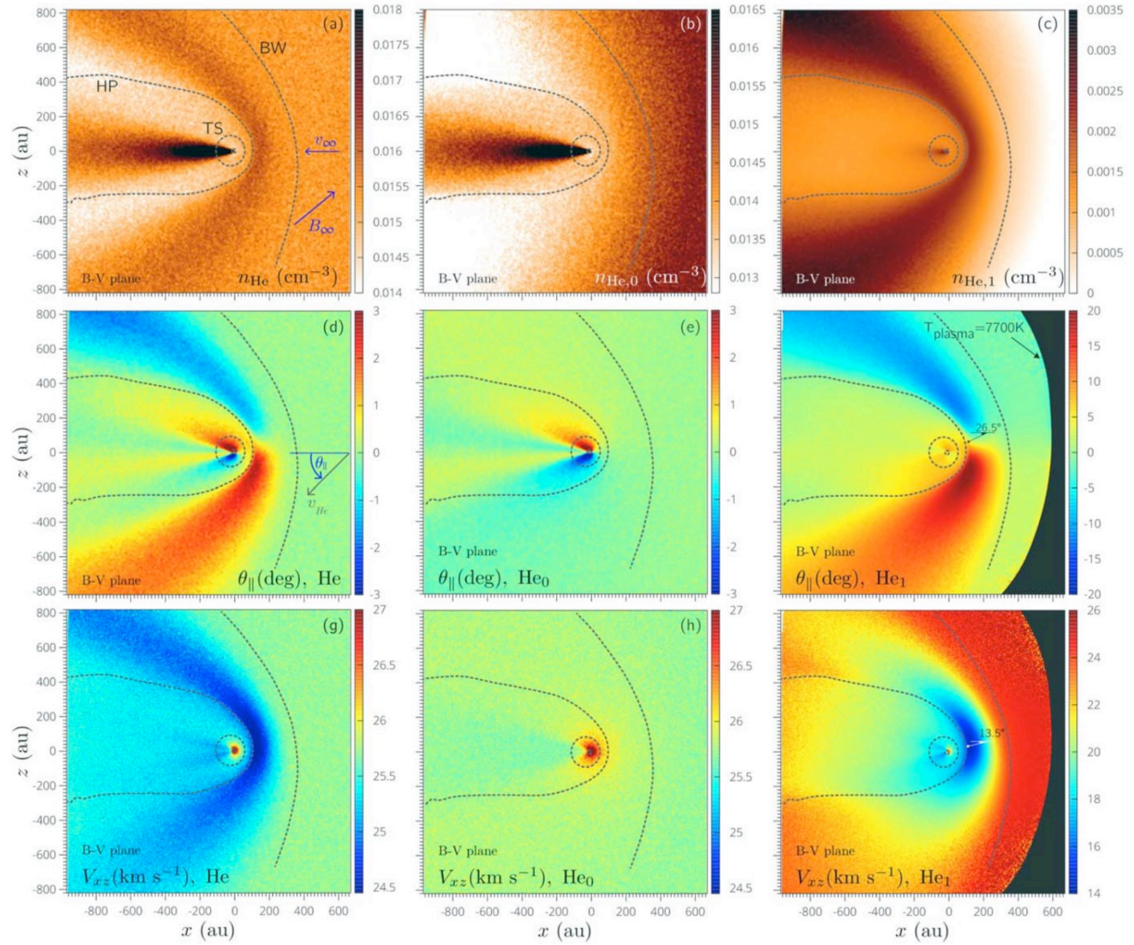


Figure 1. Helium distributions in the B–V plane. From the top to the bottom, the average number density, in-plane deflection, and speed ($V_{xz} = \langle v_x^2 + v_z^2 \rangle$) are shown. From the left to the right, we show the results for the total, pristine, and secondary helium. The orientation of the LISM velocity and ISMF vectors is shown in panel (a). The adopted definition of positive deflection for a generic particle with speed $\mathbf{v}_{He}$ is indicated in panel (d). The distributions are computed using 256^2 bins in the B–V plane, each of them with the thickness of 10 au in the y-direction and $\Delta x = \Delta z = 6$ au.

Why Frontera?

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.

We are solving the MHD equations for thermal ions coupled with two Boltzmann equations for neutral H and He atoms. We additionally solve two reduced systems of equations for PUIs and electrons, and wherever possible, the system describing the transport of turbulence.

Resource-demanding full PIC and hybrid simulations are necessary to describe shock crossings by PUIs and electrons properly.

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.

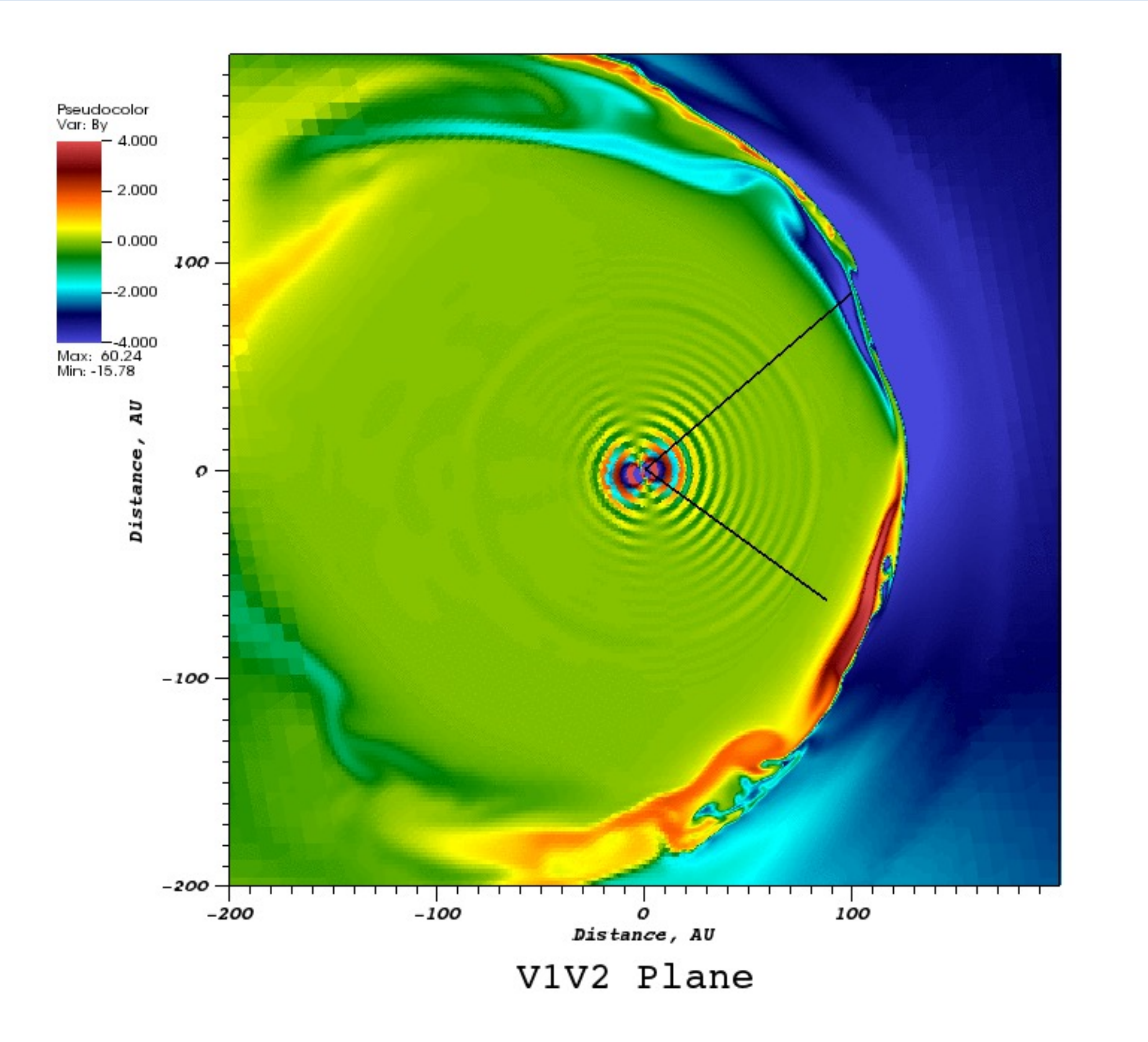
Frontera support

We greatly acknowledge support from all people on the Frontera team, especially John Cazes and Amit Ruhela, who were very instrumental in providing extended support that allowed us to increase the code performance.

Future work with our continuing Frontera allocation

1. **We will perform time-dependent simulations of the SW-LISM interaction using our coupled MHD plasma – kinetic neutrals approach.**
2. **We will continue our full PIC and hybrid simulations of the PUI crossing collisionless shock, especially paying attention to the ion isotropization behind the shock and the role of heavy ions.**
3. **Our simulations will help interpret IBEX, New Horizons, PSP, and Voyager, as well as Tibet air shower experiments.**

Instability of the heliopause and magnetic reconnection in its vicinity



Transverse component of B in the V1-V2 plane.