Simulating the time-dependent global interaction of the solar wind and the LISM with kinetic H and He neutral atoms using MS-FLUKSS

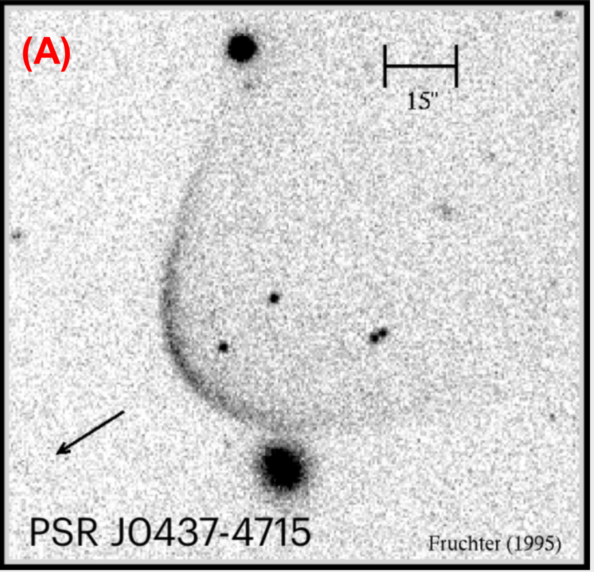
F. Fraternale[1], N. V. Pogorelov[1], V. Roytershteyn[2]

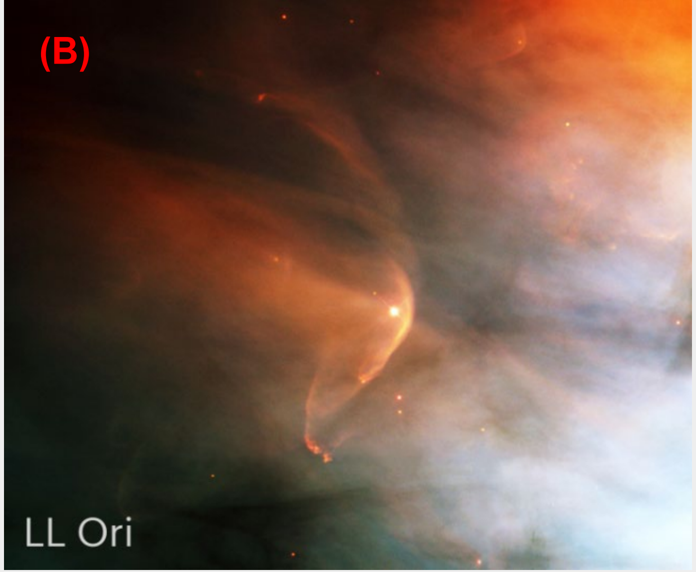
1 The University of Alabama in Huntsville, CSPAR, Huntsville AL, USA
2 Space Science Institute, Boulder CO, USA

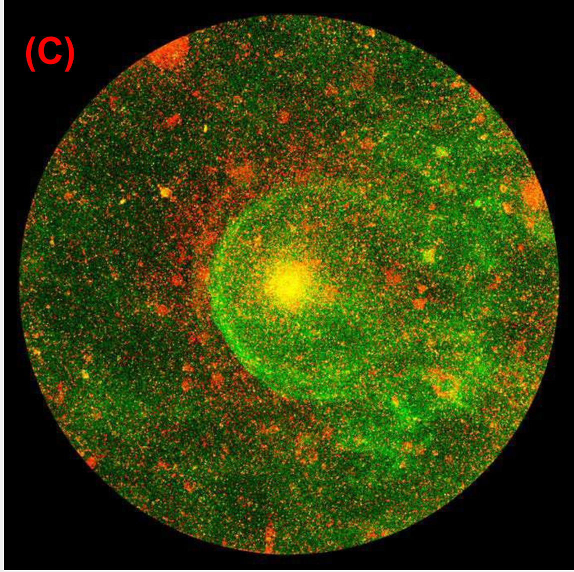
Collaborators: R. K. Bera, T. K. Kim; T. Singh (UAH); M. Gedalin (Ben Gurion U. Israel); P. Colella and B. Van Straalen (LBNL)

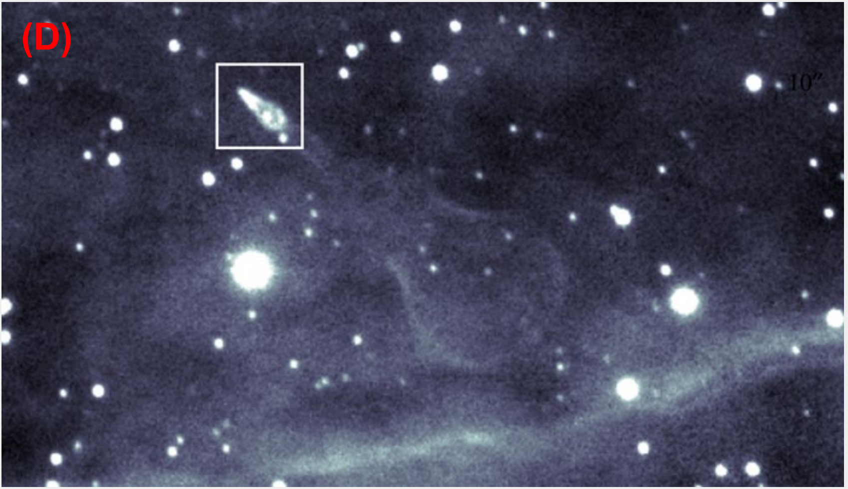
2024 Frontera User Meeting

August 4-6, Austin TX, USA





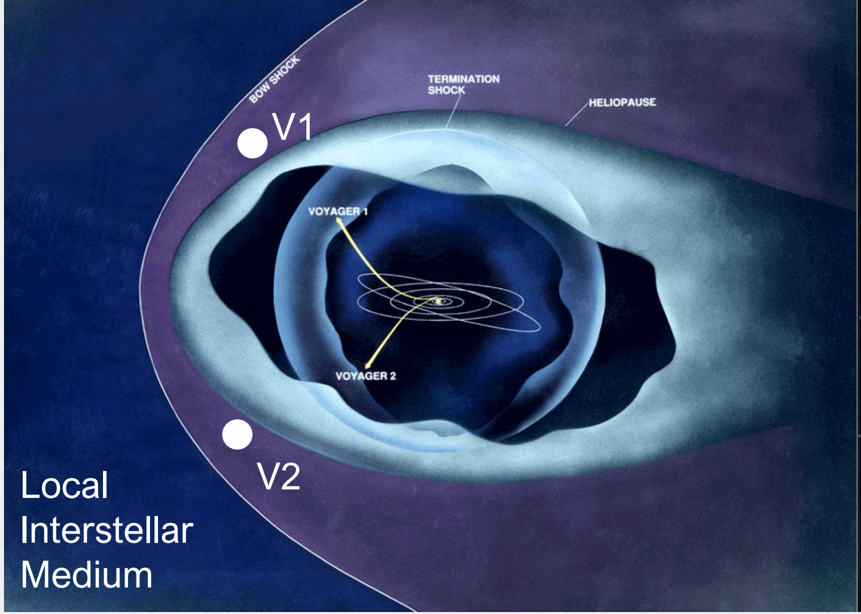


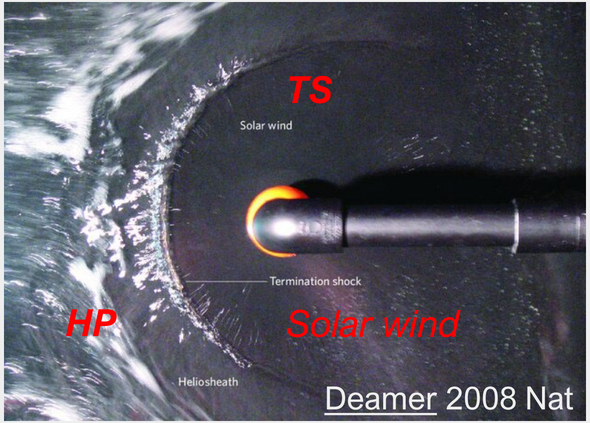


Examples of stellar winds interacting with the interstellar medium

(A) The Guitar nebula, pulsar PSR B2224+65 (from Fruchter 1995).
(B) L-L Orionis interacting with the Orion nebuls (NASA)
(C) Carbon Star IRC+10216 (from Sahai & Chronopoulos, 2010).
(D) The Guitar nebula, pulsar PSR B2224+65 (from Chatterjee & Cordes, 2002).

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

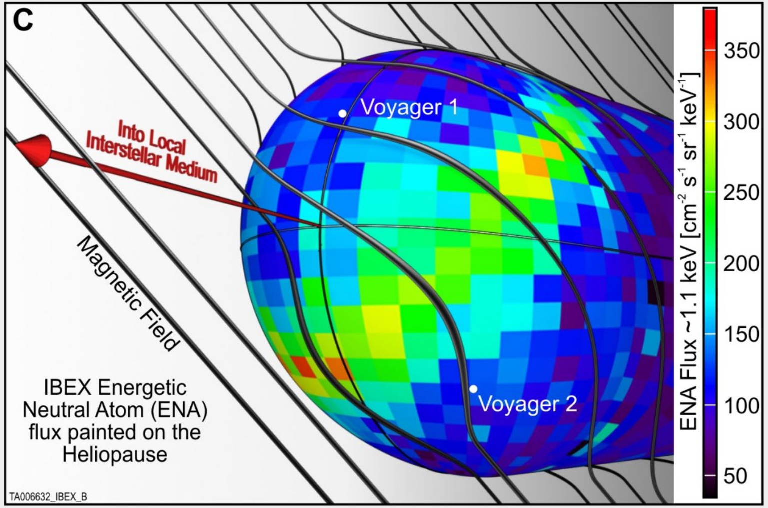




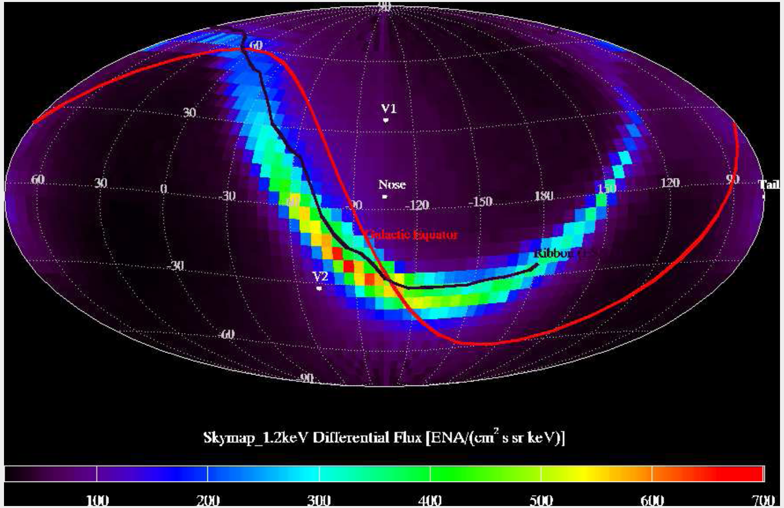
Voyager 1 and *2* *(V1* and *V2),* crossed the heliospheric termination shock *(TS)* in Dec 2004 and in Aug 2007 respectively (Stone et al., 2005, 2008).
After more than 47 years of historic discoveries, both spacecraft crossed the heliopause (HP) entering the LISM region and measures its properties directly. They acquire unique in situ data and 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 1.4×10^{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 D. J. McComas).
Our physical model made 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.



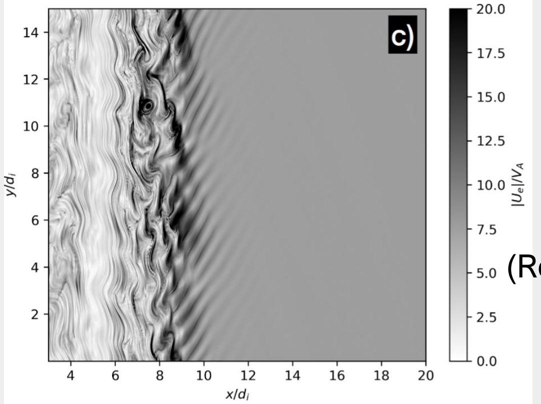
From McComas et al. (2009)



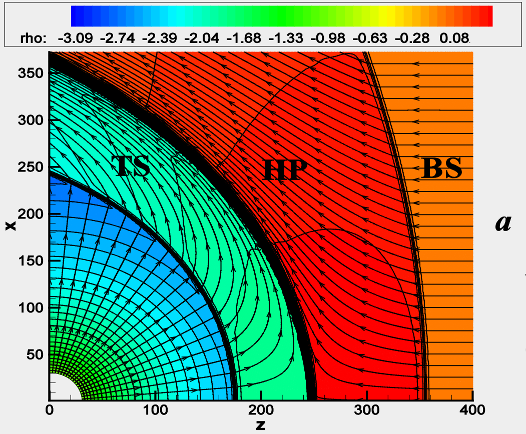
Simulated ENA flux

Project: Multi-scale, MHD-kinetic modeling of the solar wind and its interaction with the local interstellar medium (PI: N.V. Pogorelov)

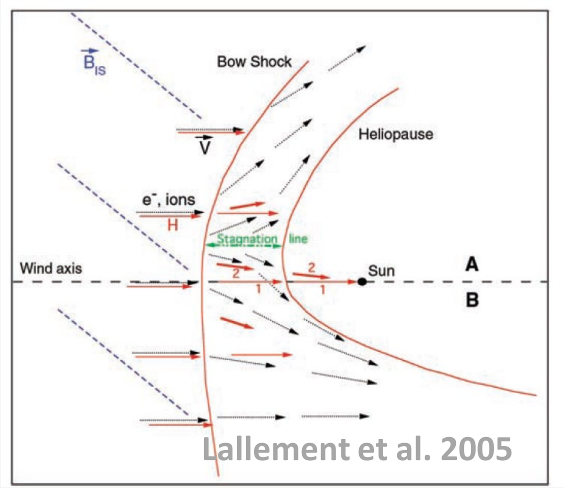
- **Objective 1.** Physical processes involving non-thermal (pickup) ions.
- **Objective 2.** MHD simulations of the solar wind (SW) – Local Interstellar Medium (LISM) interaction with pickup ions (PUIs).
- **Objective 3.** Helium in the heliosphere and the role of electrons (MHD-plasma/Kinetic neutrals models of the SW-LISM interaction

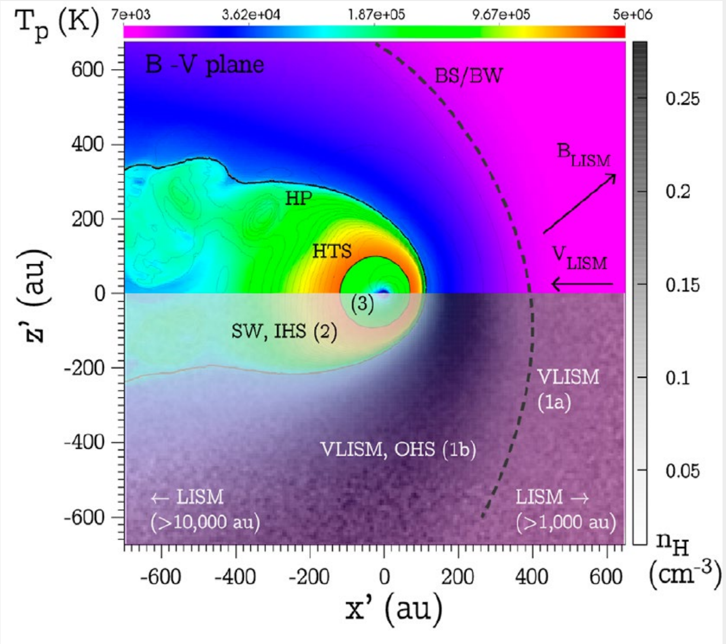


Full PIC sim. (Roytershteyn)



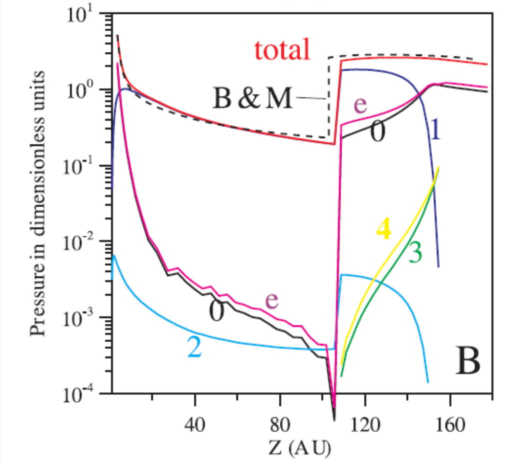
SW-LISM Interaction (Pogorelov)





Global models of the SW-LISM interaction are necessary to infer the properties of the LISM and **support the interpretation of spacecraft observations (e.g., Voyager, New Horizons, IBEX, IMAP).**

We have developed and run on Frontera a new model that incorporates both H and He atoms self-consistently (Fraternale et al ApJL 2021,2023,2024)



ISN and ENA fluxes at 1 au are used as a tool to infer the LISM properties
The mean free path (mfp) for H is ~80-100 au, for He >1000 au. Therefore, neutrals should be modeled kinetically. **Atoms reach Earth with VDFs heavily modified due to the 'filtration' effects.**

Charge exchange is one of the most important ionization processes in the outer heliosphere and VLISM. It creates secondary populations of deflected H and He atoms, and the **H and He 'walls'** in the OHS region of **compressed and heated plasma. It creates PUIs, the energetically dominant plasma component in the outer heliosphere.**

Simulation framework (SW-LISM)

MS-FLUKSS (Pogorelov et al. 2008, 2009, etc)
3D, adaptive mesh refinement (AMR),
- finite volumes (2nd order space and time)
- hybrid parallelized MPI+OpenMP (Borovikov et al., 2013).
- couples the MHD equations for the plasma mixture to the kinetic, or multi-fluid transport models for neutral atoms.

3D MHD-plasma/kinetic-neutrals:
- Boltzmann equation solved via a Monte Carlo method (e.g., Malama, 1991; Heerikhuisen et al., 2006). Statistics are gathered for the ionization source terms instead of solving the 6D Boltzmann equation directly.
- two separate kinetic modules (H and He atoms, respectively).

Latest model update presented in:

The Astrophysical Journal, 946:97 (19pp), 2023 April 1 https://doi.org/10.3847/1538-4357/acba10

The Role of Electrons and Helium Atoms in Global Modeling of the Heliosphere

F. Fraternale[1,3], N. V. Pogorelov[1,2], and R. K. Bera[1]
[1] Center for Space Plasma and Aeronomic Research, The University of Alabama in Huntsville, Huntsville, AL 35899, USA
[2] Department of Space Science, The University of Alabama in Huntsville, Huntsville, AL 35899, USA
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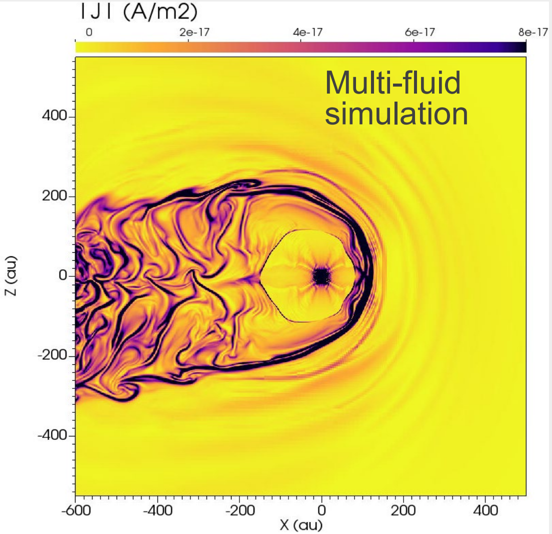
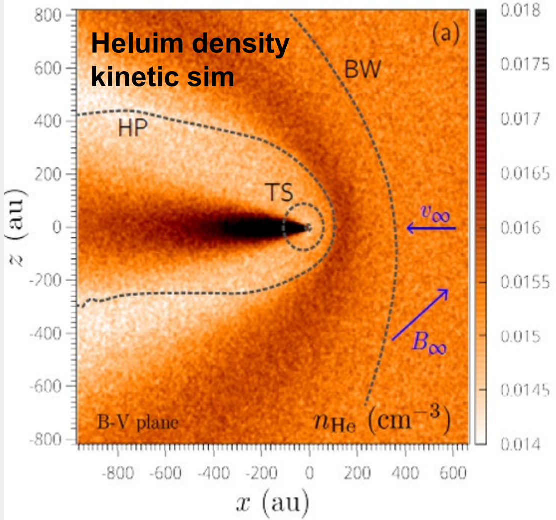
Time-dependent modeling of the SW-LISM interaction with kinetically treated H and He atoms: Should the LISM properties be revised?

Federico Fraternale,[1] Nikolai V. Pogorelov,[2,1] and Ratan Bera[1]
[1] *Center for Space Plasma and Aeronomic Research, University of Alabama in Huntsville, Huntsville, AL 35805, USA*
[2] *Department of Space Science, University of Alabama in Huntsville, Huntsville, AL 35805, USA*





A self-consistent global model with kinetic H and He, and fluid H^+, He, He^+, He^{2+}, e^-

Eqs in conservation-law form for the plasma mixture

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = \sum_s S_s^\rho, \quad (1)$$

ph-i

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + p^* \mathbf{I} - \frac{1}{4\pi}\mathbf{B}\mathbf{B}) = \sum_s \mathbf{S}_s^{\mathrm{m}}, \quad (2)$$

cx+ph-i

$$\partial_t E + \nabla \cdot ((E + p^*)\mathbf{u} - \frac{1}{4\pi}(\mathbf{B}\cdot\mathbf{u})\mathbf{B}) = \sum_s S_s^{\mathrm{E}}, \quad (3)$$

$$\partial_t \mathbf{B} + \nabla \cdot (\mathbf{u}\mathbf{B} - \mathbf{B}\mathbf{u}) = 0 \quad (4)$$

Equations for helium ions

$$\partial_t \rho_{\mathrm{He}^z} + \nabla \cdot (\mathbf{u}\, \rho_{\mathrm{He}^z}) = S^\rho_{\mathrm{He}^z}, \quad (5)$$

$$\partial_t p_{\mathrm{He}^z} + \nabla \cdot (\mathbf{u}\, p_{\mathrm{He}^z}) = (1-\gamma)\, p_{\mathrm{He}^z} \nabla \cdot \mathbf{u} + S^p_{\mathrm{He}^z} + Q^{\mathrm{C}}_{\mathrm{He}^z} \quad (6)$$

cx C-coll

$z = He^{2+}$ In the SW regions

$z = He^{+}$ In the LISM/VLISM

Pressure equation for electrons

ph-i C-coll PUI-turb

$$\partial_t p_{\mathrm{e}} + \nabla \cdot (\mathbf{u}\, p_{\mathrm{e}}) = (1-\gamma)\, p_{\mathrm{e}} \nabla \cdot \mathbf{u} + S_{\mathrm{e}}^{\mathrm{p}} + Q_{\mathrm{e}}^{\mathrm{C}} + Q_{\mathrm{e}}^{\mathrm{W}} \quad (7)$$

Bolzmann eqs: Two kinetic modules (H and He)

$$\frac{\partial}{\partial t} f + \boldsymbol{v}\cdot\nabla f + \frac{\boldsymbol{F}}{M}\cdot\nabla_{\boldsymbol{v}} f = P - L,$$

$$Q_{\varrho,\mathrm{ph}} = M_{\mathrm{n}} \sum_{i=1}^{N_{\mathrm{p}}} W(\boldsymbol{x}-\boldsymbol{x}_i)\alpha_i \beta_{\mathrm{ph},i}$$

$$Q_{\varrho,\mathrm{ex}} = \frac{M_{\mathrm{n}} - M}{n_{\mathrm{p}}} \sum_{i=1}^{N_{\mathrm{p}}} W(\boldsymbol{x}-\boldsymbol{x}_i)\alpha_i \int \beta_{\mathrm{ex},i} f_{\mathrm{p}}(\boldsymbol{v}_{\mathrm{p}}) \mathrm{d}\boldsymbol{v}_{\mathrm{p}}$$

$$\boldsymbol{Q}_{\mathrm{m,ph}} = M_{\mathrm{n}} \sum_{i=1}^{N_{\mathrm{p}}} W(\boldsymbol{x}-\boldsymbol{x}_i)\alpha_i \beta_{\mathrm{ph},i} \boldsymbol{v}_i$$

$$\boldsymbol{Q}_{\mathrm{m,ex}} = \frac{1}{n_{\mathrm{p}}} \sum_{i=1}^{N_{\mathrm{p}}} W(\boldsymbol{x}-\boldsymbol{x}_i)\alpha_i \int \beta_{\mathrm{ex},i} (M_{\mathrm{n}}\boldsymbol{v}_i - M\boldsymbol{v}_{\mathrm{p}}) f_{\mathrm{p}}(\boldsymbol{v}_{\mathrm{p}}) \mathrm{d}\boldsymbol{v}_{\mathrm{p}}$$

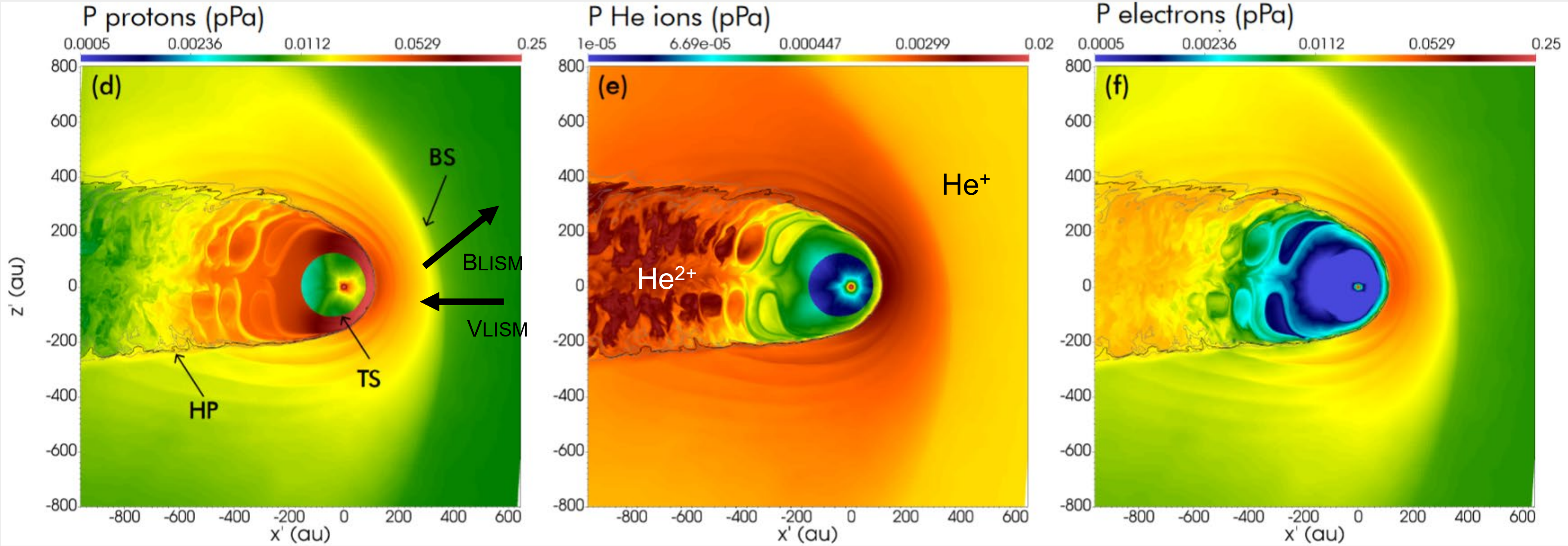
$$Q_{\mathrm{e,ex}} = \frac{1}{n_{\mathrm{p}}} \sum_{i=1}^{N_{\mathrm{p}}} W(\boldsymbol{x}-\boldsymbol{x}_i)\alpha_i \int \beta_{\mathrm{ex},i} \left(\frac{M_{\mathrm{n}} v_i^2 - M v_{\mathrm{p}}^2}{2}\right) f_{\mathrm{p}}(\boldsymbol{v}_{\mathrm{p}}) \mathrm{d}\boldsymbol{v}_{\mathrm{p}}$$

$$\beta(\boldsymbol{x}, \boldsymbol{v}, t) = \int f_{\mathrm{p}}(\boldsymbol{x}, \boldsymbol{v}_{\mathrm{p}}, t) V_{\mathrm{rel,p}} \sigma_{\mathrm{ex}}(V_{\mathrm{rel,p}}) \mathrm{d}^3 \boldsymbol{v}_{\mathrm{p}} + \beta_{\mathrm{ph}},$$

Solved with a Monte Carlo method (Malama 1991)

First solar cycle simulation with kinetic H, He atoms

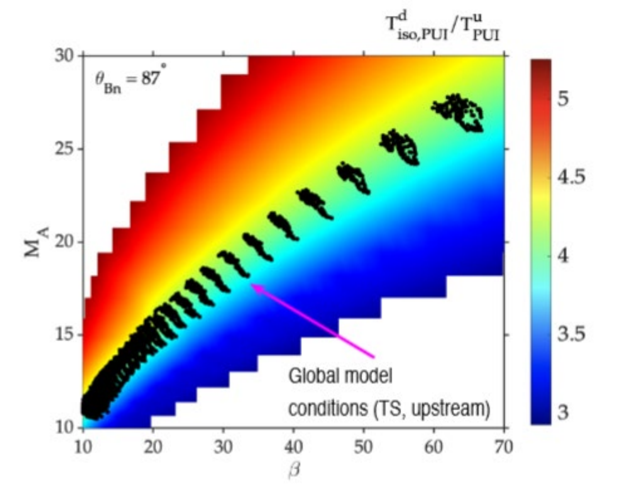
Pressure distributions of (a) protons (thermal+PUIs); (b) helium ions; (c) electrons



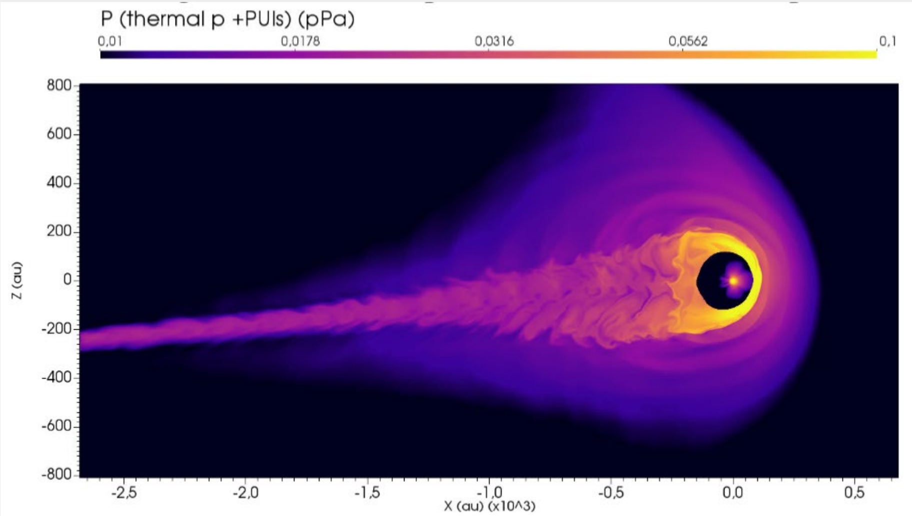
He ions and electrons become significantly heated in the tail.
Our MHD/kinetic simulation suggest that helium ENAs should be able to shed light onto the heliospheric structure, particularly in the heliotail length (e.g., see also Swaczyna+ 2019)

This model will be crucial for the interpretation of IMAP observations

Hybrid PIC solutions (> 50 sim)



Bera et al. ApJ (2023)

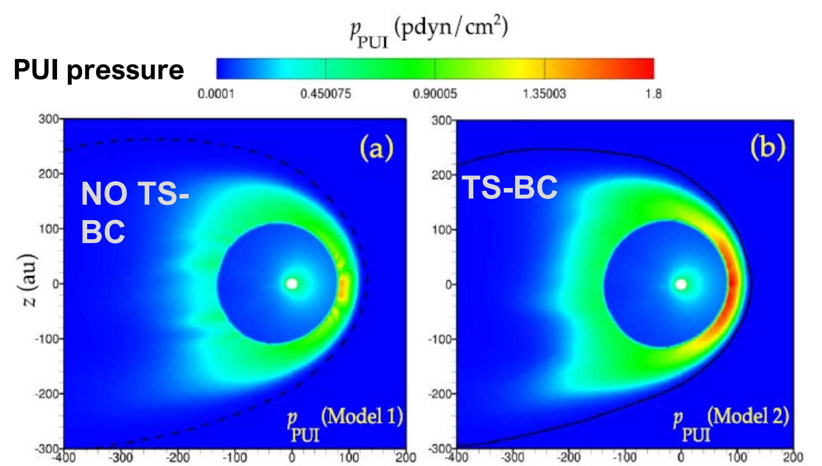


MHD models cannot describe PUI crossing of the shock

We have derived BCs for PUIs based on a set hybrid kinetic simulations

$$T^{d}_{\mathrm{iso,PUI}}/T^{u}_{\mathrm{PUI}} \approx g(M_A,\, \theta_{Bn},\, \beta)$$

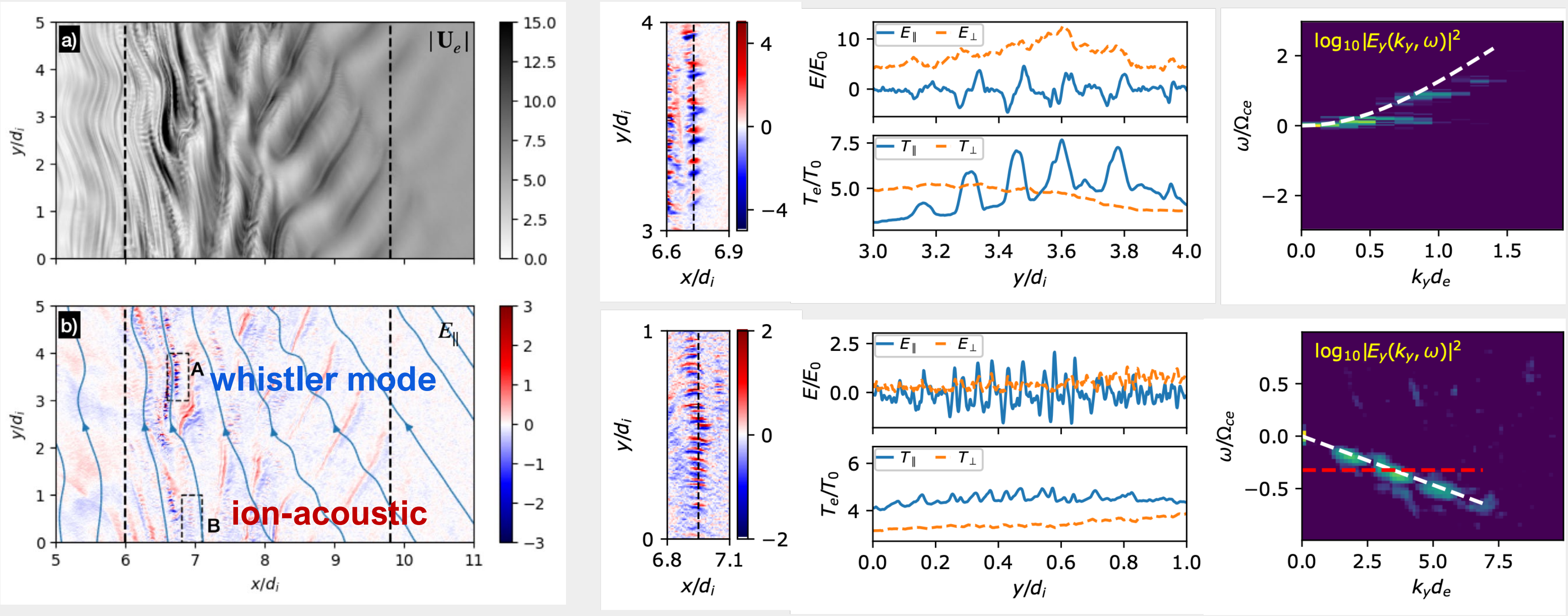
PUI pressure



Key points of Model 2 with b.c.'s at the TS:

- **PUIs become hotter than in Model 1 without TS-BC;**
- **The plasma mixture is slightly cooler due to charge exchange;**
- **The heliosheath becomes more compact (the TS moves outward more than the HP moves inward).**
- **Now extended to Cartesian grids (see top panel)**

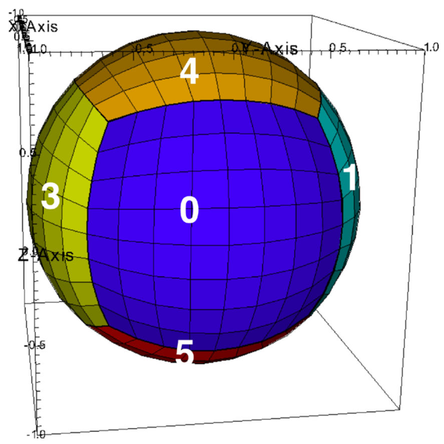
Micro- to macro-scale coupling in collisionless shocks: role of micro-instabilities in shock dynamics

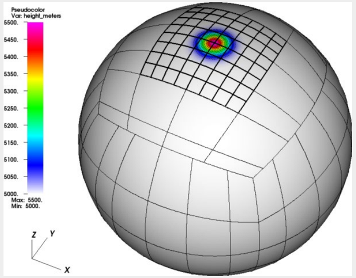


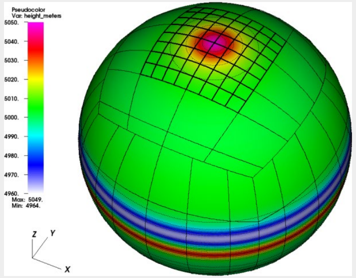
This problem is encountered in all collisionless shocks. We are using Frontera to analyze near-Earth shocks. Typical simulation, VPIC code: 512-768 nodes, MPI + 4 pthreads/rank, HDF5 output, ~200 total hours of wall-time. The simulation shows instabilities developed in a transition region of a collisionless shock with $M_A = 6.5, \theta = 65°$.

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 (‘Lion Roar’). In box B, the dominant mode is an ion-acoustic fluctuation. Solitary structures (electron and ion holes) are also present.

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







Leverage with DOE-funded activities

- Proto developed under Exascale Computing Project.
- AMR / mapped-multiblock development shared with DOE fusion modeling project.

New algorithms

- **4th – order accurate finite-volume method for MHD in spherical geometries that preserves radial solutions.**
- **Mapped-multiblock grids to eliminate pole singularity; extension to block-structured AMR.**
- **High-order coupling to boundary conditions, particularly inner BCs generated by other components of the SWQU system.**

New software framework

- **Structured-grid algorithms for PDE expressed as a composition of high-level abstractions (stencils, pointwise operations applied to data on a rectangle).**
- ***Proto* library provides a highly productive programming environment for such algorithms.**
- **Retargeted implementations of *Proto* provides performance portability across CPU, GPU architectures without needing to change an applications code.**

Software engineering methodology

- **Code verification: unit testing, convergence studies on benchmark problems, integrated into a regression testing framework.**
- **Workflow management for code validation, parameter sweeps for uncertainty quantification.**

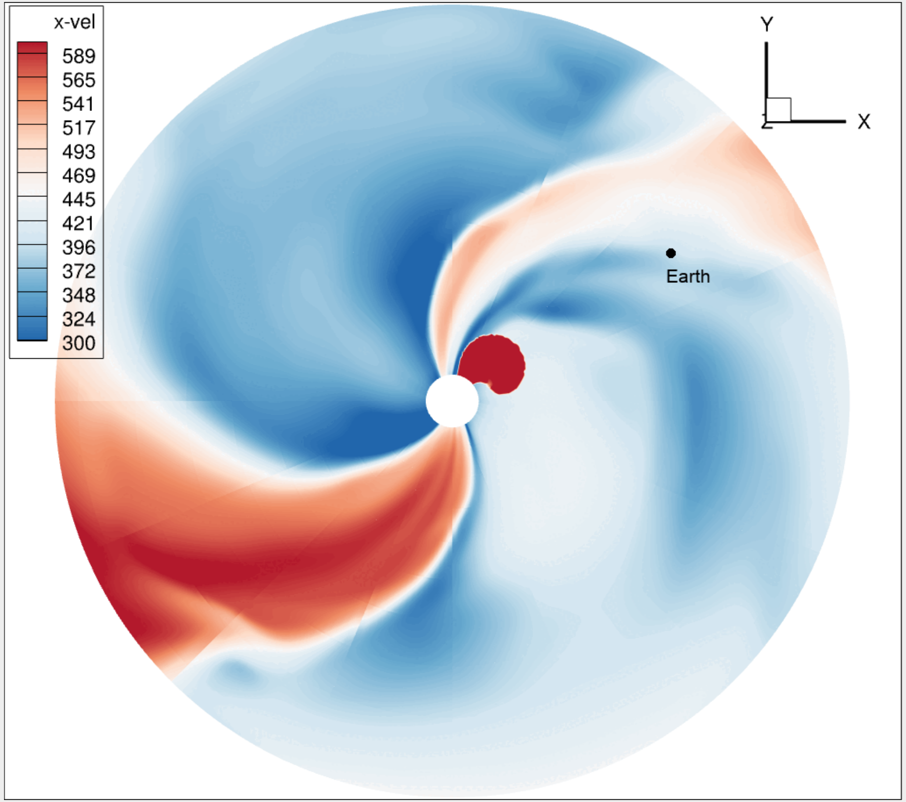
HelioCubed: 4th order finite volume method For MHD

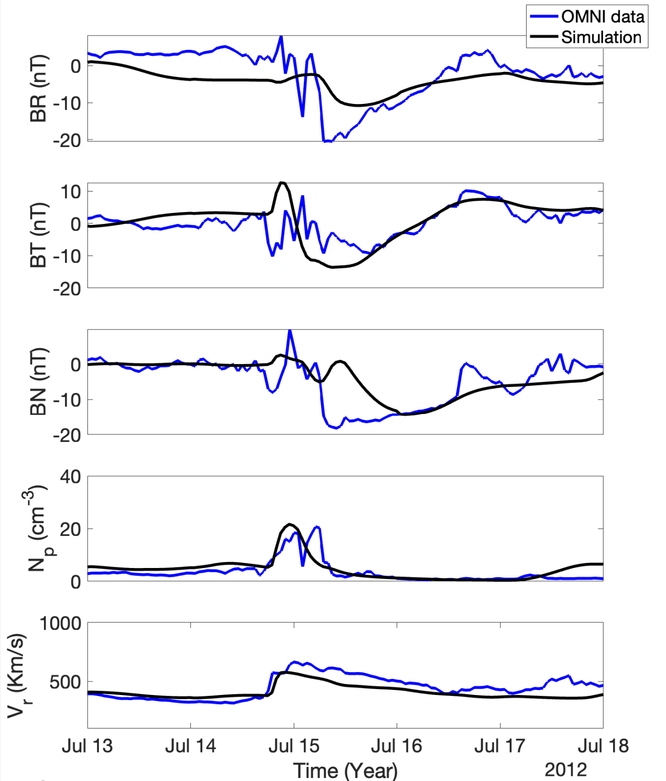
1. We use finite volume method to solve hyperbolic MHD equations in conservative form with 4th order of accuracy in space and time (for non-linear problems!). The formalism is described by Colella et al. (2011) and MacCorquodale & Colella (2011).
2. The average values of primitive variables are calculated on R and L side of the faces with 4th order accuracy and a Reimann problem solver is used to find the 4th order accurate fluxes through these faces.
3. The 4th order accurate RK4 method is used to integrate the equations with time.
4. Limiters specially designed for the 4th order accurate methods are used.
5. We have deployed both CPU and GPU execution of Proto using CUDA on NVIDIA GPU architectures and using HIP on AMD GPU architectures. The CUDA version has been optimized for the NVIDIA Tesla processor (v100) and has also been deployed on the newer Ampere graphics processor (A100).
6. We have also implemented linear and non-linear dissipation methods to suppress oscillations and retain smooth solutions with fourth-order accuracy in space. HDF5 support has been added to Proto. The radial flow will be exactly preserved on mapped grids.
7. We use the WSA predictive metric to objectively rank HelioCubed model predictions when using an ensemble of photospheric magnetic field input maps.

Space Weather applications

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

12 July 2012 CME simulation



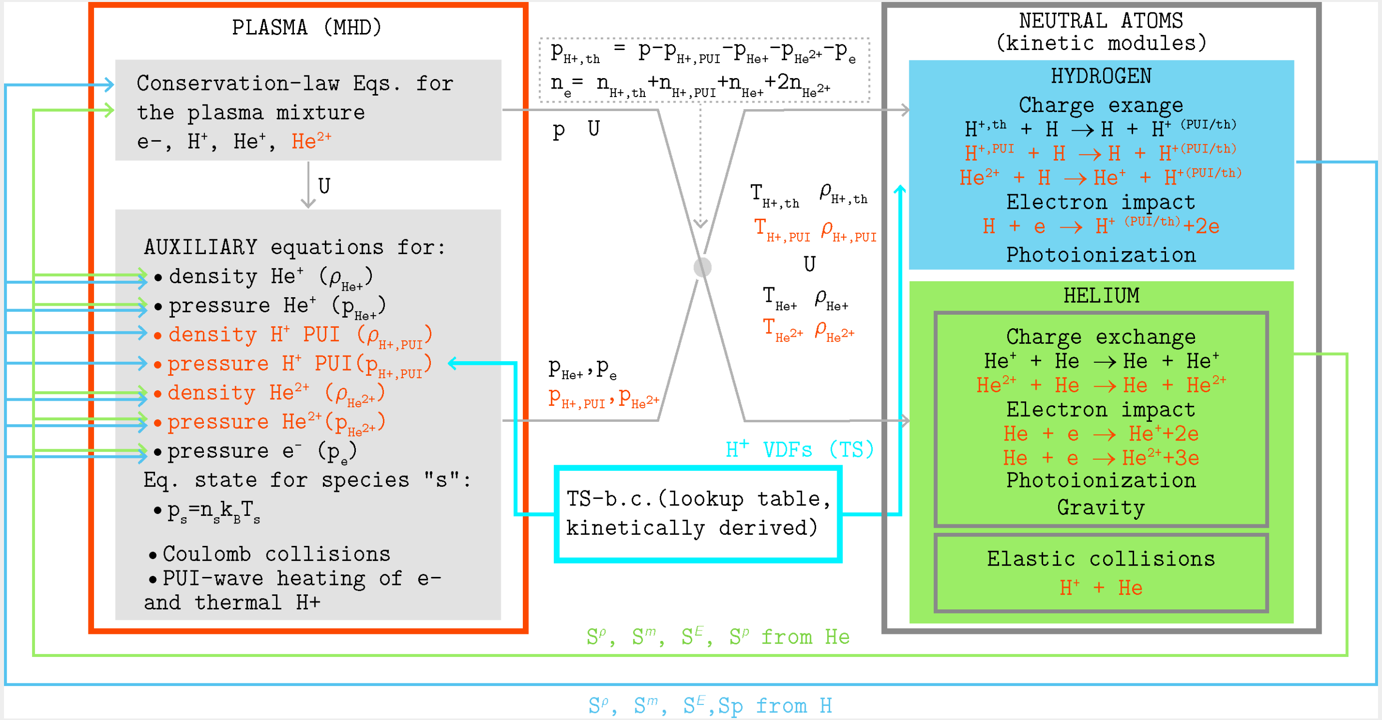


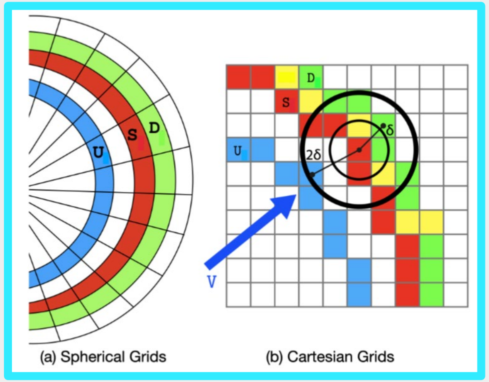
Singh et al 2022

New computational hurdles, and why Frontera?

- Implementation of new equations (PUIs, fluid electrons and helium ions)
- Implementation of kinetically-derived BCs for PUIs at the termination shock in global models (from spherical to Cartesian grids), see Bera et al JPCS, 2024, ApJ 2024 in prep
- Solving the time-dependent MHD/kinetic SW-LISM interaction problem (solar cycle effects) Fraternale et al 2024b (under review) 200k node hours per simulation on (1860^3 AU^3 box – 1.4B cells).
- Running multidimensional (2D) full Particle-In-Cell simulations with realistic electron to proton mass ratio (VPIC code, 37000x10000 cells, 1000 ppc, 1M node hours.)

MS-FLUKSS MHD/Kinetic Model development





Shock BCs for PUIs (lookup table)

AMR (Chombo framework)

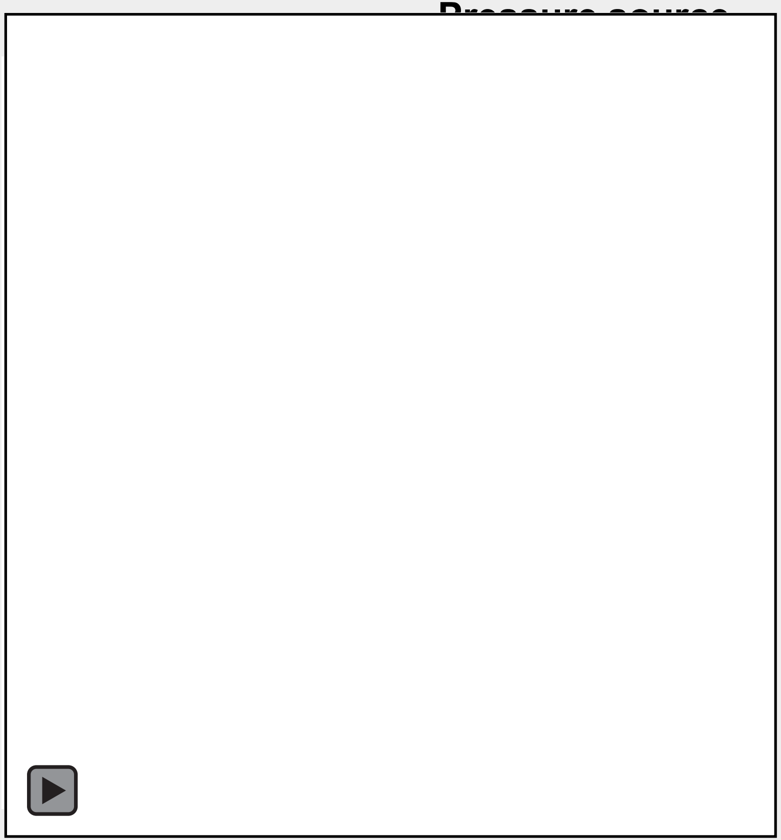
parallel I/O, HDF5 files;

A method for time-dependent MHD/kinetic models

Simulating the time-dependent, non-periodic, scenario with kinetic atoms is challenging

(Izmodenov+ 2005 – periodic solutions, Heerikhuisen+ 2013, Zirnstein+ 2015)

Pressure source



The code runs the **plasma stage** and the **kinetic stage** in an alternating way, reaching convergence iteratively, in a steady-state case. Each stage has its own time interval.

Plasma stage → kinetic source terms are kept fixed

Kinetic stage → plasma is fixed, neutral particles run.

Typical parameters: $\tau_p = 0.3$ yrs, $\tau_N = 700$ yrs

τ_N , τ_p Must be chosen carefully to avoid:

(i) smoothing out gradients or inhomogeneities in the neutral atom distributions (τ_N);

(ii) Spurious, wave-like features (τ_p);

(iii) Excessively impacting the neutral atoms VDFs (τ_N, τ_p);

(iv) Too noisy source terms (τ_N);

We managed to reduce $\tau_N \equiv \tau_p$ to **0.2 yrs**, **while keeping the same statistics for the source terms, see figure**

(Fraternale et al 2024a JPCS; 2024b ApJL – under review)

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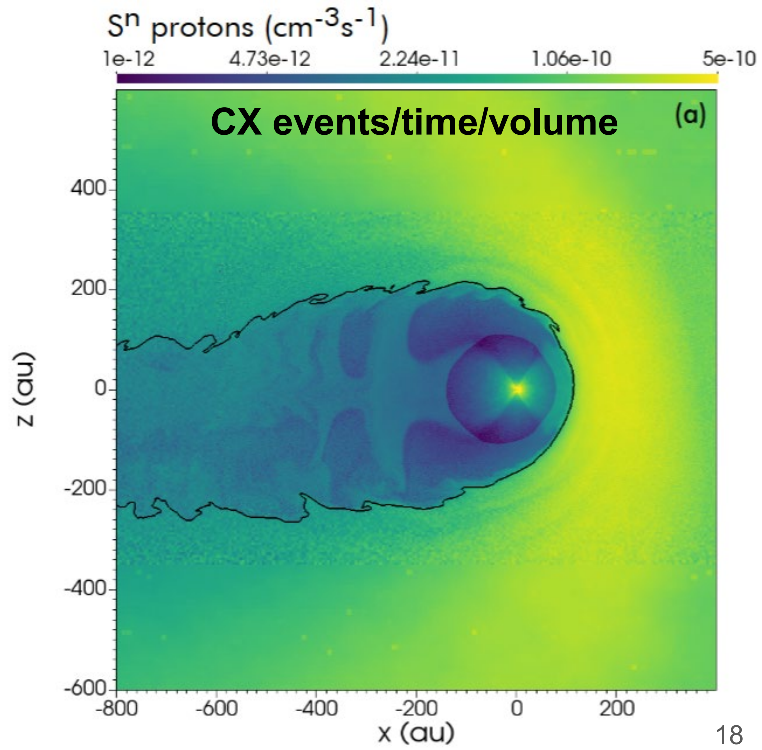


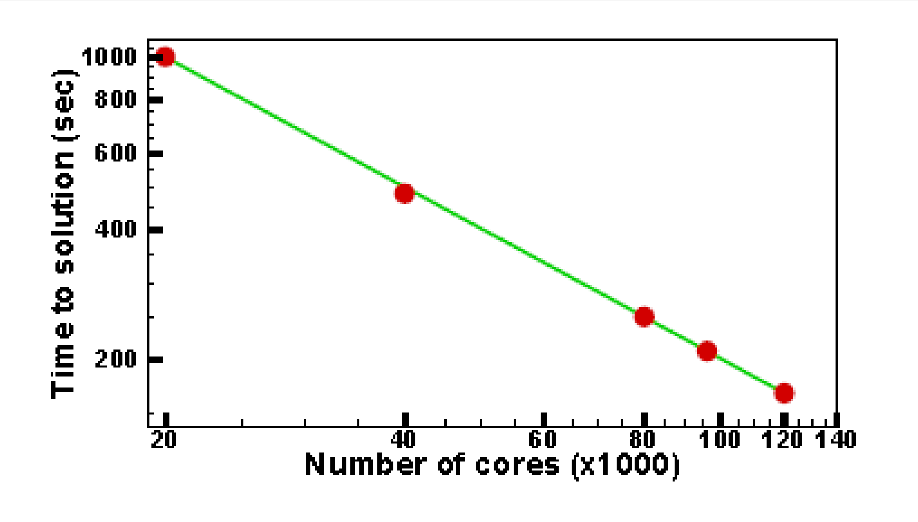
A method for time-dependent MHD/kinetic models

NOTE: each MPI task stores a copy of plasma variables needed by particles --- our memory requirement/task is large

Problem solved: a bottleneck due to *MPI_Bcast* of plasma
We benchmarked msg size and algor. (*I_MPI_ADJUST_BCAST*)

(We acknowledge support by Amit Ruhela)

Now the kinetic module determines >50% of overall code performance! Good from scaling perspective



Frontera with 2560 MPI tasks, 14 Omp threads/task → 640 Nodes, 35840 cpus

$\tau_p = N_p * \Delta t_p$ $\quad \Delta t_p \sim 20\ s$ **wall time**
$N_p \sim 15$ **(0.2 yrs phys time)**
$\tau_N \sim$ **380 s wall time**

(3B macroparticles, 80B virtual, 'split' macroparticles).
(1.4B plasma cells,
~10M cpu hours, 180k SUs, to simulate 500 yrs phys. Time)

Future directions

- MHD/kinetic code: Implementation of additional equations for alpha particles and PUIs in the MHD/kinetic code, ionization processes (cx, electron impact), elastic collisions (reduce the memory requirement – new parallelization strategy?)
- MHD/kinetic code: Implementing data-driven boundary conditions
- Full PIC, 2D simulations of collisionless shocks: investigate whether the electron kinetic effects (ω_{pe}/Ω_{ce} ratio) can affect the energy partition to a degree that would merit modifying previously obtained results (which accounted only for kinetic effects associated with ions)

Recent accomplishments are published in 16 papers; at least 27 presentations have been made

Press releases:

Research scientist's "one-of-a-kind" model of the heliosphere wins $824k NASA heliophysics grant (June 18, 2024 https://www.uah.edu/news/items/research-scientist-s-one-of-a-kind-model-of-the-heliosphere-wins-824k-nasa-heliophysics-grant)

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).

Which Way Does the Solar Wind Blow? (June 3, 2021, https://www.tacc.utexas.edu/-/which-way-does-the-solar-wind-blow-).

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).

Predicting the weather in space (November 29, 2021, https://businessalabama.com/predicting-the-weather-in-space/).

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).
9. Fraternale, F (Principal), Pogorelov, N. (Co-I), Transport of neutral helium and hydrogen throughout the heliosphere, $824,000 (1/1/2024-12/31/2026)