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).

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), SW turbulence, etc. Collisions between atoms and ions in the helio-spheric 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 a kinetic treatment.

3. We need 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?

1. The behavior of plasma and magnetic fields in the vicinity of the heliospheric termination shock (TS) and the heliopause (HP) is of major importance for the interpretation of the puzzling data from the Voyager 1 and 2 spacecraft, which are now the only in situ space mission intended to investigate the boundary of the solar system. 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). Our physical model allowed us to constraint the direction and strength of the interstellar magnetic field (ISMF) in the near vicinity of the global heliosphere.

2. With the realistic boundary conditions in the LISM, we were successful in the explanation of the sunward SW flow at V1 location, penetration of the LISM plasma into the heliosphere, etc. 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.

3. 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.
Why Blue Waters?

To analyze the stability of the heliopause (HP) and investigate the flow in the heliotail, we should perform simulations with the local resolution 5 – 6 orders of magnitude smaller than the size of our typical computational region.
Solar wind interaction with the interstellar medium

Solar wind:
$V_p = 450 \text{ km/s}, \ n_p = 7.4 \text{ cm}^{-3}, \text{ and } T_p = 51100 \text{ K}.~$

LISM:
$V_\infty = 26.4 \text{ km/s}, \ n_\infty = 0.05 - 0.07 \text{ cm}^{-3}, \ T_\infty = 6500 \text{ K}, \ n_{H_\infty} = 0.15 - 0.18 \text{ cm}^{-3}.~$


A 3D model of the nominal solar cycle, including the Sun’s rotation and charge-exchange effects (Pogorelov et al., 2009).
Three-dimensional structure of the heliosphere in the presence of the IMF and ISMF

ISMF draping around the HP and an IMF spiral: ISMF is perpendicular to the LISM velocity vector and parallel to the ecliptic plane

Magnetic pressure exerted perpendicular to the magnetic field direction compresses the heliopause in the north-south direction

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

- Pickup ion transport and turbulence models
- Adaptive mesh refinement and dynamic load balancing (Chombo)
- MHD system with collisional source terms
- \( N \times M \) Euler systems with collisional source terms
- \( N \) Boltzmann equations for different neutral species
- HDF5 files for visualization
Code parallelization

<table>
<thead>
<tr>
<th>Time (sec)</th>
<th>All MPI</th>
<th>2 threads</th>
<th>3 threads</th>
<th>6 threads</th>
<th>12 threads</th>
</tr>
</thead>
<tbody>
<tr>
<td>180</td>
<td>167</td>
<td>170</td>
<td>181</td>
<td>208</td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Number of cores</th>
<th>Time (sec)</th>
<th>Speed up</th>
<th>Ideal</th>
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</thead>
<tbody>
<tr>
<td>20,000</td>
<td>1003</td>
<td></td>
<td></td>
</tr>
<tr>
<td>40,000</td>
<td>484</td>
<td>2.07</td>
<td>2</td>
</tr>
<tr>
<td>80,000</td>
<td>251</td>
<td>1.93</td>
<td>2</td>
</tr>
<tr>
<td>96,000</td>
<td>209</td>
<td>1.20</td>
<td>1.2</td>
</tr>
<tr>
<td>120,000</td>
<td>167</td>
<td>1.25</td>
<td>1.25</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Number of cores</th>
<th>Time (sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20,000</td>
<td>164</td>
</tr>
<tr>
<td>40,000</td>
<td>159</td>
</tr>
<tr>
<td>80,000</td>
<td>168</td>
</tr>
<tr>
<td>96,000</td>
<td>177</td>
</tr>
<tr>
<td>120,000</td>
<td>167</td>
</tr>
</tbody>
</table>

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).
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)?

The first question is somewhat simpler because the magnetic field behavior on the outer side of the HP may be affected by different processes, including those described below. In principle, as seen from our solar cycle simulations (Pogorelov et al. 2009, 2012, 2013), magnetic field elevation and azimuthal angles behind the HP are varying near the average values of 25° and 190°, respectively, which agrees with Burlaga & Ness (2014).

Another possibility based on an analogy with magnetic flux transfer events in the Earth magnetosphere was proposed by Schwadron & McComas (2013).
Interaction of the periodic SW with the LISM: Negative radial velocity component and the absence of the latitudinal flow

Slow SW

\[ n_E = 8 \, \text{cm}^{-3} \]
\[ V_E = 400 \, \text{km/s} \]
\[ T_E = 10^5 \, \text{K} \]

Fast SW

\[ n_E = 3.6 \, \text{cm}^{-3} \]
\[ V_E = 800 \, \text{km/s} \]
\[ T_E = 2.6 \times 10^5 \, \text{K} \]

SW parameters are taken from McComas et al. (2000) as the median values for the fast and slow winds. The latitudinal extent of the slow SW changes periodically over 11 years from ± 35º at the solar minimum to ± 80º at the solar maximum. The tilt of the Sun’s magnetic axis to its rotation axis changes from 9º at the solar minimum to 80º at the solar maximum. The IMF polarity changes to the opposite every 11 years at the maximum.

LISM: \( n_\infty = 0.05 \, \text{cm}^{-3} \), \( V_\infty = 26.4 \, \text{km/s} \), \( T_\infty = 6527 \, \text{K} \), \( B_\infty = 3 \, \mu\text{G} \), \( n_{H_\infty} = 0.15 \, \text{cm}^{-3} \)

\( B_\infty \) belongs to the RL plane directed at 30º to \( V_\infty \), which is at 5º to the ecliptic plane.
Solar Cycle Model Based on Ulysses Observations
The tilt between the magnetic and rotation axes is taken from WSO data

Evolution of the radial velocity component in the meridional plane (Pogorelov et al 2013).
Evolution of the magnetic field magnitude in the meridional plane
Instability of the heliopause as an explanation of the “early” penetration of Voyager 1 into the interstellar medium

1) Kelvin-Helmholtz instability due to the flow shear.

2) Rayleigh-Taylor instability was suggested by Fahr et al., who blamed on the HP acceleration due to solar cycle.

3) The role of charge exchange was emphasized by Liewer et al. (1996) and Zank et al. (1999). Axially symmetric studies were performed by Florinski et al. (2005) and Borovikov et al. (2008). However, these are not applicable in 3D, so we performed 3D simulations with space resolution that resulted in the RT unstable HP in axially symmetric formulations.
Heliopause Instability May Strongly Affect Its Shape and the Distribution of Quantities in its Vicinity

Mixing of the SW and LISM plasma due to instability (from Borovikov et al. (2008)).
Heliospheric current sheet

Figure 5: The HCS shape in the plane formed by the V1 and V2 trajectories.

From Borovikov et al. (2011), also on the cover of the 2010 Voyager Senior Review Proposal.
Evolution of the heliospheric magnetic field in the inner heliosheath
Interaction of the periodic SW with the LISM: Instabilities

Parameters for SW-LISM interaction models:

(a) Solar wind at 1AU:
- \(n_p = 7.4 \text{ cm}^{-3}\)
- \(T = 51100 \text{ K}\)
- \(|u| = 450 \text{ km/s} \quad B_r = 35 \mu\text{G} \text{ or } 0 \mu\text{G}\)
(b) The same as (a), but no HMF
(c) The same as (a), but no ISMF
(d) Solar cycle model

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Slow SW</th>
<th>Fast SW</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number density, (n_e), cm(^{-3})</td>
<td>6.9</td>
<td>2.4</td>
</tr>
<tr>
<td>Radial velocity component, (V_r), km s(^{-1})</td>
<td>450</td>
<td>762</td>
</tr>
<tr>
<td>Temperature, (T), K</td>
<td>68000</td>
<td>245000</td>
</tr>
<tr>
<td>Radial component of the HMF, (B_R), nT</td>
<td>3.5</td>
<td>3.5</td>
</tr>
</tbody>
</table>

*Local Interstellar Medium at 1AU:*
- \(n_p = 0.08 \text{ cm}^{-3}\)
- \(T = 6200 \text{ K}\)
- \(|u| = 23.2 \text{ km/s} \quad B_\infty = 3 \mu\text{G} \quad n_H = 0.21 \text{ cm}^{-3}\)
- He direction: \(\lambda = 79^\circ, \beta = 4.9^\circ\)
- IMF direction: \(\lambda = 255^\circ, \beta = 44^\circ\)

The simulations are performed using a 4-fluid model (one plasma fluid and three neutral atom populations) implemented in Multi-Scale Fluid-Kinetic Simulation Suite (MS-FLUKSS). We use adaptive mesh refinement technique to achieve the resolution of about 0.4 AU in the vicinity of the heliopause.
(Right) The frontal view of the unstable HP and (left) the plasma density distribution in the meridional plane: no HMF (Borovikov & Pogorelov, 2014).
(Right) The frontal view of the HP and (left) the plasma density distribution in the meridional plane: no ISMF (Borovikov & Pogorelov, 2014).
(Right) The frontal view of the HP and (left) the plasma density distribution in the meridional plane: HMF and ISMF (0.3 nT) (Borovikov & Pogorelov, 2014).
(Right) The frontal view of the HP and (left) the plasma density distribution in the meridional plane: solar cycle (Borovikov & Pogorelov, 2014).
Voyager 1 positions with a two-year interval
Mira’s Astrotail

Observed by the Galaxy Evolution Explorer

Martin et al., 2007 Nature

Tail size is \( \sim 800,000 \text{ AU} \)
Carbon Star IRC+10216

Observed by the Galaxy Evolution Explorer

(a) Bow Shock
(b) Astropause Astrotail
Interstellar Magnetic Field Lines

The heliopause and the equatorial plane as seen from the LISM perspective. 

Movie
Magnetic Field Lines
Instabilities of the heliopause tail
Magnetic field in the heliotail
Conclusions

• The Parker spiral deteriorates at distances 800-1000 AU from the Sun creating instabilities in solar wind plasma
• Charge exchange with the neutral atoms results in the tail pressure decrease, so the heliopause is squeezed by the ISMF
• This mechanism may explain some IBEX tail observations
• The plasma flow becomes superfast magnetosonic again at distances greater than 4200 AU
• The size of the heliosphere may be around 20,000 AU
Final Conclusions

1. Observational boundary conditions are necessary to model heliospheric flows realistically.

2. We showed that a number of observational results, can be reproduced by time-dependent numerical simulations.

3. MS-FLUKSS is a suite of codes capable of solving multi-scale, fluid- and kinetic, flows of the SW plasma. The suite is very friendly regarding the format of input boundary conditions, extracts data along major spacecraft trajectories in the process of numerical simulations, and ensures strict satisfaction of the conservation laws, which is crucial for obtaining correct shock propagation velocity and strength.
Energetic charged particle transverse streaming anisotropy data can be explained by multiple crossing of the termination shock by IMF lines (Jokipii et al, 2004). The possibility of such crossings was discussed by Zank (1999). Here we show one of the calculated IMF lines that crosses the termination shock approximately at the Voyager 1 location.
Evolution of the toroidal component of the magnetic field vector in the meridional plane

Pogorelov et al. (2009).
Shock-wave interaction with a dense cloud (Dai & Woodward 1998).

$$W^L = \begin{bmatrix} 3.86859 \\ 0.0 \\ 0.0 \\ 0.0 \\ 167.345 \\ 0.0 \\ 7.73718 \\ -7.73718 \end{bmatrix}, \quad W^R = \begin{bmatrix} 1.0 \\ -11.2536 \\ 0.0 \\ 0.0 \\ 0.0 \\ 1.0 \\ 2.0 \\ 2.0 \end{bmatrix}.$$

$$x_{SW} = 0.6, \quad x_{cl} = 0.8, \quad y_{cl} = 0.5, \quad r_{cl} = 0.15, \quad \rho_{cl} = 10\rho^R, \quad t_{end} = 0.06, \quad \gamma = 5/3.$$