FINAL REPORT
ON COLLABORATIVE DOE GRANTS DE-SC0008334 and DE-SC0008721

Collaborative Research: A Model of Partially Ionized Plasma Flows with Kinetic Treatment of Neutral Atoms and Nonthermal Ions

Period of Performance: 08.01.2012–07.31.2016

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1 Executive Summary

Interactions of flows of partially ionized, magnetized plasma are frequently accompanied by the presence of both thermal and non-thermal (pickup) ion components. Such interactions cannot be modeled using traditional MHD equations and require more advanced approaches to treat them. If a nonthermal component of ions is formed due to charge exchange and collisions between the thermal (core) ions and neutrals, it experiences the action of magnetic field, its distribution function is isotropized, and it soon acquires the velocity of the ambient plasma without being thermodynamically equilibrated. This situation, e. g., takes place in the outer heliosphere - the part of interstellar space beyond the solar system whose properties are determined by the solar wind interaction with the local interstellar medium. This is also possible in laboratory, at million degrees and above, when plasma is conducting electricity far too well, which makes Ohmic heating ineffective. To attain the target temperatures one needs additional heating eventually playing a dominant role. Among such sources is a so-called neutral particle beam heating. This is a wide-spread technique (Joint European Torus and International Thermonuclear Experimental Reactor experiments) based on the injection of powerful beams of neutral atoms into ohmically preheated plasma. In this project we have investigated the energy and density separation between the thermal and nonthermal components in the solar wind and interstellar plasmas. A new model has been developed in which we solve the ideal MHD equations for mixture of all ions and the kinetic Boltzmann equation to describe the transport of neutral atoms. As a separate capability, we can treat the flow of neutral atoms in a multi-component fashion, where neutral atoms born in each thermodynamically distinct regions are governed by the Euler gas dynamic equations. We also describe the behavior of pickup ions either kinetically, using the Fokker–Planck equation, or as a separate fluid. Our numerical simulations have demonstrated that pickup ions play a major role in the interaction of the solar wind and (partially ionized) interstellar medium plasmas. Our teams have investigated the stability of the surface (the heliopause) that separates the solar wind from the local interstellar medium, the transport of galactic cosmic rays, the properties of the heliotail flow, and modifications to the bow wave in front of the heliopause due to charge exchange between the neutral H atoms born in the solar wind and interstellar ions. Modeling results have been validated against observational data, such as obtained by the Interstellar Boundary Explorer (IBEX), and made it possible to shed light on the structure of energetic neutral atom maps created by this spacecraft.. We have also demonstrated that charge-exchange modulated heliosphere is a source of anisotropy of the multi-TeV cosmic ray flux observed in a number of Earth-bound air shower experiments.

Newly developed codes are implemented within a Multi-Scale Fluid-Kinetic Simulation Suite (MS-FLUKSS), a publicly available code being developed by our team for over 12 years. MS-FLUKSS scales well up to 160,000 computing cores and has been ported on major supercomputers in the country. Efficient parallelization and data choreography in the continuum simulation modules are provided by Chombo, an adaptive mesh refinement framework managed by Phillip Colella's team at LBNL. We have implemented in-house, hybrid (MPI+OpenMP) parallelization of the kinetic modules that solve the Boltzmann equation with a Monte Carlo method. Currently, the kinetic modules are being rewritten to take advantage of the modern CPU-GPU supercomputer architecture.

The scope of the project allowed us to enhance plasma research and education in such broad, multidisciplinary field as physics of partially ionized plasma and its application to space physics and fusion science. Besides the impact on the modeling of complex physical systems, our approach to computational resource management for complex codes utilizing multiple algorithm technologies appears to be a major advance on current approaches. The development of sophisticated resource management will be essential for all future modeling efforts that incorporate a diversity of scales and physical processes. Our effort provided leadership in promoting computational science and plasma physics within the UAH and FIT campuses and, through the training of a broad spectrum of scientists and engineers, foster new technologies across the country.

2 Project Accomplishments

The project accomplishments are in agreement with the proposed work plan.

1. We have developed a model of the interaction of two streams of partially ionized plasma, which is characterized by the presence of both thermal and hot, non-thermal ion components. The latter component consists of the so-called pickup ions (PUIs). As planned, the particular physical object of investigation was the solar wind (SW) interaction with the local interstellar medium (LISM). We have implemented numerical solution of the Fokker–Planck equation in the supersonic SW region ahead of the heliospheric termination shock. As PUIs can generate magnetic turbulence that dominates the SW turbulence and affects particle transport in the outer heliosphere at distances over 10 AU, we treated the transport/acceleration of PUI and generation of turbulence in a self-consistent manner. The results were compared with simulations using well-known "engineering" turbulence models, basically based on the additional solutions of 3–5 more equations describing the turbulence properties. Simulations based on both self-consistent and semi-empirical models have been performed using data-driven boundary conditions imposed on a sphere surrounding the Sun beyond the critical surface where the radial velocity exceeds the fast magnetosonic velocity.

2. We have also performed simulations based on a kinetic treatment of PUIs in the inner helisheath (IHS) – the plasma layer between the TS and the boundary of the SW boundary (the heliopause, HP). This was done assuming that PUIs are co-moving with the core SW plasma. However, instead of solving the kinetic equation for an anisotropic distribution function of PUIs at different points of the TS for different angles between the IMF vector and the shock normal, we have derived boundary conditions for PUIs at the TS. Such boundary conditions are entirely kinetic and take into account ion reflection and acceleration. This allowed us to solve the Fokker–Planck equation assuming the distribution function to be isotropic, although not Maxwellian. As an alternative approach, we also used *Voyager* observational data at the TS. These results are in the final stage of preparation for publication.

3. In addition to the kinetic model for PUIs, we have implemented a simpler approach, where PUIs are treated as a separate fluid. This approach is also based on the co-movement assumption, which is well justified by existing kinetic analyses, so we additionally solve a continuity equation and a pressure equations for PUIs, which supplement our solution of the MHD equations for the ion mixture. This approach should necessarily involve some sort of boundary conditions for PUIs at the TS, and we followed this approach in our modeling. Numerical results obtained with a 2-ion-fluid model are consistent with *Voyager* observations and explain the apparent decrease in the IHS width by the energy withdrawal by charge exchange of the IHS PUIs with the LISM neutral H atoms.

4. We have investigated the effect of PUIs on the energetic neutral atom (ENA) fluxes and in this way revealed the 3-D features of the heliosphere. ENAs are born when either PUIs or hot core ions experience charge exchange with interstellar neutral atoms. Since their energy depends on the place of origin, ENAs bear the imprint of the plasma distribution in different regions of the SW–LISM interaction and help us understand the structure of the heliosphere. Our 2-ion-fluid model is more economical computationally as compared with kinetic model and is especially suitable for time-dependent, data-driven simulations.

5. Using a fully coupled approach, we have modeled the 3-D heliosphere in a formulation that accounts for the presence of the nonthermal component in the plasma distribution. The results are very promising and shed light onto one of the major physical phenomenon that affects the structure of the heliosphere.

6. We have performed an extensive validation of our physical model against observational data (in situ, from ACE, Ulysses, New Horizons, and Voyager, and remote, using ENA fluxes from IBEX). We addressed the physics of the energy exchange between thermal and nonthermal ions and analyzed the particle acceleration as *Voyager* proceeds toward the heliopause. These new results are being finalized and will be submitted for publication in the coming month or two.

7. In addition to the planned activity, we have analyzed the importance of charge exchange and magnetic fields on the shape and structure of the heliotail and the so-called bow wave in front of the heliopause. Such bow wave exists in the LISM plasma and may include a subshock, the existence of which is strongly dependent on charge exchange between the LISM ions and secondary neutral atoms born in the SW and propagating outward into the LISM. It has been demonstrated that the modifications to the LISM due to the presence of the heliosphere may be an explanation of the multi-TeV cosmic ray anisotropy observed in air shower observations at Tibet, Milagro, Super-Kamiokande, IceCube/EAS-Top, and ARGO-YGB observatories. We have analyzed also the effect of charge exchange on the heliopause stability and transport of galactic cosmic rays.

8. We have disseminated our results in publications and presentations for the astrophysics, space physics, and plasma physics communities. As was planned, PI Pogorelov organized a special mini-symposium at the APS DPP meeting in New Orleans, where simulations challenges and numerical approaches were shared between the space physics and fusion science teams.

3 Projects Activities

1. Over the course of this project, we developed a new plasma model with two populations of ions and neutral atoms. The first population of ions is thermal, whereas the second one (hot pickup ions, PUIs) is not in thermal equilibrium. This situation is ubiquitous in space and laboratory plasmas in the presence of charge exchange between ions and neutral atoms. To satisfy the conservation laws at discontinuities, we solve the equations for the mixture of charged particles (thermal ion, PUIs, and electrons). The thermal ions are described by the MHD equations, whereas PUIs are modeled either kinetically (Gamayunov et al., 2012), by solving a Fokker–Planck (pitch-angle averaged Boltzmann) equation, or assuming a fluid mechanics approach (Kryukov et al., 2012; Pogorelov et al., 2016). The flow of neutral atoms is modeled kinetically, using a Monte Carlo approach. By using the developed kinetic and fluid dynamics approaches, we also investigated the details of the supersonic thermal ion heating due to turbulence generated by an unstable PUI distribution function (see Fig. 1). All new features of the model have been implemented in our Multi-Scale Fluid-Kinetic Simulation Suite (MS-FLUKSS). a publicly available code being developed by our team for over 12 years. MS-FLUKSS scales well up to 160,000 computing cores (Borovikov et al., 2013) and has been ported on major supercomputers in the country. Efficient parallelization and data choreography in the continuum simulation modules are provided by Chombo, an adaptive mesh refinement framework managed by Phillip Colella's team at LBNL. Collaborator Colella led the LBNL effort to develop a fourth-order in space and time methods for solving systems of conservation laws on adaptive, cubed-sphere grids, which was successfully accomplished. We have implemented in-house, hybrid (MPI+OpenMP) parallelization of the kinetic modules that solve the Boltzmann equation with a Monte Carlo method. Currently, the kinetic modules are being rewritten to take advantage of the modern CPU-GPU supercomputer architecture.

2. A self-consistent model of the interstellar pickup protons, the slab component of the Alfvénic turbulence, and core SW protons was developed (Gamayunov, 2013a, 2013b) for distances from the Sun to up to the heliospheric termination shock (TS), where results were compared with the *Voyager 2* (*V*2) observations. Two kinetic equations were used to describe the pickup proton distribution and Alfvénic power spectral density. An additional equation described the SW temperature and included the source term due to

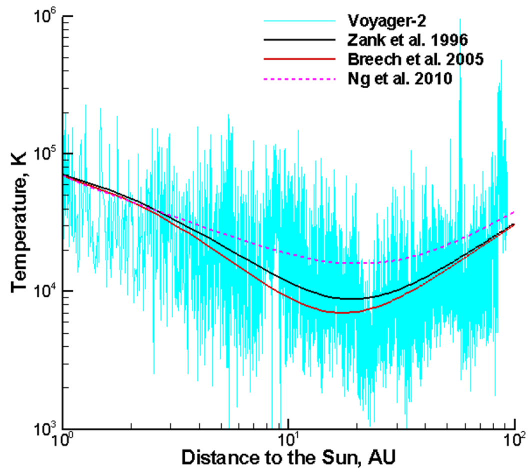

Figure 1: Comparison of the SW temperature measured by $V2$ (blue line) with the MS-FLUKSS simulations using different turbulence models.

the Alfvén wave energy dissipation. A fraction of the pickup proton free energy, which is actually released in the waveform during isotropization, was determined using quasi-linear considerations.

3. We used observational data at 1 AU to specify the strength of the large-scale turbulence driving. It was shown that PUIs generate waves which heat up the core solar wind. The wave energy is pumped into turbulence. Without this pumping, the nonlinear cascade would be suppressed and turbulence at all wavelengths would be much weaker. We used observational data at 1 AU to specify the strength of the large-scale turbulence driving. It was shown that PUIs generate waves which heat up the core solar wind through absorption of wave power at resonant frequencies. The results agree well with the spacecraft observations. We have improved this model by takeing into account ion crossing the TS. The change in the PUI energy spectrum across the TS was approximated using diffusive shock acceleration under the constraints by particle intensity observed by *Voyager* spacecraft. This allowed us to obtain the PUI distribution function along SW streamlines as they approach the heliopause. These results were further used in our iterative model describing the flow of the mixture of thermal and nonthermal ions.

4. A two-ion-population approach has been extended beyond the heliospheric termination shock using the boundary conditions determined by the Voyager observations of the energetic ion spectrum (e.g., Zhang and Schlickeiser, 2012). A more sophisticated treatment of shock acceleration using the focused particle transport equation was also developed (Zuo et al. 2013a). The approach allows us to compute the efficiency of the diffusive shock acceleration, which cannot be achieved using the standard Parker equation. The distributions of PUIs were obtained by numerical solution of the Fokker–Planck equation along the fixed streamlines in the heliosheath (a plasma layer between the TS and the heliopause, HP). The velocity distribution was obtained in an MHD simulation of the ion mixture, which is admissible since PUIs quickly acquire the bulk velocity of the surrounding medium due to the action of the motional electric field.

5. The focused transport theory is appropriate to describe the injection and acceleration of low-energy particles at shocks as an extension of diffusive shock acceleration (DSA). Zuo et al. (2013b) investigated the role of cross-shock potential (CSP) originated in the charge separation across the shock ramp on PUI acceleration at various types of shocks with a focused transport model. The simulation results of energy spectrum and spatial density distribution for the cases with and without CSP added in the model were compared. With sufficient acceleration time, the focused transport acceleration finally falls into the DSA regime with the power-law spectral index equal to the solution of the DSA theory. The CSP can affect the shape

of the spectrum segment at lower energies, but it does not change the spectral index of the final power-law spectrum at high energies. It was found that the CSP controls the injection efficiency which is the fraction of PUIs reaching the DSA regime. A stronger CSP jump resulted in a dramatically improved injection efficiency. Our simulation results also showed that the injection efficiency of PUIs is mass-dependent, which is lower for species with a higher mass. In addition, the CSP is able to enhance the particle reflection upstream to produce a stronger intensity spike at the shock front. We concluded that the CSP is a non-negligible factor that affects the dynamics of PUIs at shocks. With a sizable CSP, it is possible we can effectively injected PUI into the quasi-perpendicular termination shock for acceleration to anomalous cosec ray energies.

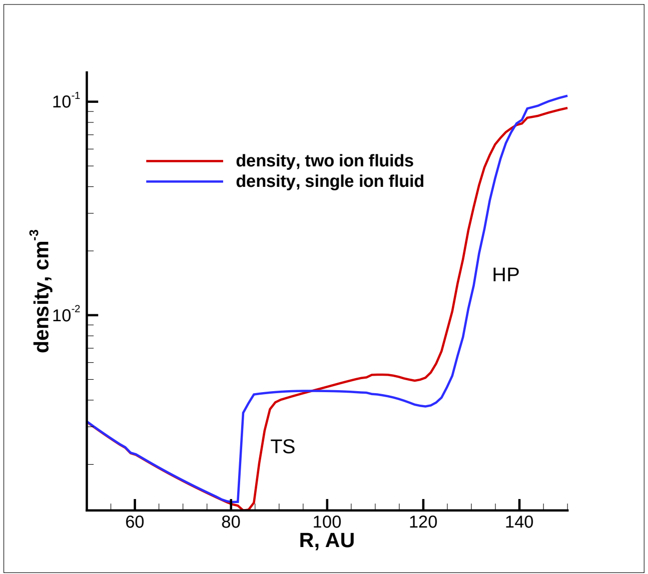

Figure 2: Ion density distributions along the *V1* trajectory shows that the TS moves farther from the Sun while the HP becomes closer to it, if PUIs are treated as a separate plasma component.

6. We extended MS-FLUKSS by adding a solar wind turbulence model (three additional differential equations) and a fluid treatment of pickup ions. This work was started in Kryukov et al. (2012) and continued by our graduate student Matthew Bedford. Numerical results of the time-dependent solar wind modeling with the observational boundary conditions were validated against *V*2 observations in the distant heliospheric region (see Fig. 2). We have also implemented a level-set method to analyze the spatial structure of flow interfaces.

7. We have analyzed (Heerikhuisen et al., 2012, 2013) the behavior of ENAs, which are created when PUIs experience charge exchange with lower-energy interstellar medium atoms. This is important for the validation of our approach since the ENA fluxes in different energy bands are measured by the *Interstellar Boundary Explorer* (*IBEX*). ENAs have properties of the parent PUIs, which makes it possible to investigate the energy spectrum of the latter.

8. We have discovered an interesting phenomenon of transition to chaos in the plasma flow due to magnetic reconnection across the heliospheric current sheet (see Fig. 3. This is of considerable importance for the description of energy transfer in collisionless, partially ionized plasma (Pogorelov et al., 2013).

9. Our MHD-kinetic simulations were used to model the transport of the interstellar dust throughout the heliosphere, which showed a strong potential of comparing dust simulations and observations for the derivation of important knowledge about the properties of the SW–LISM interaction. (Slavin et al., 2012).

10. We investigated a fundamental problem of the shock modulation in plasma due to charge exchange with neutral atoms. This was done both analytically and numerically with our MHD-kinetic code, MS-FLUKSS. Our results show strong changes in the shock strength caused by the charge-exchange induced changes in the plasma quantities upstream and downstream of the shock (Zank et al., 2013).

11. We obtained new results from three-dimensional simulations of the SW–LISM interaction using recent observations by NASA's Interstellar Boundary EXplorer (IBEX) mission estimates of the velocity and temperature of the LISM (Heerikhuisen et al., 2014). We investigated four strengths of the LISM magnetic field, from 1 to 4 μG, and adjusted the LISM proton and hydrogen densities so that the distance to the termination shock (TS) in the directions of the Voyager spacecraft became just below 90 AU, and the density of hydrogen at the TS was close to 0.09 cm-3 in the nose direction. The orientation of the magnetic field was chosen to point toward the center of the ribbon of enhanced ENA flux seen in the IBEX data. Our

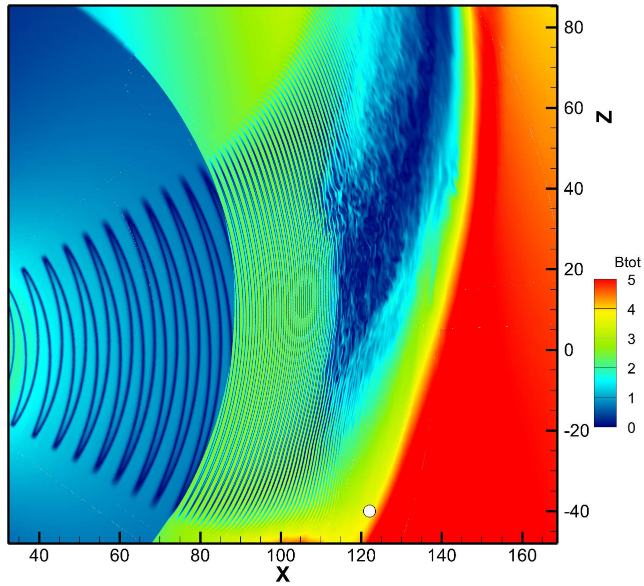

Figure 3: Transition to chaotic behavior in the IHS. Magnetic field strength distribution (in μG) is shown in the meridional plane defined by the Sun's rotation axis and the LISM velocity vector $\mathbf{V}_\infty$. The angle between the Sun's rotation and magnetic axes is 30°.

simulations showed that the plasma and neutral properties in the outer heliosheath vary considerably as a function of the LISM magnetic field strength. We also showed that the heliotail points downwind in all cases, though its structure is strongly affected by the external magnetic field. Comparison and consistency between the simulated ENA flux and the circularity of the ribbon as measured by IBEX turned out to be most consistent with a LISM magnetic field strength aligned with the center of the ribbon and a magnitude in the range 2.5-3 μG. This global simulation allowed us to constraint the LISM properties as boundary conditions for our simulations.

12. PUIs play an integral role in the multi-component nature of the plasma in the interaction between the SW and LISM. Three-dimensional MHD simulations with a kinetic treatment for neutrals and PUIs are currently under development. In light of recent ENA observations by IBEX, Zirnstein et al. (2014) addressed the complex coupling between PUIs across the heliopause (HP) as facilitated by ENAs using estimates of PUI properties extracted from a 3D MHD simulation of the SW-LISM interaction with kinetic neutrals. Firstly, we improved upon the multi-component treatment of the inner heliosheath (IHS) plasma from Zank et al. (2013) by including the extinction of PUIs through charge-exchange. We found that a significant amount of energy is transferred away from hot, termination shock-processed PUIs into a colder, "freshly injected" PUI population. Secondly, we extended the multi-component approach to estimate ENA flux from the outer heliosheath (OHS), formed from charge-exchange between interstellar hydrogen atoms and energetic PUIs. These PUIs are formed from ENAs in the IHS that crossed the HP and experienced charge-exchange. Our estimates, based on plasma-neutral simulations of the SW–LISM interaction and a post-processing analysis of ENAs and PUIs, suggest the majority of flux visible at 1 AU from the front of the heliosphere, between ~ 0.02 and 10 keV, originates from OHS PUIs, indicating strong coupling between the IHS and OHS plasmas through charge-exchange.

13. We also performed 3D simulations of the SW–LISM interaction with solar cycle effects taken into account (Pogorelov et al., 2013; Borovikov & Pogorelov, 2014). These simulations did not treat PUIs as a separate component of the SW plasma, but assumed in a thermodynamic equilibrium with the SW ions preserving the total mass, momentum, and energy of the system. The model based on Ulysses observations

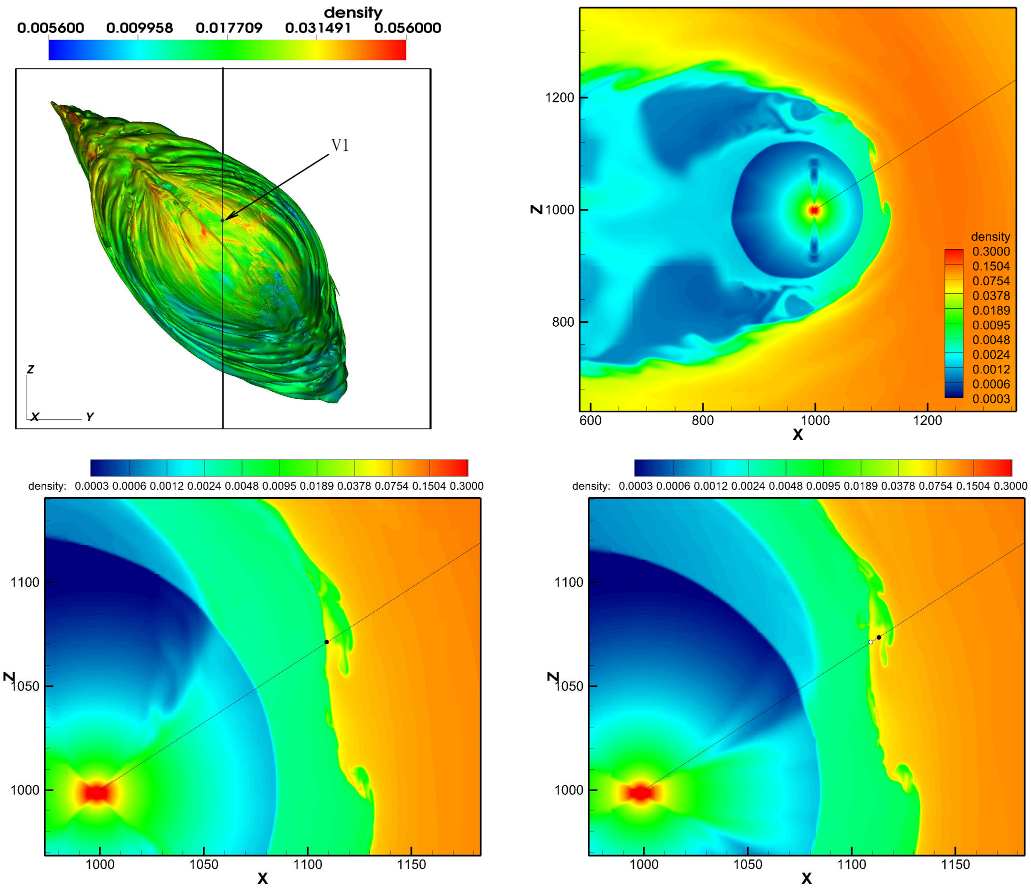

Figure 4: (*Top panel*) The heliopause colored by plasma density values (*left*) and the distribution of plasma density in the meridional plane (right) for model *d*. (*Bottom panel*) A possible scenario of Voyager 1 moving through the instability. Left panel: initial crossing of the HP. Right panel: position of *V1* two years later as the HP evolves.

allowed us to explain the observed time-dependent topology of the termination shock. We also showed that solar cycle effects, and related temporary annihilation of the heliospheric magnetic field near the heliopause (HP) due to turbulence, help destabilize the HP and result in deep penetration of the LISM plasma into the heliosphere, thus explaining Voyager 1 "early" enter into the LISM in 2012 (see Fig. 4). These phenomena are expected to be affected by PUI and therefore require further self-consistent investigation.

14. The results of our simulations have been used by Desai et al. (2014) to compare ENA spectra from the first 3 years of observations by the IBEX-Hi and -Lo ENA imagers along the lines-of-sight (LOSs) from the inner heliosphere through to the locations of Voyager 1 and 2 with results from an updated physics-based model of the three-dimensional heliosphere and its constituent ion populations. Our results showed that (1) IBEX ENA fluxes and spectra above ~ 0.7 keV measured along the LOSs of the Voyagers are consistent with several models in which the parent PUI populations originate in the inner heliosheath, and (2) a significant fraction of lower energy ENAs between ~ 0.1-0.5 keV may originate from interstellar neutral gas charge-exchanging with a non-thermalized (hot) population of PUIs in the outer heliosheath beyond the heliopause. We analyzed the implications of ENAs observed by IBEX originating from distinct parent populations as well as from two distinct locations in the heliospheric interface. These results indicate that ENA spectral measurements at various energies can be used to remotely probe distinct physical processes operating in vastly different regions of the distant heliosphere. They will also be useful for comparison with simulations

that take into account PUIs self-consistently. These results were further extended in Desai et al. (2015).

15. Kucharek et al. (2013) used the results of our simulations to identify yet another possible source of PUIs that create the ENA-flux ribbon observed by IBEX. We proposed that gyrating SW ions and PUIs in the ramp and in the near downstream region of the termination shock (TS) could provide a significant source of ENAs. A fraction of the solar wind and PUIs are reflected and energized during the first contact with the TS. Some of the solar wind can be reflected propagating toward the Sun but most of the solar wind ions form a gyrating beam-like distribution that persists until it is fully thermalized further downstream. Depending on the strength of the shock, these gyrating distributions can exist for many gyration periods until they are scattered/thermalized due to wave-particle interactions at the TS and downstream in the heliosheath. During this time, ENAs can be produced by charge exchange of interstellar neutral atoms with the gyrating ions. With a localized source and such a short integration path, this model would also allow fast time variations of the ENA flux.

16. While the solar wind is mostly ionized material from the corona, the interstellar medium is only partially ionized. The ion and neutral populations are coupled through charge-exchange collisions that operate on length scales of tens to hundreds of astronomical units. About half the interstellar hydrogen flows into the heliosphere where it may charge-exchange with solar wind protons. This process gives rise to a nonthermal proton, known as a pickup ion, which joins the plasma. In this paper we investigate the effects of approximating the total ion distribution of the subsonic solar wind as a generalized Lorentzian, or κ distribution, using an MHD neutral code. We illustrated (Heerikhuisen et al., 2015) the effect different values of the κ parameter have on both the structure of the heliosphere and the energetic neutral atom flux at 1 AU. We found that using a κ distribution in our simulations yields levels of energetic neutral atom flux that are within a factor of about 2 or 3 over the IBEX-Hi range of energies from 0.5 to 6 keV. While the presence of a suprathermal tail in the proton distribution leads to the production of high-energy neutrals, the sharp decline in the charge-exchange cross section around 10 keV mitigates the enhanced transfer of energy from the ions to the neutrals that might otherwise be expected.

17. Since 2009, observations by *IBEX* have vastly improved our understanding of the SW–LISM interaction through direct measurements of ENAs. An enhanced feature of flux in the sky, the so-called IBEX ribbon, was not predicted by any global model before the first IBEX observations. A dominating theory of the origin of the ribbon, although still under debate, is a secondary charge-exchange process involving secondary ENAs originating from outside the heliopause. According to this mechanism, the evolution of the solar cycle should be visible in the ribbon flux. We simulated a fully time-dependent ribbon flux, as well as globally distributed flux from the inner heliosheath (IHS), using time-dependent SW parameters as boundary conditions for our time-dependent heliosphere simulation (Zirnstein et al., 2015; see Fig. 5). After post-processing the results to compute H ENA fluxes, our results showed that the secondary ENA ribbon indeed should be time dependent, evolving with a period of approximately 11 yr, with differences depending on the energy and direction. Our results for the IHS flux show little periodic change with the 11 yr solar cycle, but rather with short-term fluctuations in the background plasma. While the secondary ENA mechanism appears to emulate several key characteristics of the observed IBEX ribbon, it appears that our simulation does not yet include all of the relevant physics that produces the observed ribbon.

18. The intensity of Galactic cosmic rays in the heliosphere is modulated by solar activities. The outer boundary where the solar modulation begins has always been a subject matter of debate in the cosmic-ray and heliophysics community. Various experimental methods and theoretical model calculations have been used to determine the boundary. Although the heliopause was always suspected to be the boundary, it is only until very recently after *Voyager* 1 had crossed the heliopause did we confirm that the boundary is indeed the heliopause. We used a model simulation and detailed *Voyager* observation of cosmic rays at the heliopause crossing to show that the modulation boundary, in fact, is a fraction of an AU beyond the heliopause. Such a conclusion requires a very low turbulence level of the interstellar magnetic field in the outer heliosheath. According to the quasi-linear theory, a low level of turbulence should result in a very

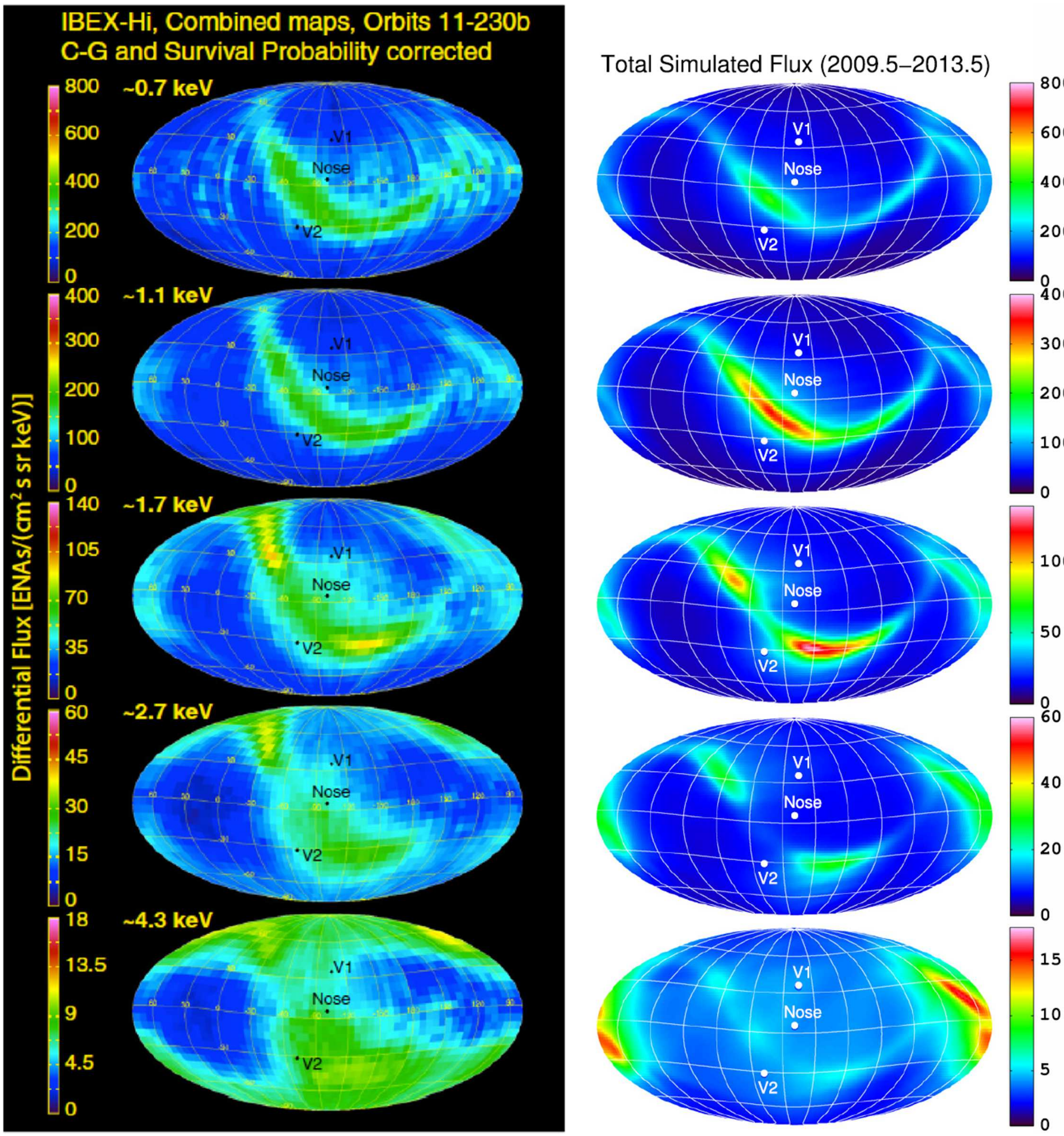

Figure 5: Comparison of the SW temperature measured by $V2$ (blue line) with the MS-FLUKSS simulations using different turbulence models.

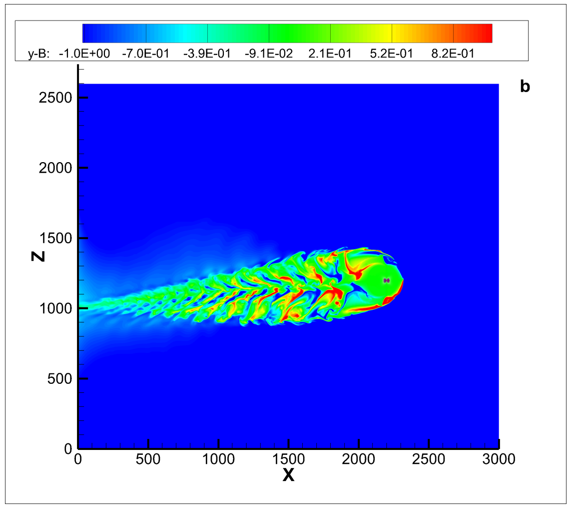

Figure 6: *IBEX* observations of H ENA ux (left), weight-averaged over the rst 5 yr of observations, Compton–Getting and survival probability-corrected, for all IBEX-Hi passbands. On the right we show simulated H ENA ux measurements, linearly averaged over the rst 5 yr.

large diffusion coefficient parallel to the magnetic field and a very small perpendicular diffusion coefficient. For the first time, we are confident that *Voyager* 1 has obtained the truly pristine local interstellar cosmic-ray spectra down to the energies below 1 MeV (Zhang et al., 2015). The cosmic-ray intensity is rapidly filtered by a thin layer of the interstellar magnetic field immediately outside of the heliopause. Its filtration amount depends on the conditions of magnetic field turbulence on the both sides of the heliopause, thus making it solar-cycle dependent as well.

19. The heliotail is formed when the SW interacts with the LISM and is shaped by the interstellar magnetic field (ISMF). While there are no spacecraft available to perform in situ measurements of the SW plasma and heliospheric magnetic field (HMF) in the heliotail, it is of importance for the interpretation of measurements of energetic neutral atom fluxes performed by Interstellar Boundary Explorer. It has been shown recently that the orientation of the heliotail in space and distortions of the unperturbed LISM caused by its presence may explain the anisotropy in the TeV cosmic ray flux detected in air shower observations. The SW flow in the heliotail is a mystery itself because it is strongly affected by charge exchange between the SW ions and interstellar neutral atoms. If the angle between the Suns magnetic and rotation axes is constant, the SW in the tail tends to be concentrated inside the HMF spirals deflected tailward. However, the twisted field soon becomes unstable and the reason for the SW collimation within a two-lobe structure vanishes. We demonstrated (Pogorelov et al., 2015, 2016) that kinetic treatment of the H atom transport becomes essential in this case for explaining the lobe absence further along the tail. We showed that the heliotail flow is strongly affected by the solar cycle that eliminates artifacts, which is typical of solutions based on simplifying assumptions. The heliopause in the tail is subject to KelvinHelmholtz instability, while its orientation and shape are determined by the ISMF direction and strength (see Fig. 6).

20. From the ideal MHD perspective, the heliopause is a tangential discontinuity that separates the solar wind plasma from the local interstellar medium plasma. There are physical processes, however, that make the heliopause permeable. They can be subdivided into kinetic and MHD categories. Kinetic processes occur on small length and time scales, and cannot be resolved with MHD equations. On the other hand, MHD instabilities of the heliopause have much larger scales and can be easily observed by spacecraft. The heliopause may also be a subject of magnetic reconnection. In Borovikov & Pogorelov (2014), we discussed mechanisms of plasma mixing at the heliopause in the context of *Voyager* 1 observations. Numerical results are obtained with a Multi-Scale Fluid-Kinetic Simulation Suite (MS-FLUKSS), which is a package of nu-

merical codes capable of performing adaptive mesh refinement simulations of complex plasma flows in the presence of discontinuities and charge exchange between ions and neutral atoms. The flow of the ionized component is described with the ideal MHD equations, while the transport of atoms is governed either by the Boltzmann equation or multiple Euler gas dynamics equations. The code can also treat nonthermal ions and turbulence produced by them.

21. We investigated physical processes related to the heliotail which is formed when the solar wind interacts with the local interstellar medium (Pogorelov, 2016). Although astrotails are commonly observed, the heliotail observations are only indirect. As a consequence, the direct comparison of the observed astrophysical objects and the Sun is impossible. This requires proper theoretical understanding of the heliotail formation and evolution, and numerical simulations in sufficiently large computational boxes. We reviewed some previous results related to the heliotail flow and show new simulations which demonstrate that the solar wind collimation inside the Parker spiral field lines diverted by the heliopause toward the heliotail is unrealistic. On the contrary, solar cycle effects ensure that the solar wind density reaches its largest values near the solar equatorial plane. We also argue that a realistic heliotail should be very long to account for the observed anisotropy of 1-10 TeV cosmic rays.

22. In Pogorelov et al. (2016), we present numerical simulation results of the 3D heliospheric interface treating pickup ions as a separate proton fluid. To satisfy the fundamental conservation laws, we solve the system of equations describing the flow of the mixture of electrons, thermal protons, and pickup ions. To find the density and pressure of pickup ions behind the termination shock, we employ simple boundary conditions that take into account the *Voyager* observations that showed that the decrease in the kinetic energy of the mixture at the termination shock predominantly contributed to the increase in the pressure of pickup ions. We show that this model adequately describes the flow of the plasma mixture and results in a noticeable decrease in the heliosheath width.

23. The outer heliosphere is a dynamic region shaped largely by the interaction between the solar wind and the interstellar medium. While interplanetary magnetic field and plasma observations by the *Voyager* spacecraft have significantly improved our understanding of this vast region, modeling the outer heliosphere still remains a challenge. We simulated (Kim et al., 2016) the three-dimensional, time-dependent solar wind flow from 1 to 80 astronomical units (AU), where the solar wind is assumed to be supersonic, using a two-fluid model in which protons and interstellar neutral hydrogen atoms are treated as separate fluids. We used 1-day averages of the solar wind parameters from the OMNI data set as inner boundary conditions to reproduce time-dependent effects in a simplified manner which involves interpolation in both space and time. Our model generally agrees with Ulysses data in the inner heliosphere and *Voyager* data in the outer heliosphere. Ultimately, we present the model solar wind parameters extracted along the trajectory of New Horizons spacecraft. We compare our results with in situ plasma data taken between 11 and 33 AU and at the closest approach to Pluto on July 14, 2015.

24. The SW emanating from the Sun interacts with the LISM, forming the heliosphere. Hydrogen ENAs produced by the solar-interstellar interaction carry important information about plasma properties from the boundaries of the heliosphere, and are currently being measured by NASA's *IBEX*. *IBEX* observations show the existence of a "ribbon" of intense ENA emission projecting a circle on the celestial sphere that is centered near the local interstellar magnetic field (ISMF) vector. We showed that the source of the *IBEX* ribbon as a function of ENA energy outside the heliosphere, uniquely coupled to the draping of the ISMF around the heliopause, can be used to precisely determine the magnitude (2.93 ± 0.08 μG) and direction ($227.^{\circ}28 \pm 0.^{\circ}69, 34.^{\circ}62 \pm 0.^{\circ}45$ in ecliptic longitude and latitude) of the pristine ISMF far ($\sim$ 1000 AU) from the Sun. We find that the ISMF vector is offset from the ribbon center by $\sim 8.^{\circ}3$ toward the direction of motion of the heliosphere through the LISM, and their vectors form a plane that is consistent with the direction of deflected interstellar neutral hydrogen, thought to be controlled by the ISMF. Our results yield draped ISMF properties close to that observed by *Voyager* 1, the only spacecraft to directly measure the ISMF close to the heliosphere, and give predictions of the pristine ISMF that *Voyager* 1 has yet to sample.

4 Publications

The following papers have been published as a result of the scientific research supported by this project.

1. Borovikov, S. N., Pogorelov, N. V., Heerikhuisen, J., Hybrid Parallelization of Adaptive MHD-Kinetic Module in Multi-Scale Fluid-Kinetic Simulation Suite, in Astronomical Society of the Pacific Conf. Ser. 474, Numerical Modeling of Space Plasma Flows: ASTRONUM-2012, eds. N. V. Pogorelov, E. Audit, and G. P. Zank, 219–225 (2013)

2. Borovikov, S. N., Pogorelov, N. V., Voyager 1 near the Heliopause, Astrophys. J., 783, L16 (2014)

3. Desai, M. I., Allegrini, F. A., Bzowski, M., Dayeh, M. A., Funsten, H., Fuselier, S. A., Heerikhuisen, J., Kubiak, M. A., McComas, D. J., Pogorelov, N. V., Schwadron, N. A., Sokól, J. M., Zank, G. P., Zirnstein, E. J., Energetic Neutral Atoms Measured by the Interstellar Boundary Explorer (IBEX): Evidence for Multiple Heliosheath Populations, Astrophys. J., 780, 98 (2013)

4. Desai, M. I., Allegrini, F., Dayeh, M. A., Funsten, H., Heerikhuisen, J., McComas, D. J., Fuselier, S. A., Pogorelov, N., Schwadron, N. A., Zank, G. P., Zirnstein, E. J., Latitudinal and Energy Dependence of Energetic Neutral Atom Spectral Indices Measured by the Interstellar Boundary Explorer, Astrophys. J., 802, 100 (2015)

5. Fermo, R. L., Pogorelov, N. V., Burlaga, L. F., Transient shocks beyond the heliopause, J. Phys. Conf. Ser., 642, 012008

6. Gamayunov, K. V., Zhang, M., Pogorelov, N. V., Heerikhuisen, J.; Rassoul, H. K., Self-consistent Model of the Interstellar Pickup Protons, Alfvénic Turbulence, and Core Solar Wind in the Outer Heliosphere, Astrophys. J., 757, 74 (2012)

7. Gamayunov, K., Zhang, M., Pogorelov, N., Heerikhuisen, J., Rassoul, H., Modeling of the Interstellar Pickup Protons, Alfvénic Turbulence, and Solar Wind in the Outer Heliosphere, in Astronomical Society of the Pacific Conf. Ser. 474, Numerical Modeling of Space Plasma Flows: ASTRONUM-2012, eds. N. V. Pogorelov, E. Audit, and G. P. Zank, 140–146 (2013a)

8. Gamayunov, K., Zhang, M., Pogorelov, N., Heerikhuisen, J., Rassoul, H., Alfvénic turbulence generated by the interstellar pickup protons in the outer heliosphere, In Solar Wind 13: Proceedings of the Thirteenth International Solar Wind Conference, AIP Conference Proceedings 1539, 171–174 (2013b)

9. Gamayunov, K., Zhang, M., Pogorelov, N., Heerikhuisen, J., Rassoul, H., Turbulent Heating of the Core Solar Wind Protons in the Outer Heliosphere, in Astronomical Society of the Pacific Conf. Ser. 484, Outstanding Problems in Heliophysics: From Coronal Heating to the Edge of the Heliosphere, eds. Q. Hu and G. P. Zank, 49 (2014)

10. Heerikhuisen, J., Pogorelov, N., Zank, G., Modeling energetic neutral atoms and the IBEX spectrum, in Physics of the Heliosphere: A 10 Year Retrospective, Proc. 10th Annual Astrophysics Conference, American Institute of Physics Conf. Ser. 1436, 221 - 226, New York (2012)

11. Heerikhuisen, J., Pogorelov, N., Zank, G., Simulating the Heliosphere with Kinetic Hydrogen and Dynamic MHD Source Terms, in Astronomical Society of the Pacific Conf. Ser. 474, Numerical Modeling of Space Plasma Flows: ASTRONUM-2012, eds. N. V. Pogorelov, E. Audit, and G. P. Zank, 195–201 (2013)

12. Heerikhuisen, J., Zirnstein, E., Kawamura, A. D., Pogorelov, N., Zank, G., Connection of the solar wind with the interstellar medium through numerical modeling, In Solar Wind 13: Proceedings of the Thirteenth International Solar Wind Conference, AIP Conference Proceedings 1539, 319–324 (2013)

13. Heerikhuisen, J., Zirnstein, E. J., Funsten, H. O., Pogorelov, N. V., Zank, G. P., The Effect of New Interstellar Medium Parameters on the Heliosphere and Energetic Neutral Atoms from the Interstellar Boundary, Astrophys. J., 784, 73 (2014)

14. Heerikhuisen, J., Zirnstein, E., Pogorelov, N., Kappa-distributed protons in the solar wind and their charge-exchange coupling to energetic hydrogen, J. Geophys. Res., 120, 1516 (2015)

15. Kawamura, A. D., Heerikhuisen, J., Pogorelov, N. V., Zank, G. P., 3D simulation of LISM oxygen flux with PUIs inside of heliosphere, SPACE WEATHER: THE SPACE RADIATION ENVIRONMENT: 11th Annual International Astrophysics Conference. AIP Conference Proceedings, Volume 1500, pp. 234-240 (2012)

16. Kim, T. K., Pogorelov, N. V., Borovikov, S. N., Clover, J. M., Jackson, B. V., Yu, H.-S., Time-dependent MHD simulations of the solar wind outflow using interplanetary scintillation observations, SPACE WEATHER: THE SPACE RADIATION ENVIRONMENT: 11th Annual International Astrophysics Conference. AIP Conference Proceedings, Volume 1500, pp. 140-146 (2012)

17. Kim, T. K., Pogorelov, N. V., Zank, G. P., Elliott, H. A., McComas, D. J., Modeling the Solar Wind at the Ulysses, Voyager, and New Horizons Spacecraft, Astrophys. J., in press (arXiv:160807655K) (2016)

18. Kryukov, I.A., Pogorelov, N.V., Zank, G.P., Borovikov, S.N., Numerical modeling of the solar wind turbulence, in Physics of the Heliosphere: A 10 Year Retrospective, Proc. 10th Annual Astrophysics Conference, American Institute of Physics Conf. Ser. 1436, 48 - 54, New York (2012)

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20. Manoharan, P., Kim, T., Pogorelov, N. V., Arge, C. N., Manoharan, P. K., Modeling solar wind with boundary conditions from interplanetary scintillations, J. Phys. Conf. Ser., 642, 012016

21. Pogorelov, N.V., Borovikov, S.N., Burlaga, L.F., Ebert, R.W., Heerikhuisen, J., Hu, Q., Kryukov, I.A., Suess, S.T., Zank, G.P., Numerical modeling of transient phenomena in the distant solar wind and in the heliosheath, in Physics of the Heliosphere: A 10 Year Retrospective, Proc. 10th Annual Astrophysics Conference, American Institute of Physics Conf. Ser. 1436, 321 - 330, New York (2012)

22. Pogorelov, N. V.; Borovikov, S. N.; Burlaga, L. F.; Ebert, R. W.; Heerikhuisen, J.; Kim, T. K.; Kryukov, I. A.; Suess, S. T.; Wu, S. T.; Zank, G. P., Numerical modeling of the solar wind flow with observational boundary conditions, SPACE WEATHER: THE SPACE RADIATION ENVIRONMENT: 11th Annual International Astrophysics Conference. AIP Conference Proceedings, Volume 1500, pp. 134-139 (2012)

23. Pogorelov, N.V., Audit, E., Zank, G.P., Numerical Modeling of Space Plasma Flows: ASTRONUM-2012, Astronomical Society of the Pacific Conf. Ser. 474, San Francisco, CA, ISBN 978-1-58381-832-9 (2013)

24. Pogorelov, N. V., Borovikov, S. N., Bedford, M. C., Heerikhuisen, J., Kim, T. K., Kryukov, I. A., Zank, G. P., Modeling Solar Wind Flow with the Multi-Scale Fluid-Kinetic Simulation Suite, in Astronomical Society of the Pacific Conf. Ser. 474, Numerical Modeling of Space Plasma Flows: ASTRONUM-2012, eds. N. V. Pogorelov, E. Audit, and G. P. Zank, 165–171 (2013)

25. Pogorelov, N. V., Suess, S. T., Borovikov, S. N., Ebert, R. W., McComas, D. J., Zank, G. P., Three-dimensional features of the outer heliosphere due to coupling between the interstellar and interplanetary magnetic fields. IV. Solar Cycle Model Based on Ulysses Observations, Astrophys. J., 772, 2 (2013)

26. Pogorelov, N. V.; Borovikov, S. N., Magnetized Plasma Near the Heliopause: Voyager 1 Measurements and Theoretical Modeling, in Astronomical Society of the Pacific Conf. Ser. 484, Outstanding Problems in Heliophysics: From Coronal Heating to the Edge of the Heliosphere, eds. Q. Hu and G. P. Zank, 174 (2014)

27. Pogorelov, N. V., Borovikov, S. N., Heerikhuisen, J., Kim, T. K., Zank, G. P., Time-dependent Processes in the Sheath Between the Heliospheric Termination Shock and the Heliopause, in Astronomical Society of the Pacific Conf. Ser. 488, Numerical Modeling of Space Plasma Flows: ASTRONUM-2013, eds. N. V. Pogorelov, E. Audit, and G. P. Zank, 167 (2014)

28. Pogorelov, N. V., Borovikov, S. N., Heerikhuisen, J., Zhang, M., The Heliotail, Astrophys. J.Lett., 812, L6 (2015)

29. Pogorelov, N. V.; Borovikov, S. N., Mixing of the Interstellar and Solar Plasmas at the Heliospheric Interface, in Astronomical Society of the Pacific Conf. Ser. 498, Numerical Modeling of Space Plasma Flows: ASTRONUM-2014, eds. N. V. Pogorelov, E. Audit, and G. P. Zank, 160 (2015)

30. Pogorelov, N. V., The Heliotail: Theory and Modeling, J. Phys. Conf. Ser., 719, 012013 (2016)

31. Pogorelov, N. V., Bedford, M. C., Kryukov, I. A., Zank, G. P., Pickup Ion Effect of the Solar Wind Interaction with the Local Interstellar Medium, J. Phys. Conf. Ser., in press (arXiv:1609.03100) (2016)

32. Slavin, J. D., Frisch, P. C., Müller, H.-R., Heerikhuisen, J., Pogorelov, N. V., Reach, W. T., Zank, G. P., Trajectories and Distribution of Interstellar Dust Grains in the Heliosphere, Astrophys. J., 760, 46 (2012)

33. Zank, G. P., Heerikhuisen, J., Wood, B. E., Pogorelov, N. V., Zirnstein, E., McComas, D. J., Heliospheric Structure: The Bow Wave and the Hydrogen Wall, Astrophys. J., 763, 20 (2013)

34. Zhang, M., Schlickeiser, R, A Theory of Bimodal Acceleration of Pickup Ions by Compressive Solar Wind Turbulence under Pressure Balance, Astrophys. J., 756, 129 (2012)

35. Zhang, M., Zuo, P., Pogorelov, N., Heliospheric Influence on the Anisotropy of TeV Cosmic Rays, Astrophys. J., 790, 5 (2014)

36. Zhang, M., Luo, X., Pogorelov, N., Where is the cosmic-ray modulation boundary of the heliosphere?, Phys. Plasmas, 22, 091501 (2015)

37. Zuo, P., Zhang, M., Rassoul, H. K., Acceleration of Low-energy Ions at Parallel Shocks with a Focused Transport Model, Astrophys. J., 767, 6 (2013a)

38. Zuo, P., Zhang, M., Rassoul, H. K., The Role of Cross-shock Potential on Pickup Ion Shock Acceleration in the Framework of Focused Transport Theory, Astrophys. J., 776, 93 (2013b)

39. Zirnstein, E., Heerikhuisen, J., Pogorelov, N., Numerical simulations of primary and secondary hydrogen ENA fluxes at 1 AU, SPACE WEATHER: THE SPACE RADIATION ENVIRONMENT: 11th Annual International Astrophysics Conference. AIP Conference Proceedings, Volume 1500, pp. 262-267 (2012).

40. Zirnstein, E. J., Heerikhuisen, J., Pogorelov, N. V., McComas, D. J., Dayeh, M. A., Simulations of a Dynamic Solar Cycle and Its Effects on the Interstellar Boundary Explorer Ribbon and Globally Distributed Energetic Neutral Atom Flux, Astrophys. J., 804, 5 (2015)

41. Zirnstein, E. J., Heerikhuisen, J., Funsten, H. O., Livadiotis, G., McComas, D. J., Pogorelov, N. V., Local Interstellar Magnetic Field Determined from the Interstellar Boundary Explorer Ribbon, Astrophys. J., 818, L18 (2016)

5 Presentations (supported or related to the project)

1. Pogorelov, N. V., Modeling Heliosheath Flow with Observational Boundary Conditions, 39th COSPAR Scientific Assembly, 14-22 July, 2012, Mysore, India.

2. Pogorelov, N. V., Solar Wind Behavior at Voyager Spacecraft from the Simulation Perspective, Voyager Science Steering Group Meeting, 4–5 September, 2012, Pasadena, CA. (Invited)

3. Pogorelov, N. V., Modeling CMEs from the Sun to the Earth Orbit, 2nd In-situ Heliospheric Science Conference, September 18-20, 2012, Laurel, MD.

4. Pogorelov, N. V., Solar Cycle Model based on Ulysses Measurements, 2nd In-situ Heliospheric Science Conference, September 18-20, 2012, Laurel, MD.

5. Pogorelov, N. V., Magnetic Fields in the Vicinity of the Heliopause, 2nd In-situ Heliospheric Science Conference, September 18-20, 2012, Laurel, MD.

6. Pogorelov, N. V., Nonstationary Phenomena in the Heliosheath, 2012 Fall AGU Meeting, December 3 - 7, 2012, San Francisco, CA.

7. Pogorelov, N. V., The Heliopause and Plasma Flow in Its Vicinity, Voyager Science Steering Group Meeting, December 2, 2012, San Francisco, CA. (Invited)

8. Pogorelov, N. V.,Magnetic Field in the Vicinity of the Heliopause: Matching Observations and Modeling, Magnetic Fields in the Universe IV: From Laboratory and Stars to Primordial Structures, February 4 - 8, 2013, Playa del Carmen, Mexico. (Invited)

9. Pogorelov, N. V., Plasma Flow and Magnetic Field in the Heliosheath and Heliotail, Interstellar Boundary Explorer SWT Meeting, March 18 - 21, 2013, Austin, TX. (Invited)

10. Pogorelov, N. V., Interpretation of Voyager Measurements in the Heliosheath, 12th Annual International Astrophysics Conference, April 15–19, 2013, Myrtle Beach, SC. (Invited)

11. Pogorelov, N. V., Physical Processes in the Vicinity of the Heliopause and Related 2-3 kHz Radio Emission, The AGU Meeting of the Americas, 14 - 17 May, 2013, Cancun, Mexico. (Invited)

12. Pogorelov, N. V., Solar Cycle Effects on the Heliospheric Interface and Related Energetic Neutral Atom Production, The AGU Meeting of the Americas, 14 - 17 May, 2013, Cancun, Mexico. (Invited).

13. Pogorelov, N. V., Time-dependent Processes in the Sheath Between the Heliospheric Termination Shock and the Heliopause, 8th International Conference on Numerical Modeling of Space Plasma Flows, ASTRONUM-2013, 1 - 5 July, 2013, Biarritz, France. (Invited)

14. Pogorelov, N. V., Three-dimensional Structure of the Time-dependent Heliosphere Interacting with the LISM, Cosmic Ray Anisotropy Workshop, 26 - 28 September, 2013, Madison, WI. (Invited).

15. Pogorelov, N. V., Solar Cycle Effect of the IBEX and Ulysses Measurements, Fall AGU Meeting, 9 - 13 December, 2013, San Francisco, CA, USA (Invited)

16. Pogorelov, N. V., Multi-scale Modeling of the Solar Wind Interaction with the Interstellar Medium and Its Connection to Voyager Results, Fall AGU Meeting, 9–13 December, 2013, San Francisco, CA, USA.

17. Pogorelov, N. V., Voyager 1 Near the Heliopause, 13th International Astrophysics Conference, Myrtle Beach, SC, 10 - 14 March, 2014. (Invited).

18. Pogorelov, N. V., Voyager Science Steering Group meeting, Dec 2013.

19. Pogorelov, N. V., ISSI meeting, Bern, Switzerland, Jan 2014, ”Heliosheath Processes and Structure of the Heliopause: Modeling Energetic Particles, Cosmic Rays, and Magnetic Fields” (team leader)

20. Pogorelov, N. V., Time-dependent Structure of the Outer Heliosphere and Its Influence on the Energetic Ion Production and Transport, 40th COSPAR Scientific Assembly, August 2014, Moscow, Russia. (Invited)

21. Pogorelov, N. V., Modeling the heliosphere using tomographic reconstruction of the solar wind from interplanetary scintillation data, 40-th AOGS Scientific Assembly, Sapporo, Japan, 28 July 1 August, 2014.

22. Pogorelov, N. V., Structure of the Heliopause and Its Implications for Voyager Observations, 40-th AOGS Scientific Assembly, Sapporo, Japan, 28 July 1 August, 2014. (Invited)

23. Pogorelov, N. V., Interstellar Mapping Probe: Scientific Challenges of the IMAP Mission, Fall AGU Meeting, San Francisco, CA, December 1519, 2014, SH21D-04. (Invited)

24. Pogorelov, N. V., Instabilities and Magnetic Reconnection near the Heliopause, Fall AGU Meeting, San Francisco, CA, December 1519, 2014, SH11B-4050

25. Pogorelov, N. V., Turbulence in the Heliosphere, International Conference Turbulence in the Sky as on Earth, Natal, Brazil, 6-16 October, 2014. (Invited)

26. Pogorelov, N. V., Modeling Heliophysics and Astrophysics Phenomena with a Multi-Scale Fluid Kinetic Simulation Suite, Blue Waters Symposium, Champaign, IL, 12 15 May, 2014. (Invited)

27. Pogorelov, N. V., MS-FLUKSS and Its Application to Modeling Flows of Partially Ionized Plasma in the heliosphere, Extreme Science and Engineering Discovery Environment Conference XSEDE14, Atlanta, GA, 13-18 July, 2014. (Invited)

28. Pogorelov, N. V., Mixing of the Interstellar and Solar Plasmas at the Heliospheric Interface, 9th International Conference on Numerical Modeling of Space Plasma Flows, Long Beach, CA, June 2014. (Invited)

29. Pogorelov, N. V., Instabilities at the Heliopause, Midwest Magnetic Field Workshop, Madison, WI, 28 29 April, 2014. (Invited)

30. Pogorelov, N. V., Modeling Nonthermal Ions in the Heliosphere, 56th Annual Meeting of the APS Division of Plasma Physics, New Orleans, Louisiana, 27 31 October, 2014.

31. Pogorelov, N. V., Challenges in Numerical Modeling of the SW-LISM Interaction, ISSI meeting Heliosheath Processes and Structure of the Heliopause: Modeling Energetic Particles, Cosmic Rays, and Magnetic Fields, Bern, Switzerland, Nov. 2014. (Team leader)

32. Pogorelov, N. V., Three-dimensional, Time-dependent Structure of the Heliopause, Voyager SSG team meeting, 14 December, 2014. (Invited)

33. Pogorelov, N. V., Heliospheric Asymmetries and Related Cosmic Ray Anisotropy, Cosmic Ray Anisotropy Workshop, Bad Honnef, Germany, 26 30 January, 2015. (Invited)

34. Pogorelov, N., AGU Fall Meeting, "Transition Region Near the Heliopause: Modeling Results from the Voyager Mission Perspective," San Francisco, CA. (December 18, 2015).

35. Pogorelov, N., Voyager Science Steering Group Meeting, "Magnetic Field Near the Heliopause," San Francisco, CA. (December 17, 2015).

36. Pogorelov, N., Magnetic Fields in the Universe V, "Magnetic Field in the Outer Heliosphere and Beyond," Cargese, France. (October 7, 2015).

37. Pogorelov, N., NORDITA Workshop Magnetic Reconnection in Plasmas, "Instabilities and Magnetic Reconnection Near the Heliopause," Stockholm, Sweden. (August 13, 2015).

38. Pogorelov, N., 26th IUGG General Assembly, "Solar Wind Interaction with the Local Interstellar Medium: Modeling Results vs. Spacecraft Observations," Prague, Czech Republic. (July 2, 2015).

39. Pogorelov, N., International Conference New Paradigms for the Heliosphere, "Magnetic Field in the Outer Heliosphere and Beyond," Bad Honnef, Germany. (June 30, 2015).

40. Pogorelov, N., Voyager Science Steering Group meeting, "Using Observations to Constrain the Properties of the VLISM," Pasadena, CA. (June 21, 2015).

41. Pogorelov, N., 10th International Conference on Numerical Modeling of Space Plasma Flows: ASTRONUM-2015, "Magnetic Field at the Edge of the Heliosphere," Avignon, France. (June 9, 2015).

42. Pogorelov, N., Midwest Magnetic Field Workshop, "The heliopause shaped by the interstellar magnetic field," Madison, WI. (May 22, 2015).

43. Pogorelov, N., Blue Waters Symposium, "Modeling Heliophysics Solar Wind Flow with a Multi-Scale Fluid Kinetic Simulation Suite," NSF, Redmond, OR. (May 12, 2015).

44. Pogorelov, N., Joint American Astronomical Society/American Geophysical Union Triennial Earth-Sun Summit, "Ion-Neutral Coupling in the Outer Heliosphere and Beyond," Indianapolis, IN. (April 27, 2015).

45. Pogorelov, N., 14th Annual Astrophysics Conference, Linear and Nonlinear Particle Energization Throughout the Heliosphere and Beyond, "Magnetic Field in the Heliosphere and Beyond," Tampa, FL, April 20-24, 2015. (April 21, 2015).

46. Borovikov, S. N., The Role of the Interstellar and Interplanetary Magnetic Fields in the Heliopause Stability, Fall AGU Meeting, December 3–7, 2012, San Francisco, CA.

47. Borovikov, S. N., Numerical simulation of the January 2012 CME event and its propagation to the Earth orbit, December 3–7, 2012, San Francisco, CA.

48. Borovikov, S. N., Investigating the heliotail structure with a MHD-kinetic model, 12th Annual International Astrophysics Conference, April 15–19, 2013, Myrtle Beach, SC. (Invited)

49. Borovikov, S. N., Investigating the Heliotail Structure with an MHD-kinetic Model, 8th International Conference on Numerical Modeling of Space Plasma Flows, ASTRONUM-2013, 1 - 5 July, 2013, Biarritz, France. (Invited).

50. Borovikov, S. N., MHD-kinetic Simulation of the Heliospheric Interface and Related 2-3 kHz Radio Emission, Fall AGU Meeting, 9–13 December, 2013, San Francisco, CA, USA.

51. Gamayunov, K., Interstellar Pickup Protons and Their Effects in the Outer Heliosphere, 12th Annual International Astrophysics Conference, April 15–19, 2013, Myrtle Beach, SC. (Invited)

52. Heerikhuisen, J., Global Modeling of the Heliosphere and the IBEX Ribbon, Fall AGU Meeting, 2012, December 3–7, 2012, San Francisco, CA.

53. Heerikhuisen, J., Simulations of Heliospheric Boundary Conditions on the Ribbon, Interstellar Boundary Explorer SWT Meeting, March 18 - 21, 2013, Austin, TX. (Invited)

54. Heerikhuisen, J., Energetic Ions and Neutrals in the Outer Heliosphere, Workshop on Reconnection, Turbulence, and Particles in the Heliosphere, Queenstown, New Zealand. February, 2015. (Invited)

55. Heerikhuisen, J., Properties of ENA Source Regions Outside the Heliosphere, American Geophysical Union Fall Meeting, San Francisco, CA. December, 2015. (Invited)

56. Heerikhuisen, J., Ion-Neutral Coupling in the Heliosphere", 11th International Conference, Monterey, CA. June, 2016. (Invited)

57. Heerikhuisen, J., Neutral H distribution in the ribbon, IBEX Science Working Team Meeting #20, Princeton, NJ. August, 2016.

58. Zank, . P., Heliospheric Structure: The Bow Wave and the Hydrogen Wall, IBEX 2012, Santa Fe, NM, November 2012. (Invited)

59. Zank, G. P., The transport of density fluctuations throughout the heliosphere, ARCETRI Workshop, Florence, Italy, November 2012. (Invited)

60. Zank, G. P., Heliospheric Structure: Overview of two sets of MHD Global Simulations, Science Steering Group Meeting, San Francisco, CA, December 2012. (Invited)

61. Zank, G. P., The transport of low frequency turbulence throughout the heliosphere, The 1st Solar Probe Plus Conference, Pasadena, CA, March 2013.

62. Zank, G. P., Heliospheric structure and the Lyman-alpha signature of the Hydrogen Wall, 13th Annual International Astrophysics Conference, Myrtle Beach, SC, April 2013.

63. Zhang, M., Applications of Stochastic Process Modeling to Particle Transport in Space Plasmas, ISSI Workshop on particle transport, May 2013. (Invited)

64. Zhang, M., Understanding the anisotropy of TeV cosmic rays, International Workshop on TeV cosmic ray anisotropy, University of Wisconsin-Madison. (Invited)

65. Zhang, M., Implications of the IBEX observation of ribbon in energetic neutral atom emissions to the transport of Galactic and anomalous cosmic rays near the heliopause, Fall AGU meeting, San Francisco, CA, December 2013

66. Zhang, M., Numerical Investigation of the 2007 cosmic ray transient decrease events observed by Voyager Spacecrafts, Fall AGU meeting, San Francisco, CA, December 2013

67. Zhang, M., Acceleration of energetic particles by intermittent compressive plasma waves, ISSI Workshop on particle transport, Jan 2014. (Invited)

68. Zhang, M., IBEX ribbon and Galactic cosmic rays modulation boundary, ISSI Workshop on particle transport, Jan 2014. (Invited)

69. Zhang, M., Applications of Stochastic Process Modeling to Particle Transport in Space Plasmas, ISSI Workshop on particle transport, Nov 2014. (Invited)

70. Zhang, M., Implications of the IBEX observation of ribbon in energetic neutral atom emissions to the transport of Galactic and anomalous cosmic rays near the heliopause, COSPAR Scientific Assembly, Moscow, Russia, Aug 2014.

71. Zhang, M., Modulation of Galactic cosmic rays near the heliopause, COSPAR Scientific Assembly, Moscow, Russia, Aug 2014.

72. Zhang, M., Acceleration of pickup ions by intermittent compressive plasma waves in interplanetary space, APS DPP meeting, New Orleans, 2014. (Invited)

73. Zhang, M., Transport of cosmic rays across the heliopause, Fall AGU meeting, San Francisco, CA, December 2015.

74. Zhang, M., Exploring the global heliospheric structure with TeV Galactic cosmic ray anisotropy, International Workshop on New Paradigm of the Heliosphere, Bad Honeff Germany, June 2015. (Invited)

75. Zhang, M., Acceleration of Pickup Ions by Compressive Plasma Waves, 14th Annual International Astrophysics Conference: Linear and Nonlinear Particle Acceleration Throughout the Heliopshere and Beyond, April 2015.

76. Zuo, P., Zhang, M., Low-energy particle acceleration at parallel shocks, 33rd COSPAR Assembly, India (2012)

6 Computer Modeling Insight

Adding new equations to any mathematical model implemented in MS-FLUKSS is straightforward. It suffices to let the code know that new equations are added. For the sake of this project, we have introduced the following three modifications: (1) in a multi-fluid model, an additional continuity equation and a pressure equation for PUIs have been added, and the possibility of imposing boundary conditions for the PUI density and pressure across the TS has been implemented; (2) to treat PUIs, we have implemented a procedure for solving numerically the Fokker–Planck equation along plasma streamlines for the pitch-angle averaged distribution function accompanied by a boundary conditions imposed on it at the TS; and (3) we have completely reworked the parallelization strategy for solving the kinetic Boltzmann equation for neutral atoms, which turned out to be essential for preforming higher-resolution, adaptive-mesh-refinement simulations.

The Boltzmann equation for neutrals and ideal MHD equations for plasma are solved self-consistently using global iterations. For the current configuration of plasma, the Monte Carlo code is run until appropriate statistics is accumulated to calculate the source terms for the plasma. After that, the plasma code is run for some time. This procedure is repeated until a steady state is reached. Our Monte Carlo method for solving the Boltzmann equations is based on injecting test particles into a computational region and gathering statistics for the charge-exchange source terms instead of solving the 6D Boltzmann equation directly. The kinetic module was successfully integrated into the MS-FLUKSS (Borovikov et al., 2013). Plasma data and arrays storing the source terms for the MHD code are shared among the cores of a single node. This is done by switching parallelization approach from a pure MPI to a hybrid (MPI+OpenMP) method, where particles are distributed between MPI tasks and threads. Load balancing is a 2-level algorithm that guarantees an even workload between nodes and threads within a single node. We have implemented a 64-bit support for the code to be able to handle more than 2 billion particles.

The plasma module in MS-FLUKSS has domain-driven parallelization, i.e., a computational region is split between processors and every MPI task computes only in the specified region. The kinetic code splits the workload between ranks by ensuring approximately even distribution of particles among cores. The plasma data is gathered into a set of arrays (each array represents a level of refinement in the plasma code) which is passed from the main C++ code to the kinetic code using a specially created interface. A similar set of arrays is created and passed to the kinetic code for collection of the source terms and the neutral atom distribution. The arrays are shared between threads that are spawned in the main subroutine of the kinetic code. When a neutral particle experience charge exchange, the information about this event should be stored in the arrays for source terms. To solve this problem efficiently, a special buffer was created as an array of special data structure representing a single charge exchange event. This user-defined data structure has the following fields: a) index of the finest level in nested grids hierarchy where charge exchange occurs; b) position where charge exchange happens; c) physical quantities of the event (mass loss, momentum and energy data). When charge exchange occurs, the corresponding data is written to the buffer, not to the global arrays. The buffer is an array of the data structure whose size is chosen on a random basis for each thread to make concurrent requests to update the arrays unlikely. Its typical size varies from 200,000 to 600,000 elements. When the buffer is full it is flushed to the main array via a critical section in the code.

	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.

The load balancing algorithm has been revised recently. An MPI task which has the largest number of particles sends excess particles to a task with the least number of particles. If the excess is too large, some particles are sent to a task having the second least number of particles, etc. Additionally, if the deficit of particles is too large on a processor, it can receive particles from different MPI tasks. Each MPI task receives information about the number of particles the other tasks have. This is the only global collective communication. This information allows each rank to calculate the average number of particles per core and determine the communication scheme for load balancing. Of interest is that each rank knows the whole communication pattern (which of them will send/receive and how many particles will be transferred). Each MPI rank initiates a series of non-blocking send or receive calls. When the communication is complete the load balancing within a node is performed using a similar approach. We have rewritten entirely the random number generator because it turned out that the GNU Fortran random number generator shares seeds among threads and uses mutexes to regulate their update. This significantly deteriorated the overall performance. We have implemented our own random number generator where each thread has its own set of seeds.

Our first test was to compare the performance with a different number of threads per MPI task. This test was performed on Cray XT5 Kraken with two six-core AMD Istanbul processors per node. We use 16 nodes and 50 million particles in our test case. The runs ranged from 192 MPI tasks and no threads, to 16 MPI tasks each spawning 12 threads. The results are summarized in Table 1. If hybrid parallelization is not used, the run time is 180 seconds. The code works faster when two threads are used, because the number of MPI calls is reduced by a factor of two. When the number of threads is further increased, the code slows down because synchronization between the threads requires more time. The case with 12 threads per MPI task gave the worst performance. This happened because of the Non-Uniform Memory Access (NUMA) design of the Kraken nodes. Each processor has its own local memory. Although processor can access the other processor memory, the memory bandwidth in this case is 20% smaller than the access time to local memory. For this reason, we observed the performance decrease by 15%.

To perform scaling tests, we used Blue Waters, which is a Cray XE6/XK7 machine. The XE6 nodes have two AMD Interlagos processors, whereas XK7 nodes contain one AMD processor and the NVIDIA GK110 "Kepler" accelerator. We used the XE6 nodes for the tests. Each Interlagos processor has 16 integer cores. There are 8 floating point units (FPU) per processors, e.g. a FPU is shared between two integer cores. Eight integer cores form a NUMA domain. To perform our runs, we used 1 MPI task per NUMA domain to keep shared data in one domain. Totally, we had 4 MPI tasks per node and each one spawned additional 8 threads. For the strong scaling tests we used 12 billion particles and the physical run time was 800 years. The strong scaling results are almost perfect (see Figure 7). Some superscaling effect may be explained by the better cache fitting speedup that overpasses the extra communication load. Figure 8 shows the weak scaling results when there is approximately an even load of 100,000 particles per core in each test. The simulation time is equal in all cases, except for some small insignificant fluctuations.

The IO performance of the code is quite good. A 650 Gb data file containing 10 billion particles can be written as fast as 32 seconds on Lustre file system, if striped over 100 Object Storage Targets (OSTs).

We are also exploring the opportunity to speed up the plasma module using available cores. Since number of grid blocks (patches) is less than the number of available cores, we needed to focus on how to speed up calculations on a single patch. We tried two different approaches: (a) auto-parallelization of low-level loops that are done by compiler and (b) dimension splitting parallelization when reconstruction and solving of the Riemann problem is done in parallel by creating one thread for each dimension. Both approaches gave approximately the same speedup, close to a factor of two. There are some methods to speed up the code even more, e.g. nested parallelism, which is also being explored. We are part of a

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

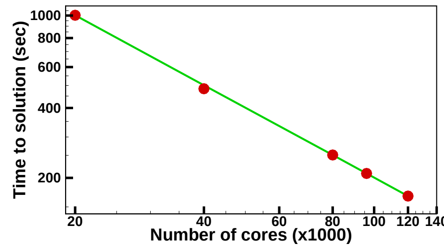

Figure 7: Strong scaling results of the kinetic code. The green line shows ideal performance. The red circles are measured time.

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

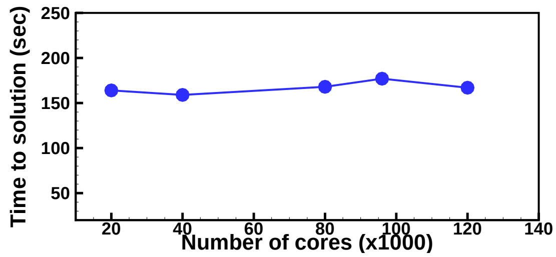

Figure 8: Weak scaling results of the kinetic code.

Blue Waters PAID team now aimed to rewrite the kinetic code using GPUs. The communication pattern implemented in Chombo as an AMR framework is quite unique and can be considered as a good stress test for HPC systems. Our experience shows that we always benefit from close collaboration with supporting staff to resolve emerging issues. As the result, a few compiler bugs and system issues were discovered and subsequently fixed by vendors.

7 Personnel

At UAH, this project supported salaries of the Professor Nikolai Pogorelov, Co-PIs Sergey Borovikov, Jacob Heerikhuisen, and Gary Zank, and partially covered graduate research assistants, Matthew Bedford, Preethi Manoharan, and Tae Kim. At FIT, this project supported salaries for Professor Ming Zhang, Co-I Konstantin Gamayunov, and postdoc P. Zuo. The UAH and FIT teams performed extensive discussions both remotely, through monthly teleconferences, and at scientific meetings.

8 Synergistic Activity

UAH PI Pogorelov organized sessions at 2012 COSPAR Scientific Assembly, Mysore, India and at all 2012-2015 Fall AGU Meetings, San Francisco, CA, where the subjects related to this proposal were discussed. FIT PI organized a session at 2014 COSPAR Scientific Assembly in Moscow, Russia. Co-PI Zank organized the 12–14 International Astrophysics Conference. UAH PI Pogorelov was the Chair of five international conferences on Numerical Modeling of Space Plasma Flows (ASTRONUM-2012 in Big Island, Hawaii, ASTRONUM-2013 in Biarritz, France, ASTRONUM-2014 in Long Beach, California, ASTRONUM-2015 in Avignon, France, and ASTRONUM 2016 in Monterey, California). UAH PI Pogorelov also organized a session “Nonthermal Ions in Space and Laboratory Plasmas” (co-conveners C. C. Cheng, W. Heidbrink, and M. Zhang) at the APS DPP Meeting in New Orleans, LA, where representatives from both space physics and fusion communities discussed issues related to physical phenomena in partially ionized plasmas in presence of nonthermal, hot ion component.

9 Summary

This project has been productive and considerable achievements have been made that contributed to our understanding of interactions between partially ionized plasma flows in the presence of a nonthermal, hot ion component. 41 papers were published (21 in the refereed journals and 18 in refereed proceedings), 2 papers are in press, and 76 talks (38 of them invited) have been supported or are the result of work partially supported by these grants. Only a few results remained unpublished, but the papers are either to be accepted or in the last stage of preparation. The goals of the projects have been completed.