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Simulating Coupling Complexity in Space Plasmas

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Abstract. With the support of a National Science Foundation Information Technology Research (ITR) grant, we are attempting to advance computational physics by developing a new class of computational code for plasmas and neutral gases that integrates multiple scales and multiple physical processes and descriptions. We are developing a highly modular, parallelized, scalable code that incorporates macroscopic scales and "microscales" by synthesizing initially three simulation technologies: 1) Computational fluid dynamics (hydrodynamics or magneto-hydrodynamics-MHD) for the large-scale plasma; 2) direct Monte Carlo simulation of atoms/neutral gas, and 3) transport code solvers to model highly energetic particle distributions. If the code development proceeds satisfactorily, we will also incorporate hybrid simulations for microscale structures and particle distributions. By synthesizing continuum and kinetic descriptions for plasmas and gases, we will provide a computational tool that will advance our understanding of the physics of neutral and charged gases enormously. Besides making major advances in basic plasma physics and neutral gas problems (e.g., reconnection, shock wave physics, etc.), this project will address 3 Grand Challenge space physics problems that reflect our research interests: 1) To develop a temporal global heliospheric model which includes the interaction of solar and interstellar plasma with neutral populations (hydrogen, helium, etc., and dust), kinetic pickup ion acceleration at the termination shock, anomalous cosmic ray production, interaction with galactic cosmic rays, while incorporating the time variability of the solar wind and the solar cycle. 2) To develop a coronal mass ejection and interplanetary shock propagation model for the inner and outer heliosphere, including wave-particle interactions and particle acceleration at travelling shock waves and compression regions. 3) To develop an advanced adaptive Geospace General Circulation Model (GGCM) that includes Hall and kinetic subgrid physics and is capable of realistically modelling space weather events, in particular the interaction with CMEs and geomagnetic storms. Our progress to date is summarized in this report.

1. Introduction

The NRC Panel Report on *Theory, Modeling, & Data Exploration* identified "coupling complexity" as a central challenge facing the further development of modelling and simulation in space physics over the next decade. Here, coupling complexity refers to the class of problems or systems that consist of significantly different scales, regions, or particle populations, and for which more than one set of defining equations or concepts is necessary to understand the system. This somewhat dry definition is best illustrated by an example describing one part of the grand challenge problems that we propose to address using a new class of numerical code that is currently under development with the support of a National Science Foundation Information Technology Research (ITR) grant ATM 0428880. Consider a shock wave propagating through the outer heliosphere (Figure 1). The solar wind into which the shock propagates is mediated by the charge exchange interaction of solar wind protons and interstellar neutral atoms. The charge exchange mean free path and the neutral collisional mean free path exceeds 100 AU, implying that the neutral atoms and plasma do not equilibrate, so necessitating a kinetic description of the neutral gas (i.e., solving the Boltzmann equation by, typically, a direct Monte Carlo simulation). The "pickup ions" created through the charge exchange interaction form a distinct suprathermal particle distribution in the solar wind, and some of these particles are reflected preferentially at the shock front. The reflected pickup ions modify the micro-structure of the shock itself, on scales corresponding to the gyroradii of reflected solar wind and pickup ions. Consequently, the particles must be described kinetically at and in the immediate vicinity of the shock to resolve the relevant shock scales and microphysics. Some of the reflected ions may be further energized by diffusive shock acceleration, so that they become anomalous cosmic

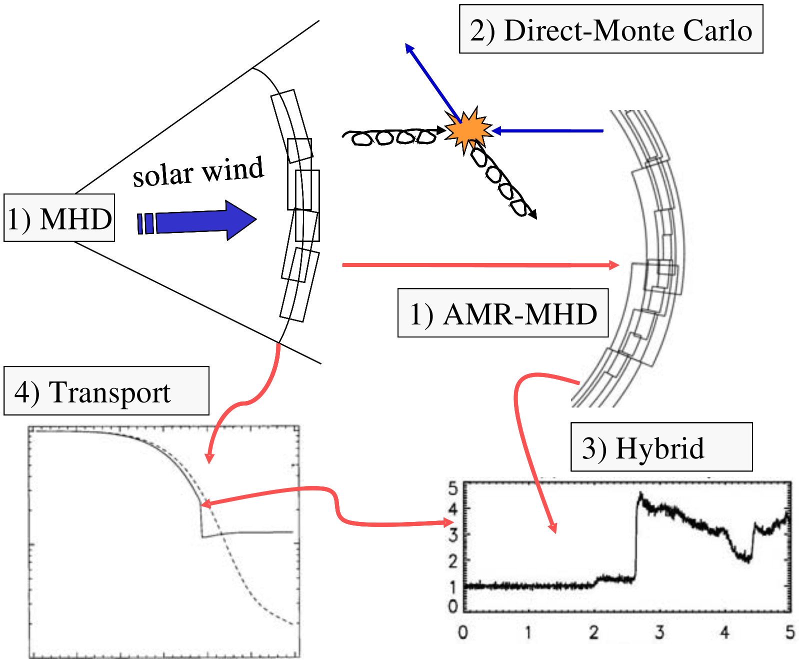

Figure 1. Qualitative diagram illustrating "coupling complexity." 1) MHD description of the large-scale solar wind and associated AMR. 2) Direct Monte Carlo simulation of neutral atoms. 3) Hybrid simulation of the micro-scale structure of the shock. 4) Transport code for energetic ions. See text for details.

rays (ACRs) with energies of many 10's of MeV. These particles have gyroradii that far exceed the micro-scale shock transition scales and may have an energy density sufficiently large to modify the macro-structure of the shock, introducing an extended precursor. The ACRs require a separate kinetic treatment, based on a transport description. The overall shock location and the large-scale solar wind can be described adequately by an MHD description. Thus, to model this apparently simple problem fully requires the use of at least four distinct simulation technologies: 1) Computational fluid dynamics (CFD) (hydrodynamics or magneto-hydrodynamics-MHD) for the large-scale plasma and shock wave location; 2) direct Monte Carlo simulation (DMCS) of neutral interstellar atoms/gas; 3) hybrid simulations to model the micro-scale structure of the shock and particle distributions in the vicinity of the shock, and 4) transport code solvers to model highly energetic particle distributions, and all of these must be coupled self-consistently since, as alluded to above, all scales affect each other (Figure 1); for example, the physics of the particle distributions in the vicinity of the micro-scale shock transition determines the "injection" of particles into the diffusive shock acceleration process, which affects the macrostructure of the shock and the shock evolution characteristics.

Related papers in this volume that discuss some of the specific numerical schemes for this project are Pogorelov et al. (3D MHD and multi-fluid), Heerikhuisen et al. (DMCS of neutral gas), Florinski et al. (cosmic ray transport), Kryukov et al. (adaptive mesh refinement - AMR), Shaikh et al. (turbulence), and Borovikov et al. (visualization, mesh generation, and code integration).

2. Results for large-scale heliospheric modelling

Complexity in plasma and neutral gas problems arises from coupling across space and time scales (e.g., turbulence at boundary layers), the coupling of multiple constituents (e.g., the interaction of the solar wind with neutrals in the interstellar medium) and the linkage of different regions (e.g., the ejection of plasma from the surface of the sun and its interaction with the Earth's magnetosphere). Distinct plasma regions and regimes are invariably coupled in a highly nonlinear dynamical fashion, with the implication that each region or physical process cannot be considered in isolation. Multiple plasma regions can be coupled through events which transfer mass, momentum, and energy from one system to another, such as the eruption and propagation of a coronal mass ejection from the solar surface through interplanetary space to the Earth's magnetosphere and beyond. To make major advances in the fields of atmospheric, plasma, space, astro-physics, and even engineering, over the next decade requires a new approach to computation and modelling. Although great successes have been achieved on the basis of very sophisticated algorithms, the use of adaptive mesh refinement, parallelization, etc., we have reached the point where we need to go well beyond the relatively simple hydrodynamic or MHD framework. The Theory, Computation, and Data Exploration sub-panel of the Space Physics Decadal Survey 2003 recognized this as the most significant challenge to computational space physics in the coming decade. To advance, computational tools need to be developed that embrace the highly nonlinear dynamical coupling and feedback of different and disparate scales, processes, and regions. The goal of our project is to develop a flexible, modular code that can simultaneously incorporate multiple spatial and temporal scales and multiple populations of charged and neutral particles. Here we describe a single example on which we have focussed our attention, namely the interaction of the solar wind with the partially ionized local interstellar medium.

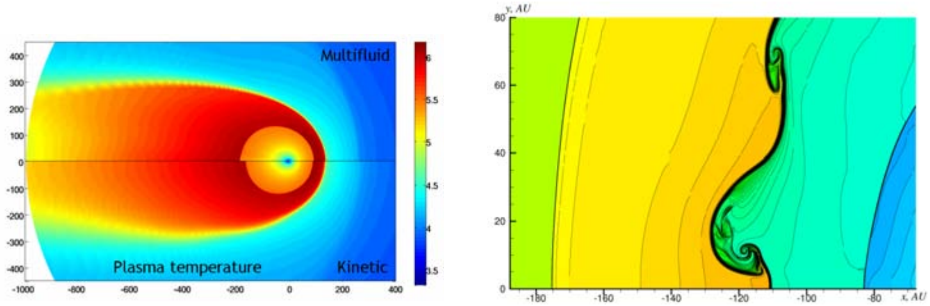

Figure 2. Left: A comparison of a coupled plasma-neutral H multi-fluid simulation (top half-plane) and a corresponding coupled plasma-kinetic neutral H simulation (bottom half-plane) showing the plasma temperature. Differences in the global morphology are relatively slight. (Heerikhuisen et al. 2006) Right: Snapshot of a section of the highly unstable heliopause, contrasting the extreme range of scales demanded of this simulation. The scales range from the scale of the heliopause itself (1000 AU) to the charge exchange mean free path in this region ($\sim$ 100 AU) to the large-scale (10's of AU) and embedded fine-scale structure ($<$ 0.1 AU) of the unstable structures themselves. Adequate resolution of the heliopause requires the use of adaptive mesh refinement techniques (Kryukov et al. 2006)

The heliospheric-local interstellar medium (LISM) plasma environment is composed of three thermodynamically distinct regions: (i) the supersonic solar wind, with a relatively low temperature, large radial speeds, and low densities; (ii) the shock-heated heliosheath solar wind with much higher temperatures and densities, and lower flow speeds, and finally (iii) the LISM, where the plasma flow speed and temperature is low. As discussed in detail by Zank et al., 1996, each of the thermodynamically distinct regions contributes a distinct population of neutral atoms produced by charge exchange with the ambient plasma and neutrals entering the region. The self-consistent inclusion of neutral hydrogen in models of the solar wind-LISM interaction is absolutely fundamental to understanding the large-scale structure of the heliosphere.

Two basic classes of model have been developed to describe neutral H in and around the heliosphere: multi-fluid models of varying degrees of sophistication (Pauls et al. 1995; Zank et al. 1996; Williams et al. 1997; Liewer et al. 1996; Wang & Belcher 1998; Pauls & Zank 1997; Fahr et al. 2000; Florinski et al. 2003; Zank & Mueller 2003; Pogorelov et al. 2004, 2006) which treat the neutral atoms as a multi-fluid, and kinetic models which solve the the neutral atom kinetic equation, either by a Monte Carlo technique (Baranov & Malama 1993, 1995; Izmodenov et al. 1999; Heerikhuisen et al. 2006) or by a particle-mesh method (Lipatov et al. 1998; Müller et al. 2000). The long charge exchange mean free path for neutral hydrogen may mean that the fluid description for neutrals within the heliosphere is not completely justifiable. Multi-fluid and Boltzmann models differ in the detailed predictions that each admits for the neutral atom distribution and this can lead to 10–15% differences in predicted neutral H densities and temperatures within the heliosphere. Nevertheless, the basic morphological predictions of both models remain the same (Figure 2, see in particular Alexashov & Izmodenov 2005 and Heerikhuisen et al. 2006). The heliospheric and LISM plasma is described by the magnetohydrodynamic equations

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} &= Q_\rho; && (1)\\
\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + (\gamma - 1)\nabla e + (\nabla \times \mathbf{B}) \times \mathbf{B} &= \mathbf{Q}_m; && (2)\\
\frac{\partial}{\partial t}\left(\frac{1}{2}\rho u^2 + e + \frac{B^2}{8\pi}\right) &+ \\
\nabla \cdot \left[\left(\frac{1}{2}\rho u^2 + \gamma e\right)\mathbf{u} + \frac{1}{4\pi}\mathbf{B} \times (\mathbf{u} \times \mathbf{B})\right] &= Q_e, && (3)\\
\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{u} \times \mathbf{B}) &= \mathbf{0}; && (4)\\
\nabla \cdot \mathbf{B} &= 0, && (5)
\end{aligned}$$

together with the equation of state $e = 2nk_{\mathrm{B}}T/(\gamma - 1) = p/(\gamma - 1)$. The proton and electron temperatures are assumed equal in these models. The remaining variables have their usual definitions and $Q_{(\rho,m,e)\mathrm{p}}$ denote the source terms for plasma density, momentum, and energy. They are listed in Pauls et al. (1995) and Zank et al. (1996). The coupling to the neutral component is accomplished by solving the Boltzmann equation for interstellar neutrals

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \left(\frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}}\right) f = P - L, \qquad (6)$$

where $f(\mathbf{x}, \mathbf{v}, t)$ is a particle distribution function expressed in terms of position $\mathbf{x}$, velocity $\mathbf{v}$ and time t. $\mathbf{F}$ is the force acting on a particle of mass m, typically gravity and radiation pressure. The terms P and L describe the production and loss of particles at $(\mathbf{x}, \mathbf{v}, t)$, and both terms are functions of the assumed plasma and neutral distributions. Multi-fluid equations can be derived from (6) when appropriate source terms for different regions are constructed (Pauls et al. 1995). The set of equations (1)–(6) are solved self-consistently.

The neutral kinetic codes, when coupled self-consistently to the background solar wind and LISM plasma, are computationally intensive, and so both kinetic approaches compromise in the scope of the problems they attack. The Monte Carlo approach has the potential to yield good neutral atom statistics since it is assumed that the solar wind is inherently steady state. Thus, very long integration times can be used to build up particle statistics. The drawback, however, is that solar wind properties vary on an 11-year scale (Lazarus & McNutt 1990; McComas et al. 2000). Since the time for a neutral atom to enter the heliosphere and reach 1 AU is $\sim$ 15–20 years, the local neutral atom distribution has experienced both a variable charge exchange and photoionization rate, as well

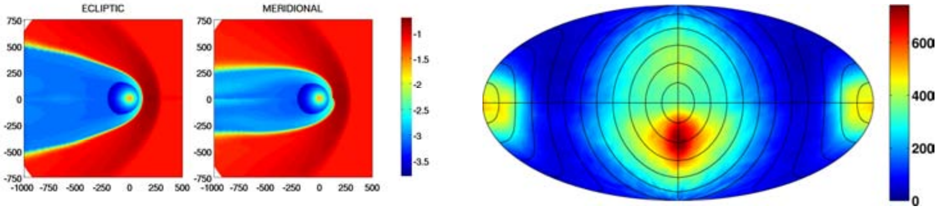

Figure 3. 3D plasma temperature plot for a multi-fluid MHD model with an assumed interstellar magnetic field in the ecliptic plane at 90 degrees to the flow (left). (right) All sky ENA maps of heliospheric neutral atoms observed at 1 AU for an energy of 200eV for the plasma profile. The map uses a Mollweide projection to plot heliospheric latitude horizontally and longitude vertically. The interstellar flow originates from the center of the plot, with the heliotail showing at the extreme left and right.

as a supersonic solar wind whose extent, in both latitude and longitude, velocity and density is highly variable (McComas et al. 2000; Pauls & Zank 1997, 1995; Tanaka & Washimi 1999). Thus, the problem of neutral atom interaction with the solar wind is inherently time-dependent and non-stationary. Neutral atom characteristics will therefore depend on solar cycle, with the overall distribution being a mixture of atoms created in temporally different solar wind environments, since they cannot be lost to the system on time scales shorter than the solar cycle. This requires a time dependent approach to the modelling of the solar wind-LISM neutral atom interaction. We have developed such a time-dependent Monte Carlo code for interstellar hydrogen (Heerikhusen et al. 2006). Nonetheless fast 3D simulations typically continue to use a multi-fluid framework (Pogorelov et al. 2006). Figure 3 illustrates an example 3D MHD simulation using a multi-fluid model (left panel), and the right panel shows the 3D distribution of energetic neutral H at 1 AU. Finally, the pickup ions should in principle be described separately on the basis of a focussed transport equation (e.g., Florinski et al. 2006 or le Roux et al. 2006) and the cosmic rays by the cosmic ray transport equation (Florinski et al. 2003), both of which should be coupled self-consistently to the global plasma-neutral H models. These efforts are underway but not discussed here.

3. Conclusions

For the purposes of this report, we focused on our activities in developing state-of-the-art 2D and 3D codes to model the outer heliosphere and its interaction with the partially ionized local interstellar medium (LISM). These codes couple self-consistently a fluid MHD description of the solar wind and LISM plasma to either a multi-fluid or a kinetic/Boltzmann model of interstellar neutral gas. This work led to the prediction of the "hydrogen wall" and its subsequent discovery by Linsky & Wood (1996) and Gayley et al. (1997). The coupling of the solar wind to the local interstellar medium occurs through the intermediary of neutral interstellar atoms (beyond some 10–15 AU, the dominant constituent of the heliosphere, by mass, is neutral interstellar H). Charge exchange couples the plasma and neutral atom populations, yielding a highly non-equilibrated, nonlinear system in which the characteristics of both populations are strongly modified (and the creation of new particle populations such as pickup ions, anomalous cosmic rays, energetic neutral atoms (ENA), for example). The self-consistent coupling of disparate plasma regimes, each governed by possibly distinct plasma physical processes, is a challenge that must be addressed by a new generation of computational modelling. The code that we are developing takes the first steps in this direction.

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References

The Sun to the Earth - and Beyond, Panel Reports, 2003 National Research Council Decadal Review of Solar and Space Physics, Chair, L. Lanzerotti.
Alexashov, D., & Izmodenov, V. 2005, Astron. Astrophys., 439, 1171
Baranov, V. B., & Malama, Y. G. 1993, J. Geophys. Res., 98, 15157
Baranov, V.B., & Malama, Y. G. 1995, J. Geophys. Res., 100, 14755 1995.
Fahr, H. J., Kausch, T., & Scherer, K. 2000, Astron. Astrophys., 357, 268
Florinski, V., Zank, G. P., & Pogorelov, N. V. 2003, J. Geophys. Res., 108(A6), 1228, doi:10.1029/2002JA009695
Florinski, V., le Roux, J. A., & Zank, G. P. 2006, Adv. Space Res., in press
Gayley, K. G., Zank, G. P., Pauls, H. L., Frisch, P. C. & Welty, D. E. 1997, Astrophys. J., 487, 259
Heerikhuisen, J., Florinski, V., & Zank, G. P. 2006, J. Geophys. Res., 111, A06110, doi:10.1029/2006JA011604
Izmodenov, V. V., Geiss, J., Lallement, R., Gloeckler, G., Baranov, V. B., & Malama, Y. G. 1999, J. Geophys. Res., 104, 4731
Kryukov, I. A., Borovikov, S. N., Pogorelov, N. V., & Zank, G. P. 2006, this volume
Lazarus, A. J. & McNutt, Jr., R. L. 1990, in Physics of the Outer Heliosphere, ed. S. Grzedzielski & D. E. Page (Pergamon)
le Roux, J.A. Webb, G. M., Florinski, V., & Zank, G. P. 2006, ApJ, in press
Liewer, P. C., Karmesin, S. R., & Brackbill, J. U. 1996, J. Geophys. Res., 101, 17119
Linsky, J. L., & Wood, B. E. 1996, ApJ, 463, 254
Lipatov, A. S., Zank, G. P., & Pauls, H. L. 1998, J. Geophys. Res., 103, 20631
McComas, D. J., Barraclough, B. L., Funsten, H. O., Gosling, J. T., Santiago-Muñoz, E., Skoug, R. M., Goldstein, B. E., Neugebauer, M., Riley, P., & Balogh, A. 2000, J. Geophys. Res., 105, 10419
Müller, H.-R., Zank, G. P., & Lipatov, A. S. 2000, J. Geophys. Res., 105, 27419
Pauls, H. L., Zank, G. P., & Williams, L. L. 1995, J. Geophys. Res., 100, 21595
Pauls, H. L., & Zank, G. P. 1997, J. Geophys. Res., 102, 19779
Pogorelov, N. V., Zank, G. P., & Ogino, T. 2004, ApJ, 624, 1007
Pogorelov, N. V., Zank, G. P., & Ogino, T. 2006, ApJ, 644, 1299
Tanaka, T., & Washimi, H. 1999, J. Geophys. Res., 104, 12605
Wang, C., & Belcher, J. W. 1998, J. Geophys. Res., 103, 247
Williams, L. L., Hall, D. T., Pauls, H. L., & Zank, G. P. 1997, ApJ, 476, 366
Zank, G. P. 1999, Space Sci. Rev., 89, 413
Zank, G. P., & Müller, H.-R., 2003, J. Geophys. Res., 108(A6), 1240, doi:10.1029/2002JA009689
Zank, G. P., Pauls, H. L., Williams, L. L., & Hall, D. T. 1996, J. Geophys. Res., 101, 21639