Structure-Preserving Kinetic Models for Magnetic Reconnection

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1 Statement of Problem

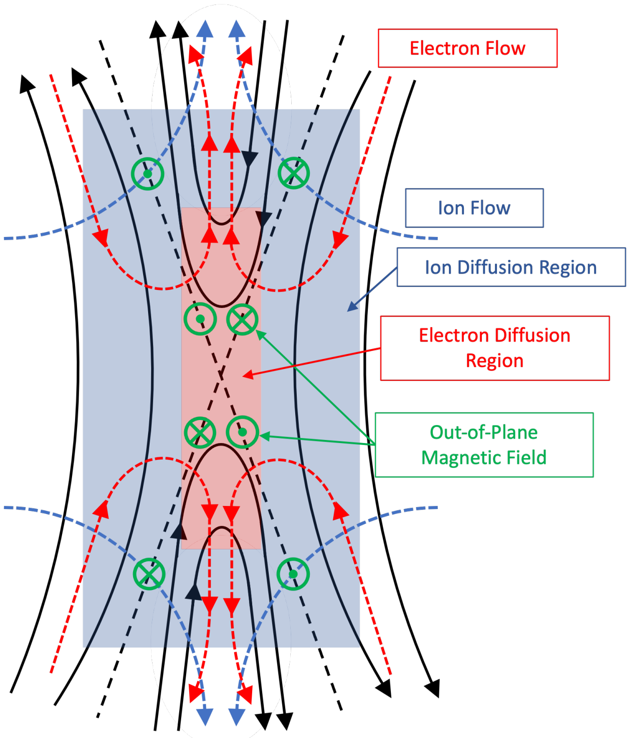

Figure 1: Kinetic description of magnetic reconnection. Electrons (red dashed lines) and ions (blue) flow in the reconnection plane together with reconnecting field line components (black solid lines) projected in the reconnection plane. The green marks are out-of-plane field components. From Yamada et al. (2014).

How magnetic reconnection converts magnetic field energy into plasma kinetic energy is the question at the core of stellar (and more locally solar) physics. Numerous plasma systems, such as flares (Su et al., 2013), coronal mass ejections (CMEs; J. Lin et al., 2000; Riley, Linker, et al., 2002; Riley, Lionello, et al., 2007), and the Earth's magnetotail (Baker et al., 1976; Borg et al., 2007), depend on magnetic reconnection for the creation of highly energetic particles. In the magnetotail, electron energies reach hundreds of thousands of electron volts, whereas the typical electron energies associated with large-scale reconnection-driven flows are just a few electron volts. Microscale plasma processes play a critical role in energizing these electrons, along with nearby ions. However, these microscopic dissipation process are always under the influence of macroscopic physics, as the microscopic kinetic regions are surrounded by global macroscopic systems. Given the inherent multiscale nature of magnetic reconnection, developing accurate and scalable numerical approaches to magnetic reconnection is essential.

Advancements in computational magnetic reconnection models have provided key frameworks for matching and predicting emissions from reconnection events. These models are essential in planning future space missions, as they give insights into what kinds of energy emissions and spectra can be expected in various environments. Accelerated ions are a major hazard to naval assets posed by reconnection events in space. While electrons are responsible for driving the general dynamics of the plasma system, ions plays a key role in determining the dangerous radiation environment (Laming et al., 2023). The multiscale nature of reconnection events makes constructing a single algorithm a significant challenge, though. Traditional fluid-based MHD approaches can capture large-scale dynamics but are dependent on assumptions of local thermal equilibrium and collisionality that limit their accuracy at microscales.

Furthermore, MHD models fail to predict observed heating within plasma systems. Kinetic plasma descriptions, shown in Figure 1, based on the Vlasov-Maxwell (or Fokker-Planck) equations are the primary tool for studying microscale collisionless magnetic reconnection, as they self-consistently include key reconnection physics and the feedback of energetic particles in the reconnection region. These approaches can more accurately estimate heating rates within plasmas as well as other key parameters. The inclusion or exclusion of inter- and intra-species collisions in the plasma affects the flow of particles along electromagnetic lines, providing key insights into reconnection dynamics in a variety of environments. Thus, capturing ion and electron interactions in varying degrees of collisionality is a vital piece of any computational approach.

Of particular interest is the production of nonthermal particles, in which a fraction of the plasma population is driven to energies considerably larger than the ambient plasma. In solar flares, upwards of 50 percent of the energy released can appear as energetic nonthermal electrons (R. P. Lin and Hudson, 1971; R. P. Lin, Krucker, et al., 2003). These nonthermal electrons can cause microscopic plasma instabilities and generate electromagnetic emission across the entire spectrum, including radiowaves (Wild et al., 1963; McLean et al., 1985), hard X-rays (HXRs) (R. P. Lin and Hudson, 1971; R. P. Lin, Krucker, et al., 2003), and gamma rays (Pesce-Rollins et al., 2021). Significant observational evidence has been found for the additional acceleration of ions inside the Earth's magnetosphere/magnetotail over the last few decades (Bingham et al., 2020; Lu et al., 2020; Richard et al., 2022). However, observing energized nonthermal ions in the solar atmosphere has proved a more difficult task, as nonthermal ions do not have as convenient energy signatures as electrons (Shih et al., 2009; Emslie et al., 2012). New instrumentation allows techniques (Kerr et al., 2023), utilizing Lyman α and β lines, to provide a better framework for detecting deka-keV nonthermal ions produced by magnetic reconnection events.

Extensive efforts have been expended in recent years to cast a fully collisional Vlasov-Maxwell-Landau set of equations in terms of a metriplectic formulation, consisting of separate Hamiltonian and dissipative solvers (Adams, Samtaney, et al., 2010; Adams, Hirvijoki, et al., 2017). Metriplectic systems combine an infinitesimal generator of Hamiltonian transformations $\mathcal{H}$ with a generator of entropy-generating transformations $\mathcal{L}$. The symmetric generator is a Casimir of the Poisson bracket, $\{\mathcal{H}, \mathcal{L}\} = 0$, and the symplectic generator is a Casimir of the metric bracket, $[\mathcal{L}, \mathcal{H}] = 0$. The PETSc particle-in-cell (PETSc-PIC; Pusztay et al., 2022; D. S. Finn et al., 2023; D. Finn, 2023) algorithm is a newly developed, scalable and composable toolkit for structure-preserving plasma simulations based in the Portable, Extensible Toolkit for Scientific Computation library (PETSc; Balay, Gropp, et al., 1997; Balay, Abhyankar, et al., 2023). The PETSc-PIC algorithm is capable of simulating electrons and ions inside conditions experienced in a variety of magnetic reconnection environments, such as the solar atmosphere, and running at larger scales than previous kinetic approaches have achieved. As a composable toolkit, individual tools from the PETSc-PIC library can, additionally, be placed inside existing methods to improve scalabilty, accuracy, and a variety of other aspects of kinetic simulations.

Fully kinetic simulations are more expensive than traditional fluid methods and limited in scale. To resolve this increased computational cost, hybrid kinetic-fluid methods, in which electrons are treated as a thermally equilibrated fluid and ions as particles, have been considered. However, questions of accuracy between fully kinetic and hybrid methods are still prominent. Thus, considering methods capable of scaling up fully kinetic computational models is a desirable alternative. During my postdoctoral research I will use kinetic methods to model microscale magnetic reconnection processes and consider how these microscale dynamics play a role in the macroscale plasma systems. This model will provide valuable insight into how the inclusion of nonthermal ions and inter-/intra-species particle collisions affects the transport of energy from magnetic field to particles. Furthermore, I will study how magenetic reconnection dynamics are affected by environmental plasma parameters, such as temperature, mean free path, conductivity, and the ratio of the thermal plasma pressure to the magnetic field pressure, β.

2 Background: Introduction to Magnetic Reconnection

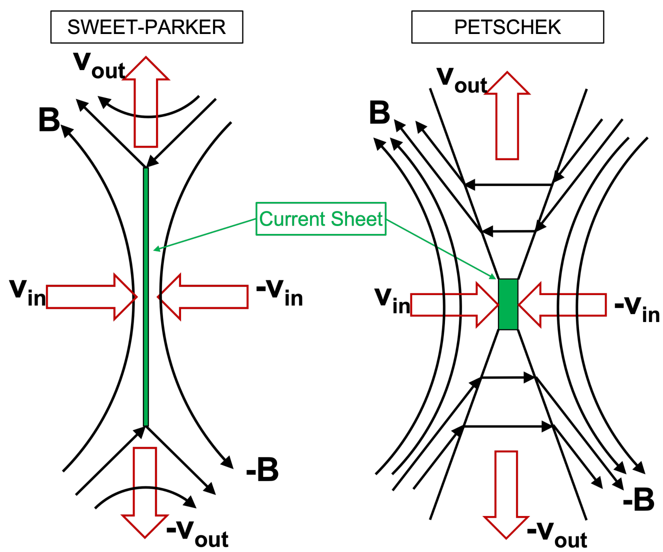

Figure 2: The two basic fluid models of reconnection. *Left*: Sweet-Parker's long thin current sheet model with all plasma flow across the sheet. *Right*: Petschek's small (unspecified) diffusion region/slow shock model. The proposed slow shocks are the four separatrices emanating from the corners of the diffusion region in this figure.

The classical view of electron acceleration during magnetic reconnection events, based on the Sweet-Parker model (left side of Figure 2; Parker, 1957), consists of a laminar reconnection scenario with a Y-type current flow. The Sweet-Parker model is characterized by slow reconnection rates, thus forming elongated, thin current sheets where the reconnection takes place. These reconnection rates, however, are not matched by observations in the solar atmosphere and magnetotail (Patel et al., 2020). To resolve the inconsistencies between the model and observations, Petschek modified the Sweet-Parker model of reconnection to account for a finite electrical conductivity only in a narrow region of space (Petschek, 1964), characterized by the presence of magnetic X-lines. This small highly-resistive reconnection site (right side of Figure 2) locally affects just a narrow flow channel. In order to deviate the flow and fields outside the reconnection site, it becomes the source of four slow shocks forming separatrices through which remaining flow can pass outside the resistive reconnection site.

When magnetic reconnection develops in multiple X-lines, the outflow plasmas from neighbor reconnection sites form low density structures with strong magnetic fields. These magnetic islands, or "plasmoids", are organized as beads in a chain, as shown in Figure 3. The existence of plasmoids in a reconnection system can be indicated by the plasma Lundquist number, S, which describes a plasma's conductivity. In high Lundquist plasmas ($S \sim 10^4$), such as those in the solar atmosphere, plasmoid chains are highly dynamic configurations which can rapidly grow by coalescence, bounce and eject smaller plasmoids. The development of plasmoids is inherently a macroscale fluid process. However, these plasmoids accelerate local electrons and ions at the microscale (Drake et al., 2006), which in turn makes subsequent reconnections faster. Numerical simulations of reconnection at high Lundquist number regimes (Lapenta, 2008; Huang et al., 2010; Uzdensky et al., 2010) have demonstrated that reconnection rates in such systems are faster than predicted by Sweet-Parker and even Petschek reconnection.

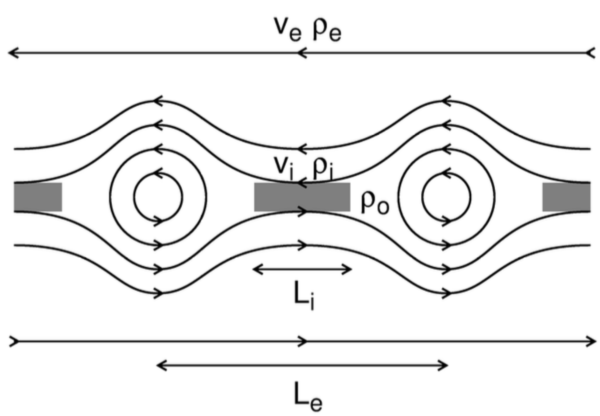

Figure 3: Schematic diagram of a reconnection current sheet with characteristic external scale length L_e, and interior length of diffusion region (shown in gray), formed around an X-line of L_i. The exterior and interior flow velocities are v_e and v_i, respectively. Magnetic islands form either side of the diffusion regions, and are the sites of electron heating as they evolve and merge. From Laming et al. (2023).

The Sweet-Parker and Petschek models depend on fluid approximations, such as local thermal equilibrium, making them accurate at larger scales (Leake, Lukin, Linton, and Meier, 2012; Leake, Lukin, and Linton, 2013). As we have discussed, reconnection is, however, necessarily a localized process, though its effect is usually global, since the formal smallness of the flux conservation breaking terms in Ohm's law requires a strong enhancement of local gradients. A fluid model usually requires some dissipation to prevent solutions from becoming singular. Hence, we can distinguish between collisional, quasi-collisionless and fully collisionless processes. In the collisional case, the reconnection time scale depends sensitively on the value of the dissipation coefficient. In the quasi-collisionless and fully collisionless cases, however, where the role of dissipation is not different from the coarse-graining process required to introduce irreversibility and dissipation in Vlasov theory, the scale is essentially independent thereof. The collisionalilties of plasmas are primarily indicated by the plasma density, temperature and mean free path, which can vary greatly between systems.

Magnetic reconnection is often observed in regions with low densities and high mean free paths, indicating a collisionless plasma. In this regime, the electrons and ions are mainly accelerated in the current layer formed at the center of the exhaust and are ejected along the field lines. The dissipation, or resistivity around the X-line, in this case, is caused by the transport of the electron momentum in a diffusion region scaled by the electron kinetic scales. The momentum transport of the electrons is achieved due to the Speiser-type motions in the vicinity of the X-line and/or the wave-particle interactions that disturb the electron motions (Speiser, 1970). The Speiser-type motions generate electron pressure tensor terms in the generalized Ohm's law. The energy conversion, then, occurs around the X-line so that electrons obtain significant energy from the electric and magnetic field. Recent observations (Bingham et al., 2020; Richard et al., 2022; Kerr et al., 2023) indicate, however, that a large amount of the released energy from the reconnection event is absorbed by the ions, which have a much larger mass than the electrons and thus must play a vital role in the energy transfer system. In denser systems, such as the chromosphere, where mean free paths are low, collisions hinder the rearrangement of magnetic field lines, slowing reconnection rates.

3 General Methodology

The primary computational challenge in modeling reconnection events lies in the multiscale nature of the system. Numerical methods for modeling plasmas, whether in space or laboratories, have traditionally been separated into two categories: kinetic and fluid. Fluid-like MHD models, an extension of simple hydrodynamic methods to electrically conducting fluids, have long been the primary choice in simulating magnetic reconnection (Bradshaw et al., 2013; Nicholeen et al., 2020) and other solar phenomena due to their ability to capture large-scale, slowly-evolving plasma dynamics. Given the scale of global dynamics on the Sun, along with the historic limitations of computing power, this choice has been the only feasible one and made way for a general understanding of the dynamics of these processes. MHD algorithms, however, are unable to capture kinetic processes, such as the acceleration of electrons and ions from the released magnetic energy, in microscopic regions which enable the macroscale dynamics. In the microscale regimes, MHD methods also struggle with problems of *non-locality* (Cho, 2010) and, furthermore, are fundamentally dependent on the particle distribution being Maxwellian and thermally equilibrated. This assumption of thermal equilibrium often breaks down when non-local effects become more pronounced. The presence of these small scale kinetic effects warrants the need for structure-preserving kinetic algorithms capable of accurate, scalable runs. The governing equations of continuum MHD must be supplemented, or supplanted, with kinetic models, such as the Vlasov-Maxwell-Landau equation.

Previous work has been done in constructing kinetic algorithms for the Vlasov-Maxwell-Landau equation. However, these algorithms often fail to preserve fundamental thermodynamic qualities of the plasma, such as conservation of energy, or ignore certain dynamics of the plasma that may be more impactful than previously thought. Metriplectic particle-in-cell (PIC) methods (Evstatiev et al., 2013; Kraus et al., 2017) offer an alternate approach for systems,

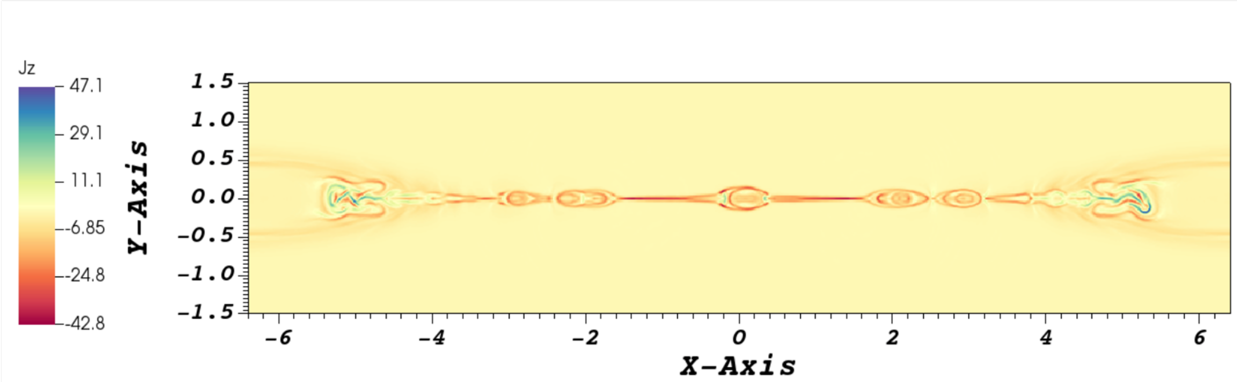

Figure 4: Out-of-plane current J_z from MHD simulation of magnetic reconnection in Harris current sheet representing post-CME current sheet in the solar corona. From Laming et al. (2023).

such as the Vlasov-Maxwell-Landau equation, that display both Hamiltonian and dissipative dynamics. Metriplectic formulations for kinetic plasma descriptions are desirable in regimes where MHD and other kinetics approaches fail to capture a complete picture of the plasma because they preserve the energy of the system as well as guarantee a local algebraic charge conservation law, long-time fidelity and stability of simulations. Furthermore, the use of well understood methods such as adaptive mesh refinement (Adams, Hirvijoki, et al., 2017), high-order accurate discretizations, as well as the effective use of modern heterogeneous hardware can ameliorate computational challenges posed by the high dimensionality of PIC models. All of these methods have been implemented and tested in the PETSc library and will be utilized during this project. It is important to note, however, that the long-time fidelity achieved by these methods are relative to kinetic scales, which are shorter than those considered in MHD models. Kinetic methods become too computationally costly when considering the scales traditionally treated with MHD models. An ideal approach to constructing a model for magnetic reconnection lies in the coupling of kinetic and MHD algorithms (Baumann et al., 2012; Lapenta et al., 2020).

All of these methods require mathematical expertise and add to the software complexity, which puts a high premium on extensible, community implementations that can be easily embedded in existing simulators. Moreover, structure-preserving discretizations can produce algebraic problems that pose difficulties for iterative solvers, and require new approaches for scalability on supercomputers. Finally, this structure must be preserved when different computational models are combined, such as particle-based kinetic formulations and continuum methods.

This proposed work utilizes tools built in PETSc, a well-known library for numerical methods. PETSc provides parallel data management, structured and unstructured meshes, linear and nonlinear algebraic solvers and preconditioners, optimization algorithms, time integrators and many more functions. The approach taken in the development of simulation algorithms in PETSc differs from that in previous literature in that the goal is to develop a toolkit of solvers is desired instead of monolithic “Application Codes.” By building a suite of individual composable solvers, that are parallelized by construction, a wide range of simulations can be built with little effort. In this work, we utilize the existing PETSc particle-in-cell (PETSc-PIC) algorithm to study magnetic reconnection under a variety of plasma conditions. The PETSc-PIC algorithm is highly scalable and capable of using cost reducing techniques, such as adaptive mesh refinement (AMR) and multigrid methods. With these scalable methods, the PETSc-PIC algorithm can approach (if not match) the larger scales considered by many of the hybrid PIC methods, as well as some MHD approaches.

4 New Particle-In-Cell Methods

For a kinetic approach to be successful, we must define a small subsection of the reconnection system to model. In this work, we will focus on a simple Harris-type plasma current sheet model (Harris, 1962), shown in Figure 4, consisting of an initial magnetic field $\mathbf{B}(z) = B_0 \tanh(z/\delta)\mathbf{e}_x$, where B_0 is the asymptotic magnetic field magnitude, and δ is the current sheet half-width. The initial plasma density contains the Harris sheet $n_1(z) = n_0 \operatorname{sech}^2(z/\delta)$, where n_0 is the peak density of the Harris current sheet, and a background plasma density $n_2(z) = n_b$. This system has been previously modelled using a variety of MHD (Adams, Samtaney, et al., 2010) and kinetic (Fujimoto, 2018; Lu et al., 2020) solvers. For example, the Geospace Environmental Modeling (GEM; Birn et al., 2001) test case, a particular 2D collisionless case of the Harris current sheet model, has become a popular system for testing both fluid and kinetic models.

A key aspect of utilizing computational models is validating models against existing reconnection observations and predicting future reconnection events. Simulations must be designed to output parameters, such as electron and ion energy flux profiles, spectra and magnetic field profiles. Laming et al. (2023) found that if magnetic islands form and merge under conditions that render the electrons collisionless, non-Maxwellian electron velocity distribution functions may result in subsequent effects in the ionization of the CME ejecta and distortion of the charge state distribution from that expected with Maxwellian electrons. The non-Maxwellian electron distributions can be best characterized by kappa-distributions. Using kinetic methods, which can accurately track the evolution of non-Maxwellian distributions, will provide valuable insight into how these electron distributions evolve in reconnection systems.

Comparing the computational results to observational reconnection evidence remains, however, a significant challenge as microscale observational data is scarce. The primary mode of accuracy verification in this project will, thus, be testing the PETSc-PIC algorithm against existing methodologies. These methodologies will include kinetic algorithms, such as those presented in (Fujimoto, 2018) and (Lu et al., 2020), and MHD tests of small scale reconnection, such as the one considered in (Laming et al., 2023).

The first step of this work will be including magnetic solvers into the PETSc-PIC algorithm. Previous work with PETSc-PIC has been done on the magnetic-free Vlasov-Poisson-Landau system. However, the magnetic field solve utilizes the same methodology used to calculate the electric field at each time step. Thus, the magnetic solve can be included in the PETSc-PIC algorithm with relative ease. In simple cases, we may consider a single species (electrons) system with an charge neutralizing background of ions. This simplification assumes the ions undergo little change in the PIC time/space scales considered in verification tests. However, when considering more complex reconnection systems, ions will be modeled as a separate species of particles.

The magnetic and electric fields generated by the charged particles are solved for at each time step using finite element methods. Early tests of the PETSc-PIC algorithm have utilized H^1 finite elements (Logg et al., 2011) which have shown to be accurate in simple plasma tests, such as Landau damping. H^1 finite elements, however, do not preserve the continuity and smoothness of the electric and magnetic fields across spatial cell boundaries. In more complex plasma systems, such as magnetic reconnection, these discontinuities will affect the accuracy of the field solves. Introducing a mixed weak form for the electric and magnetic equations, however, allows for the use of $H(div)$ finite elements, such as the Raviart-Thomas (Raviart et al., 1977) and Brezzi-Douglas-Marini (BDM) (Brezzi et al., 1985) elements. These mixed methods maintain the continuity of the electric and magnetic fields across cell boundaries, making them desirable in magnetic reconnection systems, and plasma applications in general. The particle pushing is then simultaneously conducted at each time step by conservative timesteppers, such as symplectic and implicit Runge-Kutta integrators (Hairer et al., 2002). With a full Vlasov-Maxwell solver implemented, we will verify the accuracy of the PETSc-PIC algorithm against existing computational work.

Having verified the accuracy of the PETSc-PIC algorithm in magnetic reconnection events against existing collisionless computational methods, we will develop a collisional Harris current sheet test case. The collisionality of the plasma has been shown to play a role in the transfer of energy from the magnetic field to the particles. In the strongly collisional plasmas, such as magnetic reconnections in solar/stellar photosphere and chromosphere, the plasma resistivity induces a reconnection electric field as described by the Sweet-Parker model, which leads to a rather slow reconnection with low reconnection rate. By contrast, in the weakly collisional or collisionless regime, such as those occurring in magnetopause and magnetotail, the induced reconnection electric field results in a fast reconnection that is independent of the plasma collision rate. In an effort to study a multitude of plasma systems, it is, therefore, important to construct a computational framework, such as PETSc-PIC, capable of capturing varying plasma parameters, such as β, density, temperature, and mean free path.

In the final stage of this work, we will use the developed computational framework to consider a variety of initial plasma states and field conditions present in various reconnection environments. Theoretical and computational studies have shown that the evolution of electric and magnetic fields depends heavily on the plasma properties (Biskamp, 1997), in particular, the collision rate and the plasma β. Most early work (Hoshino et al., 2001; Drake et al., 2006; Oka et al., 2010) in modelling reconnection with kinetic methods focused on relatively high-β ($\beta > 0.1$) environments, where the energization does not strongly modify the particle distribution function. Recent kinetic models (Guo et al., 2014; Werner et al., 2016; Li et al., 2017), as well as observations (Alaoui et al., 2019), however, have shown that in low-β environments ($\beta << 1$), common in the solar atmosphere and elsewhere, particle distributions can develop into broken power-laws or kappa distributions. This makes kinetic approaches highly desirable, as they can capture evolving, non-maxwellian distributions.

5 Expected Results

Simulation of plasmas is among the most demanding computational physics tasks. Important behavior occurs on many, widely separated, but tightly coupled scales in both space and time. Correctly capturing the multi-scale physics which underpins these processes, in a way that is tractable with existing hardware resources, is dependent on access to structure-preserving discretizations of the Vlasov-Maxwell-Landau system and its variants. This project will integrate the development of long-time structure-preserving discretizations and solvers with deployment in open-source community software to provide complete applications to the computational science community that employ state-of-the-art software engineering practices and leverage modern heterogeneous hardware effectively. We will extend the theory and development of these structure-preserving methods for plasmas with a focus on energy transfer in magnetic reconnection events. The high degree of scalability of the PETSc-PIC algorithm provides a good framework for modelling reconnection systems considerably larger than previous kinetic methods have achieved.

At the core of this research project is the question; how is energy, expelled during magnetic reconnection events, captured by local particles? This question has plagued plasma physicists for decades. Thus, we cannot expect to resolve it in its entirety during this project alone. We have, therefore, isolated three smaller problems within this question that we will pursue during this project. **First (year 1), we will construct magnetic field solvers in the existing PETSc-PIC framework and consider how the inclusion of ion dynamics affects reconnection rates and plasma heating.** Observations from the magnetosphere/magnetotail, along with more recent observations from the solar atmosphere, indicate ions play a significant role in capturing energy from reconnection and may drive the dynamics of the plasma due to their higher masses than more easily observed electrons. Furthermore, ions are responsible for creating dangerous radiation which poses a serious threat to naval assets in space. Comparing models with and without ions will give valuable insight into how energy is captured by each species of particle. **Secondly (year 1-2), we will develop a fully metriplectic collisional test case to study the impact of collisions on reconnection.** Inter- and intra-species collisions slow the flow of particles along electromagnetic field lines by dissipating the total energy away from the particles. Collisionless assumptions are often accurate in low-β plasma environments but lack versatility in modelling a wider array of reconnection scenarios. **Lastly (year 2), we will use the PETSc-PIC algorithm to study a wide range of plasma states and conditions.** Varying plasma parameters, such as β, density, temperature, and mean free path, will provide insight into how reconnection is modified by its environment. We will primarily focus on two different plasma environments: the solar corona and chromosphere. The development and application of the PETSc-PIC framework to these environments will be a major step forward in modelling and understanding magnetic reconnection and its effect on plasmas. It will not only aid in the study of magnetic reconnection in this project, but provide an open-source computational toolkit to the astrophysical community as a whole.

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