Global magnetohydrodynamic magnetosphere simulation with an adaptively embedded particle-in-cell model

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Key Points:

- We perform a global simulation of a geomagnetic storm event with kinetic modeling of the magnetotail reconnection
- The kinetic region is adaptively embedded to the MHD model and the reconnection sites are identified by physical criteria during the runtime
- The global scale, mesoscale and electron scale features are observed simultaneously in one simulation

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Abstract

We perform a geomagnetic event simulation using a newly developed magnetohydrodynamic with adaptively embedded particle-in-cell (MHD-AEPIC) model. We have developed effective criteria to identify reconnection sites in the magnetotail and cover them with the PIC model. The MHD-AEPIC simulation results are compared with Hall MHD and ideal MHD simulations to study the impacts of kinetic reconnection at multiple physical scales. At the global scale, the three models produce very similar SYM-H and SuperMag Electrojet (SME) indexes, which indicates that the global magnetic field configurations from the three models are very close to each other. At the mesoscale we compare the simulations with in situ Geotail observations in the tail. All three models produce reasonable agreement with the Geotail observations. The MHD-AEPIC and Hall MHD models produce tailward and earthward propagating fluxropes, while the ideal MHD simulation does not generate flux ropes in the near-earth current sheet. At the kinetic scales, the MHD-AEPIC simulation can produce a crescent shape distribution of the electron velocity space at the electron diffusion region which agrees very well with MMS observations near a tail reconnection site. These electron scale kinetic features are not available in either the Hall MHD or ideal MHD models. Overall, the MHD-AEPIC model compares well with observations at all scales, it works robustly, and the computational cost is acceptable due to the adaptive adjustment of the PIC domain.

1 Introduction

A geomagnetic storm is a major disturbance of Earth's magnetosphere that occurs when a significant amount of energy is deposited into the geospace. The most widely used and successful simulation tools to study the gomagnetic storms are based on the magnetohydrodynamic (MHD) description, which is computationally feasible to solve. The first global MHD models were developed in the 1980s (LeBoeuf et al., 1981; Wu et al., 1981; Brecht et al., 1981, 1982). Later on, models with more advanced numerical algorithms have been developed, such as the Lyon-Fedder-Mobarry (LFM) (J. G. Lyon et al., 1986; J. Lyon et al., 2004), the OpenGGCM (Raeder et al., 1995, 1996) and the GUMICS (Grand Unified Magnetosphere Ionosphere Coupling Simulation) model (Janhunen, 1996).

In this paper, we use the University of Michigan's Space Weather Modeling Framework (SWMF (Tóth et al., 2012)) which also includes an MHD model, the Block Adaptive-Tree Solar-wind Roe-type Upwind Scheme (BATS-R-US) (Powell et al., 1999) as its global magnetosphere (GM) component. The SWMF has been applied to many storm event simulations (Tóth et al., 2007; Glocer et al., 2009; Haiducek et al., 2017), which is also been selected as the physics-based model at the Space Weather Prediction Center based on a thorough model comparison (Pulkkinen et al., 2013).

Magnetic reconnection plays a key role in the magnetosphere both at the dayside and in the tail. Despite all the successful applications MHD models have achieved, magnetic reconnection in the global MHD models relies on either Hall resistivity, or ad hoc anomalous resistivity, or simply numerical resistivity. None of these approximations truly describe the physical processes responsible for collisionless reconnection. It is very important to properly represent kinetic reconnection physics in a global simulation and check if it plays an important role in contributing to the larger scale processes that eventually produce geomagnetic disturbances and space weather effects. Furthermore, the MHD approximation assumes that the distribution functions of the ions and electrons are Maxwellian. Numerous observations suggest that this condition is violated especially near the magnetic reconnection sites (L.-J. Chen et al., 2016; Burch et al., 2016; Hwang et al., 2019; Lotekar et al., 2020).

The MHD with embedded Particle-In-Cell (MHD-EPIC) model (Daldorff et al., 2014) enables kinetic physics to be introduced into a global MHD model. The MHD-EPIC

model has been successfully used to study the interaction between the Jovian wind and Ganymede's magnetopshere (Tóth et al., 2016; Zhou et al., 2019, 2020); flux transfer events (FTEs) at the Earth's dayside magnetopause (Y. Chen et al., 2017); Mars' magnetotail dynamics (Y. Ma et al., 2018) and the dawn-dusk asymmetries discovered at the Mercury's magnetotail (Y. Chen et al., 2019). However, the iPIC3D (Markidis et al., 2010) code, which is the PIC model used in the MHD-EPIC simulations, can only run on a fixed Cartesian grid. The magnetotail (and the associated current sheet that contains the reconnection sites) typically exhibits a flapping motion (Tsutomu & Teruki, 1976; Volwerk et al., 2013) during a geomagnetic storms. Covering the whole domain of interest where reconnection can occur in the magnetotail would require a very large PIC grid and would result in a massive computational cost. This may be feasible for a short simulation time (up to an hour or so) but geomagnetic storms that usually happen last for days, the computational cost would become prohibitive.

To tackle this problem, we have developed the MHD with Adaptively Embedded PIC (MHD-AEPIC) alogorithm. Shou et al. (2021) introduces this idea and verifies that by dynamically changing the region of the computational domain where the PIC model is applied, the numerical solution doesn't change essentially compared to a larger fixed PIC domain. In this paper, we further improve this method and make it more flexible: 1. The size and shape of the active PIC regions can be adapted during the runtime; 2. The adaptation of the active PIC region is fully automatic. To realize the first feature, instead of iPIC3D, we use the FLexible Exascale Kinetic Simulator (FLEKS) (Y. Chen et al., 2021) as the PIC model. FLEKS inherits all numerical algorithms from MHD-EPIC, and also accommodates an adaptive PIC grid that allows PIC cells to be turned on and off during the simulation. In addition, FLEKS employs a particle splitting and merging scheme to improve the simulation efficiency and accuracy. FLEKS is described in more detail in Section 2.2.

We have developed a reliable and efficient algorithm to identify potential reconnection sites in the magnetotail using three local criteria. The criteria are easy to compute and provide the information to the FLEKS code to adapt its grid to cover the reconnection sites. This newly developed MHD-AEPIC model is applied to simulate a magnetic storm. The SWMF simulation involves BATSRUS, FLEKS, the ionosphere electrodynamics model RIM (Ridley et al., 2004) and the inner magnetosphere model RCM (Wolf et al., 1982; Toffoletto et al., 2003). This is the first simulation of a real event with kinetic reconnection physics in the magnetotail scaling from the global scales of the magnetosphere to the electron scales near the reconnection sites.

The computational methods are described in Section 2, the demonstration of the adaptation feature and comparisons between models and observations are shown in Section 3 and we summarize in Section 4.

2 Methods

2.1 Global Magnetosphere Model: BATS-R-US

The Block-Adaptive Tree Solar-wind Roe-type Upwind Scheme (BATS-R-US) is used as the Global Magnetosphere (GM) model in our simulation. In the Hall MHD and MHD-AEPIC simulations in this paper, the Hall MHD equations (Tóth et al., 2008) are solved. The Hall term is handled with a semi-implicit scheme. The spatial discretization uses a 2nd order accurate TVD scheme with the Artificial Wind Riemann solver (Sokolov et al., 1999) and the Koren limiter (Koren, 1993) with $\beta = 1.2$. The hyperbolic cleaning (Dedner et al., 2003) and eight-wave scheme (Powell et al., 1999) are used to keep the magnetic field approximately divergence-free.

The Hall MHD equations with a separate electron pressure equation are

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u}) \tag{1}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} = -\nabla \cdot \left[\rho \mathbf{u}\mathbf{u} + (p + p_e)\bar{I} + \frac{B^2}{2\mu_0}\bar{I} - \frac{\mathbf{B}\mathbf{B}}{\mu_0} \right] \tag{2}$$

$$\frac{\partial e}{\partial t} = -\nabla \cdot \left[(\epsilon + p)\mathbf{u} + p_e \mathbf{u}_e + \mathbf{u}_e \cdot \left(\frac{\mathbf{B}^2}{\mu_0}\bar{I} - \frac{\mathbf{B}\mathbf{B}}{\mu_0} \right) \right] + p_e \nabla \cdot \mathbf{u}_e \tag{3}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \left[\mathbf{u}_e \times \mathbf{B} + \frac{\nabla p_e}{ne} \right] \tag{4}$$

$$\frac{\partial p_e}{\partial t} = -\nabla \cdot (p_e \mathbf{u}_e) - (\gamma - 1) p_e \nabla \cdot \mathbf{u}_e \tag{5}$$

where $\bar{I}$ is the identity matrix, ρ is the mass density, $\mathbf{u}$ is the plasma bulk velocity, $\mathbf{B}$ is the magnetic field, p_e is the electron pressure, p is the ion pressure and $\mathbf{j} = \nabla \times \mathbf{B}/\mu_0$ is the current density. The Hall velocity and electron bulk velocity are defined as

$$\mathbf{v}_H = -\frac{\mathbf{j}}{ne} = -\frac{M_i}{e}\frac{\mathbf{j}}{\rho} \tag{6}$$

$$\mathbf{u}_e = \mathbf{u} + \mathbf{v}_H \tag{7}$$

where $n = \rho/M_i$ is the number density, M_i is the ion mass, and e is the elementary charge. The total energy density is defined as

$$e = \epsilon + \frac{B^2}{2\mu_0} = \frac{1}{2}\rho \mathbf{u}^2 + \frac{p}{\gamma - 1} + \frac{\mathbf{B}^2}{2\mu_0} \tag{8}$$

where $\epsilon = \rho \mathbf{u}^2/2 + p/(\gamma - 1)$ is the hydrodynamic energy density of the ions and $\gamma = 5/3$ is the adiabatic index. The thermal energy density of the electrons is $\epsilon_e = p_e/(\gamma - 1)$. We note that the $e + \epsilon_e$ is conserved both analytically and numerically as the non-conservative source terms $\pm p_e \nabla \cdot \mathbf{u}$ in equations (3) and (5) cancel out. Apart from $(\rho, \mathbf{u}, \mathbf{B}, p, p_e)$, other variables are derived quantities.

The continuity equation (1), momentum equation (2), energy equation (3) and electron pressure equation (5) are solved with an explicit time stepping scheme. In the induction equation (4), the convection term $\mathbf{u} \times \mathbf{B}$ and pressure gradient term $\nabla p_e/ne$ are solved using an explicit scheme, while the Hall term $\mathbf{v}_H \times \mathbf{B}$ is advanced with an implicit scheme. The Hall MHD equations introduce whistler mode wave, which has a characteristic wave speed inversely proportional to the wavelength. The shortest wavelength that exists in a numerical simulation is proportional to the cell size Δx, so the fastest whistler wave speed in a simulation is proportional to $1/\Delta x$. The time step in a fully explicit scheme is limited by the Courant-Friedrichs-Lewy (CFL) condition: $\Delta t < \Delta x/c_{\max}$, where $c_{\max}$ is the fastest wave speed, which leads to a time step proportional to $1/(\Delta x)^2$. We use a semi-implicit scheme (Tóth et al., 2012) to handle the stiff Hall term in the induction equation, so that the time step of the explicit part is only limited by the fast magnetosonic wave speed instead of the whistler speed.

A three-dimensional block-adaptive Cartesian grid is used to cover the entire computational domain $-224R_E < x < 32R_E$, $-128R_E < y, z < 128R_E$ in GSM coordinates. The Hall effect is restricted to $x \in [-100R_E, 20R_E], |y| < 30R_E$ and $|z| < 20R_E$ box region excluding a sphere of radius $3R_E$ centered at the Earth to speed up the simulation. Outside this region the Hall effect is neglected by setting $\mathbf{v}_H = 0$. The cell size in the magnetotail is refined to the resolution with $\Delta x = 1/4R_E$. About fourteen millions cells are used in total.

At the inner boundary $r = 2.5R_E$, the density is calculated by the formula $\rho_{\text{inner}} = 28 + 0.1\text{CPCP}$ amu/cm^3, where CPCP is the average of the northern and southern cross polar cap potentials measured in keV. This boundary condition has been used successfully in previous geomagnetic storm simulations (Pulkkinen et al., 2013). The pressure

and magnetic field $\mathbf{B}_1$ have zero gradient at the inner boundary, while the radial velocity is set to zero and the tangential velocity is calculated from the corotation and the $\mathbf{E}\times\mathbf{B}$ drift, where the electric field $\mathbf{E}$ is provided by the Ridley Ionosphere Model (RIM) (Ridley et al., 2004).

2.2 Particle-in-cell Model: FLEKS

The FLexible Exascale Kinetic Simulator (FLEKS) (Y. Chen et al., 2021) is used as the particle-in-cell (PIC) model (PC component in the SWMF) to resolve kinetic physics. FLEKS uses the same two-way coupling method as MHD-EPIC (Daldorff et al., 2014) and the Gauss's law satisfying energy-conserving semi-implicit method (GL-ECSIM) (Y. Chen & Tóth, 2019) for the PIC solver. To enable the adaptation in MHD-AEPIC, FLEKS introduces an adaptive grid that allows changing simulation region dynamically. Figure 1 shows a schematic plot of the adaptive grid.

FLEKS provides a particle merging and splitting scheme to maintain the number of particles per cell within bounds. Merging particles in a cell with high number of particles can improve load-balancing and speed up simulation, while splitting particles in a cell with few particles can reduce noise and improve accuracy for the PIC simulation. This feature is very useful keeping the number of particles per cell about uniform during a long geomagnetic storm simulation.

2.3 Selection Criteria of PIC Regions

As described in the previous section, FLEKS allows patches to be turned on and off during the simulation. To make the active PIC patches only cover the regions of interest, where magnetic reconnection is happening or will be triggered soon, the MHD model should locate these regions and pass this information to FLEKS. Finding the locations of magnetic reconnection sites can be done in various ways including tracing field lines (Glocer et al., 2016). For sake of efficiency and generality, here we use local criteria based on the local MHD solution only.

Magnetic reconnection usually happens in current sheets where the current density j is strong and the magnetic field B is weak. In particular, the field $B_\perp$ that is perpendicular to the current $\mathbf{j}$ should be close to zero, while the guide field parallel to the current can be non-zero. We define the following non-dimensional relation as our first criterion

$$\frac{J\Delta x}{B_\perp + \varepsilon} = \frac{J^2\Delta x}{|\mathbf{J}\times\mathbf{B}| + J\varepsilon} > c_1 \tag{9}$$

where $\mathbf{J} = \mu_0\mathbf{j} = \nabla\times\mathbf{B}$ and ε is a small dimensional constant in units of the magnetic field introduced to avoid dividing by zero. We use $\varepsilon = 1\,\mathrm{nT}$ in our simulations presented here, which is much smaller than the typical magnetic field intensity in the tail current sheet. Δx is the local cell size that is used in calculating the curl of the magnetic field, so that $J\Delta x$ is the jump of the transverse magnetic field between neighboring grid cells. We set $c_1 = 0.8$ in this work to select the cells that are close to the reconnection sites.

While criterion (9) works quite well in general, we sometimes find that it selects the axis of flux ropes, or O-lines, in addition to X-lines, especially if ε is very small. Reconnection does not occur at O-lines, so we developed a second criterion that distinguishes X- and O-lines based on the divergence of the magnetic field curvature vector:

$$[\nabla\cdot(\mathbf{b}\cdot\nabla\mathbf{b})](\Delta x)^2 > c_2 \tag{10}$$

where $\mathbf{b} = \mathbf{B}/|\mathbf{B}|$ is a unit vector along the magnetic field. We use $c_2 = -0.1$ to identify X-lines where the curvature vectors point away from the X-line, so their divergence is positive.

The above two criteria are identifying potential magnetic reconnection sites through local plasma properties in a general scenario. However, current sheets in the solar wind can also satisfy those two criteria. To make the selection more selective, we need to introduce a third criterion to exclude the volume outside the magnetosphere. Observations show that specific entropy is two orders of magnitude larger in the magnetosphere than in the magnetosheath (X. Ma & Otto, 2014) and our simulations properly reproduce these properties. Here we use the specific entropy as the third criterion:

$$\frac{p}{\rho^\gamma} > c_3 \tag{11}$$

where p is the plasma thermal pressure, ρ is the plasma density, and $\gamma = 5/3$ is the ratio of the specific heats (Birn et al., 2006, 2009). Different from the c_1 and c_2 introduced above, this criterion is dimensional and we use the threshold value $c_3 = 0.02\,\mathrm{nPa/cm^{-3\gamma}}$.

The three criteria combined can identify X-lines in the magnetotail well. To make the active PIC region large enough around the X-lines, we flag all patches where all three criteria are met, and then activate all patches within a distance L_x, L_y and L_z from these flagged patches in the x, y and z directions, respectively. We use $L_x = 4R_E$ and $L_y = L_z = 2R_E$ in this work.

Each MPI process of BATS-R-US calculates the above criteria on their respective sub-domains overlapping with the PIC grid and activate the patches of the PIC grid where all 3 criteria are satisfied. Then the processors collect the information: a PIC patch is activated if any of the BATS-R-US processes activated it. Since the status of all PIC patches (on/off) is stored in each MPI processor of BATS-R-US, using the default logical array would consume a lot of memory. To reduce the memory use, the status is stored by a single bit, which is 32 times smaller than the size of the default logical variable in Fortran. The information is conveniently collected with the bitwise "or" operator `MPI_BOR` used in the `MPI_ALLREDUCE` call.

2.4 Ionospheric Electrodynamics Model: RIM

The Ionospheric Electrodynamics (IE) is simulated by the Ridley Ionosphere Model (RIM) (Ridley et al., 2004) that solves a Poisson-type equation for the electric potential on a 2-D spherical grid. In this work, the grid resolution is set to 2° in both longitude and latitude directions. The lower latitude boundary is at 10° where the electric potential is set to zero.

The BATS-R-US and RIM models are two-way coupled every 5 seconds. To calculate the Poisson-type equation, RIM obtains the field-aligned currents (FAC) calculated at $3R_E$ from the BATS-R-US model and maps them down to its grid. The F10.7 flux is also an input parameter of RIM that is used together with the FAC to calculate the particle precipitation and conductances based on an empirical model. The electric field calculated by the RIM is mapped back to the inner boundary of BATS-R-US to obtain the $\mathbf{E} \times \mathbf{B}/B^2$ velocity for its inner boundary condition. The cross polar cap potentials (CPCP, (the difference of the maximum and minimum potentials in the two hemispheres) are also sent to BATS-R-US to set the density at the inner boundary.

2.5 Inner Magnetosphere Model: RCM

The Inner Magnetosphere (IM) is modeled by the Rice Convection Model (RCM) (Wolf et al., 1982; Toffoletto et al., 2003). The standard RCM settings are used, including an exponential decay term with a 10-hour e-folding rate. The decay term makes the Dst index recover better after strong storms.

The RCM model is one-way coupled with RIM and two-way coupled with BATS-R-US every 10 seconds. RIM sends the electric potential to RCM, where it is used to

advect the field lines with the $\mathbf{E}\times\mathbf{B}/B^2$ drift. In the two-way coupling between BATS-R-US and RCM, BATS-R-US identifies the closed field line regions and calculates field volume integrals of pressure and density (De Zeeuw et al., 2004). The integrated pressure and density are applied to RCM as the outer boundary condition with the assumption of 90% H^+ and 10% O^+ number density composition. From RCM to BATS-R-US, the GM grid cell centers are traced to the RCM boundary along the magnetic field lines (De Zeeuw et al., 2004) and the BATS-R-US pressure and density are pushed towards the RCM values with a 20s relaxation time.

3 3D Global Simulation with Kinetic Physics in the Magnetotail

3.1 Simulation Setup

We apply the MHD-AEPIC method to the geomagnetic storm event of Aug. 6. 2011 with an observed minimum Dst −126 nT. Previous modeling works show frequent flapping motion of the megnetotail current sheet during the storm (Tsutomu & Teruki, 1976; Volwerk et al., 2013), so the adaptive embedding feature is perfect for only covering the current sheet during the simulation. We start our simulation at 2011-08-05 15:00:00 and end it at 2011-08-06 07:00:00. This time range covers the main phase and the early recovering phase of the storm when the largest geomagnetic impact happens. The solar wind inputs are shown in Figure 2. First the BATS-R-US and RIM models are run to reach an quasi-steady state after 50k iteration steps using local time stepping. Figure 3 shows the plasma density along with the different refinement level boundaries of the AMR grid in the meridional plane for the steady state solution. Then the SWMF is switched to a time-accurate mode with FLEKS and RCM models turned on. The computational domain of FLEKS is determined by the selection criteria introduced above. For sake of comparison, we also conduct two other simulations without FLEKS: one with Hall MHD model and the other with ideal MHD model.

3.2 PIC Region Adaptation

In this subsection, we highlight the utility and efficiency of the adaptive embedding scheme. Figure 4 illustrates how the PIC region is changing over the simulation. Panels (a)-(f) are snapshots from six different times. The color contours show the j_y component of the current density on the meridional plane to show the magnetospheric current system. Boundaries of the active PIC region are shown by the gray isosurface. Snapshots 4 (a) and (b) are taken before the sudden commencement of the storm. At this time, the IMF B_z is pointing northward and the solar wind speed is about 400 km/s. From the isosurface plot, the PIC region is covering the tail current sheet tilting southward. In Figure 4 (b), the tail current sheet is kinked and the PIC region adjusts its shape to accommodate the tail current sheet. Snapshots 4 (c)-(f) are taken after the sudden commencement of the storm. Here we observe a much compressed magnetosphere as well as an enhanced current density. In the last two snapshots, the tail current sheet is tilting northward and it is well covered by the PIC region. From the snapshots, we can conclude that the PIC region selection criteria work well in identifying the tail current sheet, which can make the PIC region accommodate with the flapping motion of the magnetotail. The red line in Figure 4 (g) is the volume of the active PIC region (smoothed every 60 seconds), the Dst index is also presented in the background for reference. The volume of the PIC region increase after the sudden commencement and start dropping at the recovering phase. This reflects the tail current system intensity related to the solar wind condition. Notice that the volume is less than 2000 R_E^3 for the entire storm simulation, which is only about 1.4% of a large PIC box extending from $-100R_E$ to $-10R_E$ on x direction and $-20R_E$ to $20R_E$ in y and z directions. This implies that the MHD-AEPIC method saves substantial amount of computational resources.

3.3 Global Scale: Geomagnetic Indexes

To evaluate the models' performance at the global scale, we use the SYM-H and SME as evaluation metrics. The SYM-H index approximates the symmetric portion of the northward component of the magnetic field near the equator based on measurements at six ground magnetometer stations. This index characterizes the strength of the ring current (Ganushkina et al., 2017) and it is an indicator of storm activity. The SuperMAG electrojet (SME) index is an indicator of substorms and auroral power (Newell & Gjerloev, 2011). SME utilizes more than 100 ground magnetometer stations at geomagnetic latitudes between $+40°$ and $+80°$, which resolves the large and extreme events more effectively than the traditional Auroral Electrojets (AE) index (Davis & Sugiura, 1966; Bergin et al., 2020).

In our model, the simulated SYM-H is calculated by evaluating the Biot-Savart integral at the center of the Earth from all currents in the simulation domain. Calculating SME is more complicated: the magnetic field disturbances are calculated at the positions of the 100+ ground magnetometer stations and the simulated SME is obtained following the SuperMAG procedure. From Figure 5, the MHD-AEPIC produces geomagnetic indexes close to the other two MHD models. The SYM-H plot shows that the initial, main and recovery phases of the storm event are reproduced by all three models reasonably well. However, the models cannot reproduce the lowest SYM-H values that correspond to the strongest observed geomagnetic perturbations. This feature can also be observed in the SME plots: all three models produce increased auroral electrojets, however the second and third enhancements are weaker than the observed values. The geomagnetic indexes demonstrate that introducing kinetic physics in the magnetotail does not change the global configuration of the simulated magnetosphere significantly relative to the ideal and Hall MHD simulations. It is to be seen if this trend persists for other storms, especially extreme events.

3.4 Mesoscale: Magnetotail Dynamics

During the storm event, the Geotail spacecraft was in the magnetotail at $x \approx -29\,R_E$ crossing the equatorial plane and approaching to the meridional plane. Figure 6 shows the magnetic field and ion moments observed by Geotail and compares them with the ideal-MHD, Hall-MHD and MHD-AEPIC simulations. The MHD-AEPIC model shows a reasonable agreement with the Geotail number density observation before $t =$ 2011-08-06 00:00, including the current sheet crossing event between $t =$ 2011-08-05 22:00 and $t =$ 2011-08-05 23:00 while the Hall-MHD model overestimates the ion number density substantially. However, all three models generate much higher number density than observed after $t =$ 2011-08-06 00:00. None of the three models show perfect agreement with the magnetic field observations. The B_x component gives us information about which side of the current sheet the satellite is. The comparison plot shows that the virtual satellites in the simulations are all on the opposite side of the current sheet than Geotail before $t =$ 2011-08-05 22:00. Between $t =$ 2011-08-05 23:00 and $t =$ 2011-08-06 01:00, Geotail is crossing the current sheet from the north side to the south side, and this is captured by all three models. However, the next current sheet crossing at around $t =$ 2011-08-06 01:30 is not captured by MHD-AEPIC and ideal-MHD. The Hall-MHD simulations produces a similar structure but with a 30-minute time shift. The B_y and B_z components give information about flux rope structures. All three models provide good agreement with the observation in terms of overall field magnitude, while it is difficult to tell which one is better in capturing fine details. Geotail observed a B_z reversal along with a relatively strong core B_y at around $t =$ 2011-08-06 05:00, which indicates a flux rope. A similar structure is produced by MHD-AEPIC with a 30-minute delay, while there is no similar signal from the ideal-MHD and Hall-MHD simulations. Geotail observed high ion speed around 1000 km/s at $t =$ 2011-08-06 02:00 and $t =$ 2011-08-06 03:00. The MHD-AEPIC model only generates around 500 km/s ion speeds. Although the ideal-

MHD and Hall-MHD models can produce maximum ion speeds around 1000 km/s, they also generate large scale oscillations that are not present in the observations. Overall, introducing kinetic physics in the magnetotail did not improve plasma and magnetic features compared to the ideal MHD simulation at the mesoscale. The Hall MHD simulation, on the other hand, produces significantly more oscillations than observed in multiple time periods.

Since Geotail only observes along a single trajectory, it cannot provide insight into the full dynamics of the magnetotail. To compare the different models, we plot results on 2-D surfaces. Figure 7 shows the magnetosphere simulation results from three models at the same time 2011-08-05 19:40:00. Figure 7 (a1), (b1) and (c1) show the x component of the ion bulk velocity and magnetic field lines in the meridional plane ($-80\,R_E < x < -5\,R_E$ and $-20\,R_E < z < 10\,R_E$) from MHD-AEPIC, Hall MHD and ideal MHD simulations, respectively. The global configurations of the magnetosphere share a lot of similarities but there are several differences as well. All three models give a southward tilted magnetotail that is compressed most in the z direction at around $x = -40R_E$ as a result of the IMF structure. In terms of the reconnection feature, all three models generate X-lines in the tail current sheet at around $x = -20\,R_E$ and $z = -5\,R_E$ Diverging reconnection ion jets are generated at the major X-line for all three models.

To analyze physical quantities in the current sheet better, we extract the quantities along a surface where $B_x = 0$ and project this surface to the $x-y$ plane for plotting. The bottom row in Figure 7 shows the z coordinate of the center of the current sheet. The structure is similar as in the meridional plane plots: the current sheets are at $z \approx 0$ near Earth and at $z \approx -15\,R_E$ at far tail for MHD-AEPIC and Hall MHD models, while $z \approx -12\,R_E$ for ideal MHD. Figure 7 (a2)-(c2) show the ion bulk flow speed on the current sheet surface. There are significant differences among the three models in the earthward ion flow structures. For ideal MHD, the earthward ion flow is distributed roughly symmetrically at $-3\,R_E < y < 3\,R_E$. The earthward ion jet generated by Hall MHD can only be observed on the dawn side at $-5\,R_E < y < 0$. The MHD-AEPIC simulation produces earthward ion jet both on the dawn and dusk sides. However, the ion jet on the dawn side is further away from the earth than the jets on the dusk side. Also, the earthward ion jets can be observed from $-5R_E$ to $7R_E$ in the y direction, which agrees with the observations that earthward flows are observed at a wide range of y values (Angelopoulos et al., 1994).

Although the earthward ion flow from MHD-AEPIC is different from pure MHD models, the similar magnetic field structure and current sheet position indicate that these snapshots from different models represent the same physical state of the magnetosphere. Hence, it is valid to examine the flux rope features based on these results. As first proposed to be formed in the Earth's magnetotail (Schindler, 1974), magnetic flux ropes are reported to be closely related to magnetic reconnection by various observations and simulations (Hones Jr et al., 1984; Slavin et al., 1989; Daughton et al., 2006; Markidis et al., 2013). The observational characteristics of the flux ropes are a pair of positive and negative B_z signatures with a core magnetic field B_y in between. Hence, we plot the B_z and $|B_y|$ components on the current sheet surface in Figure 7(a-c)(2-3). Panels (c3) and (c4) shows only one flux rope at $-40\,R_E$ and there is no evidence indicating flux rope exists at the near earth plasma sheet from $-40\,R_E$ to the Earth based on the ideal MHD model results. The Hall MHD and MHD-AEPIC give very different flux rope occurrence (Figure 7 (a-b)(3-4)) from ideal MHD. In addition to the moving directions of the flux ropes, the diameter of the flux ropes also varies: the earthward flux ropes are observed as smaller ones. This difference has been reported in a thorough analysis of Geotail observations (Slavin et al., 2003). By examining the flux ropes as a mesoscale feature, we can conclude that by modeling the reconnection physics better, the MHD-AEPIC and Hall MHD simulations produce more flux ropes in the magnetotail than ideal MHD as well as distinguish two types of the flux ropes. However, there is no evidence support-

ing that MHD-AEPIC can produce better mesoscale features than Hall MHD. This could be the case because the spatial scale of the flux ropes is much larger than the kinetic scale which PIC model is resolving.

3.5 Kinetic Scale: Electron Velocity Distribution Function

In this subsection, we will demonstrate that the kinetic physics at the reconnection site is also properly captured by the MHD-AEPIC model. The magnetic reconnection is regarded as one of the most fundamental physical processes to transfer energy from magnetic field to plasma. Since the launch of the Magnetospheric Multiscale (MMS) mission (Burch et al., 2016), magnetic reconnection has been observed at the electron scale during multiple satellite crossings of the electron diffusion region (EDR) (Webster et al., 2018). The EDR encounters exhibit electron agyrotropy, which can be recognized by a crescent-shaped electron distributions (Torbert et al., 2018).

Figure 8 compares the MHD-AEPIC simulation with MMS observations (Hwang et al., 2019). Panel (a) is a contour plot of ion bulk velocity in the meridional plane at $t =$ 2011-08-05 23:20:00 The ion jets, a clear signature of magnetic reconnection, are shown by the blue and red colors. Panels (b) and (d) show the electron velocity distribution functions (VDF) from the model and the MMS observation. The simulation VDF of the electrons is collected inside an ellipsoid region centered at $(-30.6, 0.5, -0.9)$ R_E with principle semi-axes $(0.3, 2.5, 0.3)$ R_E in the (x, y, z) directions, respectively. The choice of the ellipsoid shape is based on panel (c) that shows where the MMS observations were taken with respect to the reconnection site according to Figure 2 by Hwang et al. (2019). The red circle in panel (a) is the cross section of the ellipsoid on the meridional plane. To compare with observation by MMS3 (Hwang et al., 2019) at $(-18.1, 7.30, 0.66)$ R_E is presented aside. Although the simulation and observation are not from the same event and the EDR is not at the same position, the electron data is collected at a similar location relative to the X-point and the $y-z$ coordinates from the simulation are closely aligned with the $M - N$ coordinates from the observation (see panels (a) and (c)).

This suggests that we can directly compare the two VDF plots in panels (b) and (d), and they indeed agree very well. The agreement is not only qualitative, but in fact quantitative. Since we are using an ion-electron mass ratio of 100 in the PIC code, the simulation electron velocity is multiplied by $\sqrt{\frac{\mathrm{m_{i,real}}}{\mathrm{m_{e,real}}} / \frac{\mathrm{m_{i,simulation}}}{\mathrm{m_{e,simulation}}}} \approx \sqrt{18.36} \approx 4.28$ to be comparable with the observations. In both panels the velocity distribution extends to $\pm 40.000\,\mathrm{km/s}$ in the z direction and $(-40,000, 20,000)\,\mathrm{km/s}$ in the y direction. A non-Maxwellian core distribution can also be clearly identified in both panels at $-20,000\,\mathrm{km/s} < v_y < 10,000\,\mathrm{km/s}$) and $|v_z| < 10,000\,\mathrm{km/s}$. Hence, we can conclude that an MHD-AEPIC global simulation can generate electron phase space distribution that is very close to the MMS observation, and resolves the electron scales in reconnection physics.

4 Conclusions and Discussions

In this paper, we introduced a newly developed magnetohydrodynamic with adaptively embedded particle-in-cell (MHD-AEPIC) model. The MHD-AEPIC allows PIC grid cells to be turned on and off during the simulation based on the physical criteria provided. Different from the previous MHD-EPIC model, which requires a fixed Cartesian box to cover the PIC region, the MHD-AEPIC model enables PIC regions moving with the reconnection sites to save computational resources substantially. During the main phase of the storm, from $t =$ 2011-08-06 00:05:00 to $t =$ 2011-08-06 02:54:00, when the volume of the PIC domain is about $1500\,R_E^3$. The relative timings are the following: 72.72% of CPU time is used on FLEKS, 13.26% is for BATS-R-US and 10.35% is taken by the coupling between FLEKS and BATS-R-US. The rest 3.67% of CPU time is consumed by RIM, RCM and the overhead of the SWMF. For the entire 16-hour geomagnetic storm simulation, the total wall time is 256.29 hours on 5600 CPU cores.

We also introduced three physics based criteria to identify the reconnection regions in the magnetotail. To demonstrate the feasibility of the MHD-AEPIC model, we have performed a geomagnetic storm event simulation with kinetic physics embedded for the first time. The flapping motion of the magnetotail current sheet during the geomagnetic storm highlights the advantage of the adaptation feature of the MHD-AEPIC model.

We have also simulated the same event using Hall MHD and ideal MHD models and compared the three models at multiple physical scales. We examined the global scale features by comparing the SYM-H and SME indexes which reflect the equatorial and auroral region disturbances, respectively. All three models properly capture the global scale disturbances such as the main phase of the storm or the increase of the auroral electrojet. However, all three models fail to produce the strongest intensity for the geoindices. Hence no significant difference is found among the three different models at the global scale for this event. This indicates that the global magnetosphere configuration from the three models are very close, the kinetic model embedded in the magnetotail does not improve the global scale feature for this geomagnetic storm. If this trend persists for other storms, especially extreme events, is still to be investigated.

We analyze the mesoscale features by comparing the magnetic field components and ion profiles between the Geotail observation and the simulations. All three models show fairly good agreement with the Geotail observations, however, none of the three models can match all features such as all the current sheet crossing or flux rope signatures. The Hall MHD simulation shows more oscillations than observed during a few time periods. In this storm event, MHD-AEPIC and ideal MHD models produce similar agreement with the in-situ observations of Geotail.

In addition to comparing with the Geotail observations, we also compare the three models with respect to flux rope structures in the current sheet. Only one major flux rope can be observed from the ideal MHD simulation at the selected time, while Hall MHD and MHD-AEPIC can produce flux ropes at a wider range in the dawn-dusk direction. The difference of two types of the flux ropes: earth-ward with smaller spatial scale and tail-ward with a lager spatial scale is also illustrated by the MHD-AEPIC simulations, in agreement with several observations (Slavin et al., 2003).

The electron scale kinetic physics is well reproduced by the MHD-AEPIC model. We collect electron macro-particle velocities at the same side of the electron diffusion region as the MMS3 satellite did (Hwang et al., 2019). The velocity distribution functions show excellent agreement between the simulation and the MMS3 observation. This demonstrates that MHD-AEPIC can properly produce the electron scale features within a single self-consistent global model while simulating a complete geomagnetic storm event. In this particular simulation, including the kinetic reconnection physics does not improve agreement with observations at meso- and global scales. This suggests that in this storm event, the magnetosphere is mostly driven by the external solar wind and interplanetary magnetic field and not by the internal reconnection dynamics.

It is to be investigated if the kinetic physics can have a more pronounced influence on the physical condition of the magnetosphere when the external drivers are relatively constant. Another important question is to compare the impact of kinetic versus numerical reconnection during extreme events. In addition to studying the Earth's magnetosphere, we also expect the novel MHD-AEPIC model will find its applications in various collisionless plasma systems that form small regions where kinetic effects are important inside a large spatial domain.

Data Availability Statement

The Geotail data is publicly available at Data ARchives and Transmission System (DARTS) of Institute of Space and Astronautical Science (ISAS) (https://darts.isas.jaxa.jp).

The MMS observation plot is acquired with consent from Dr. K.-J. Hwang (jhwang@swri.edu). The SWMF code (including BATS-R-US and FLEKS) is publicly available through the csem.engin.umich.edu/tools/swmf web site after registration. The simulation output and scripts used for generating figures in this paper can be obtained online through the University of Michigan's Deep Blue Data repository, which is specifically designed for U-M researchers to share their research data and to ensure its long-term viability.

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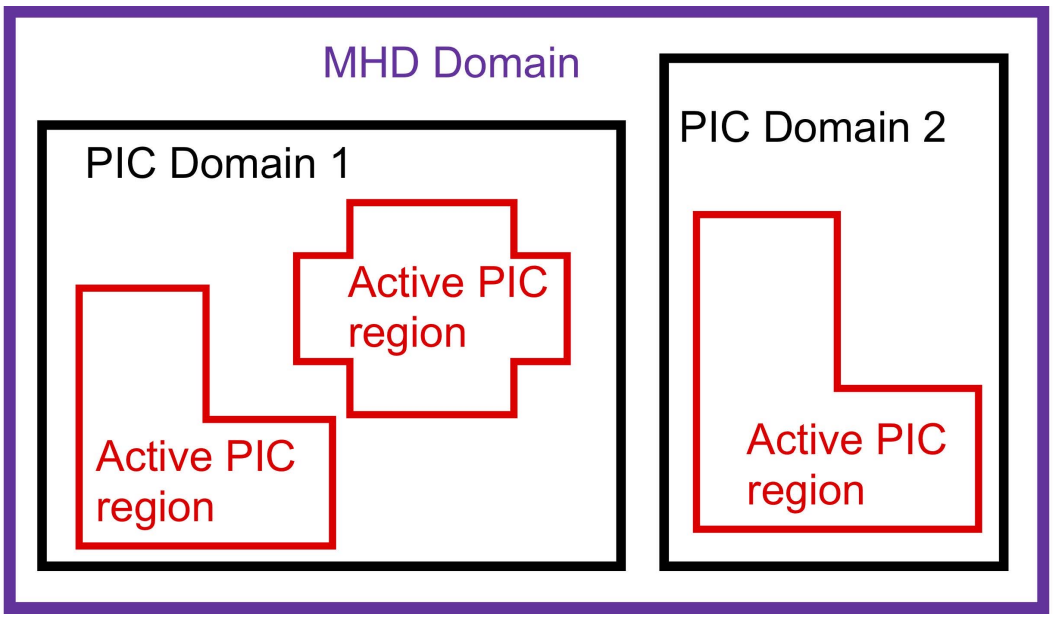

Figure 1. The schematic plot of the FLEKS adaptive grid. The red line boundary shows the flexibility of turning on and off the PIC patches during the simulation.

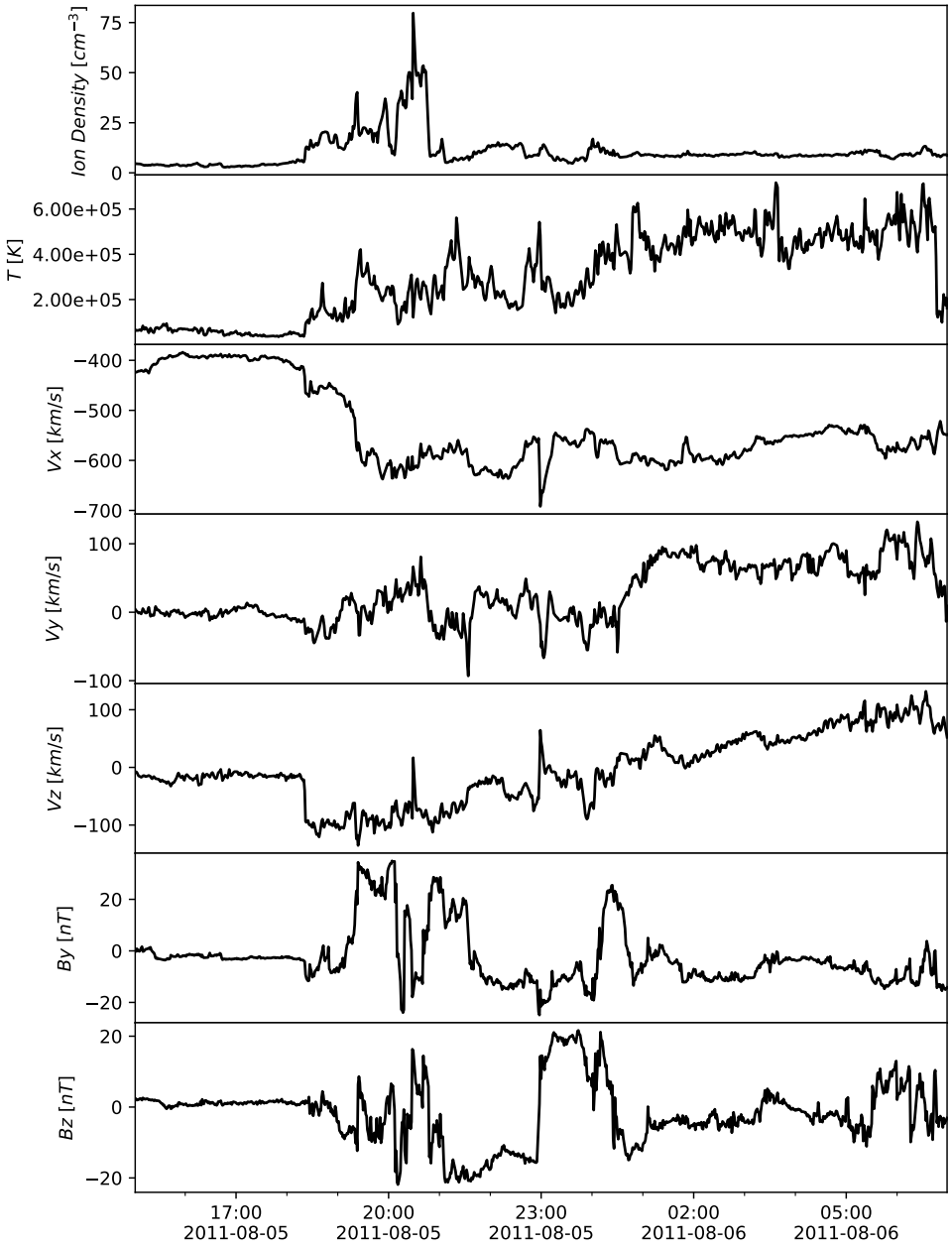

Figure 2. The solar wind bulk plasma and interplanetary magnetic field input in Geocentric Solar Magnetospheric coordinates (from top panel to the bottom: plasma density, plasma temperature, x, y and z components of the plasma flow velocity, y and z components of the magnetic field) for the simulation in this paper. The x-component of the magnetic field is set to be 0. The solar wind data is obtained from the ACE spacecraft observation and propagated to the bow shock position (Pulkkinen et al., 2013).

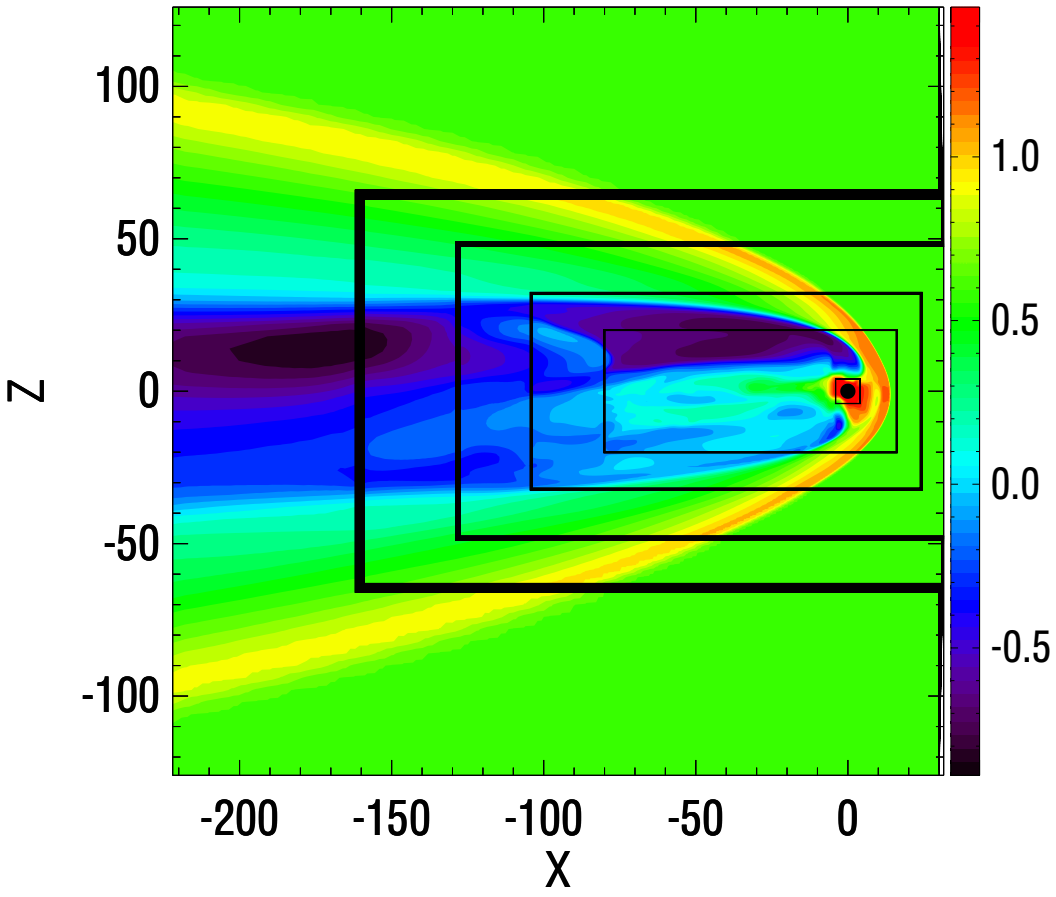

Figure 3. The meridional plane of the simulation domain. The color contour shows the plasma density of the steady state on a logarithmic scale. The black lines show the boundaries between different refinement levels. The refinement ratio between two adjacent levels is 2. The grid resolution near Earth is $1/8\,R_E$ it is $1/4\ R_E$ on the dayside and the magnetotail out to $x > -80\,R_E$.

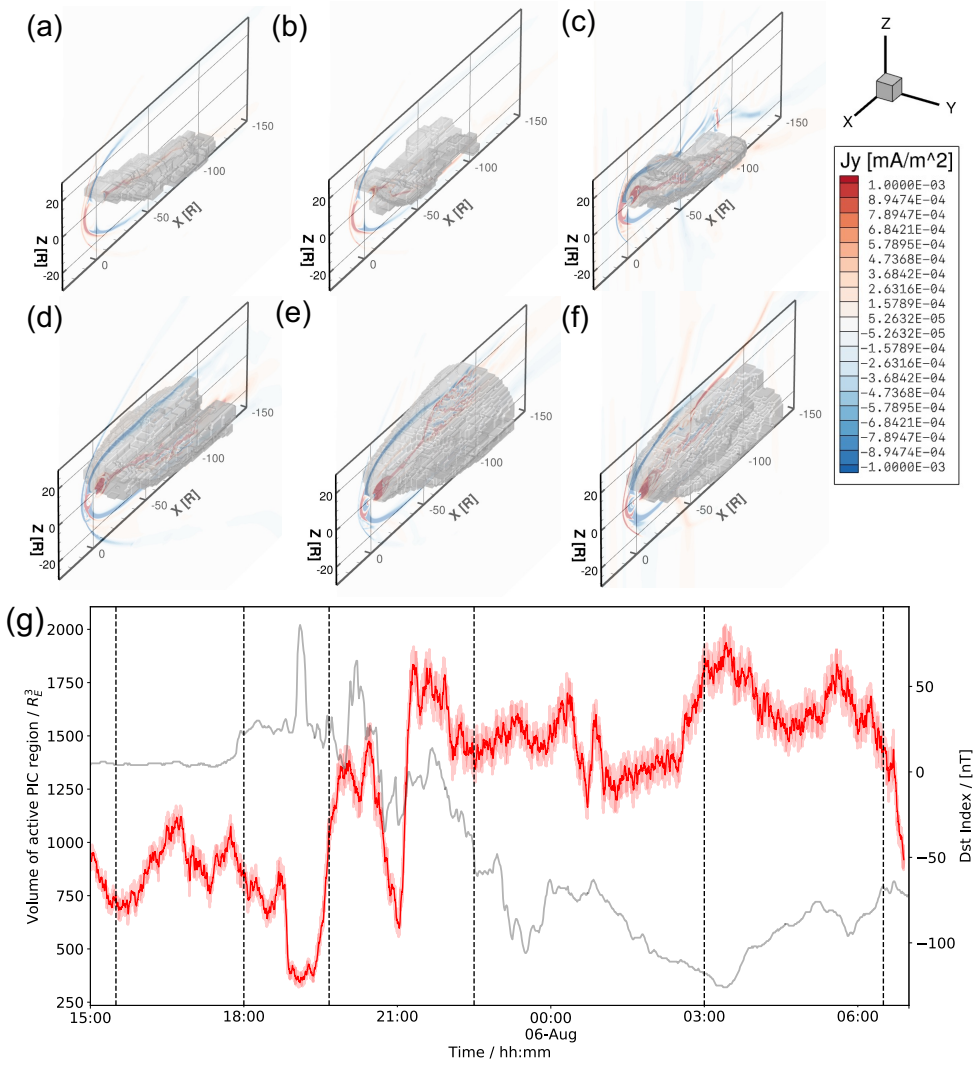

Figure 4. (a-f) Demonstration of PIC region adaptation during the simulation. The contour plot of j_y in the meridional plane is showing the general condition of the magnetospheric current system. The active PIC region boundary is shown by a gray isosurface. (g) Time evolution of the active PIC region volume (red line). The Dst index is plotted as a gray line for reference. The six vertical dashed lines correspond to the times of the snapshots (a)-(f), respectively.

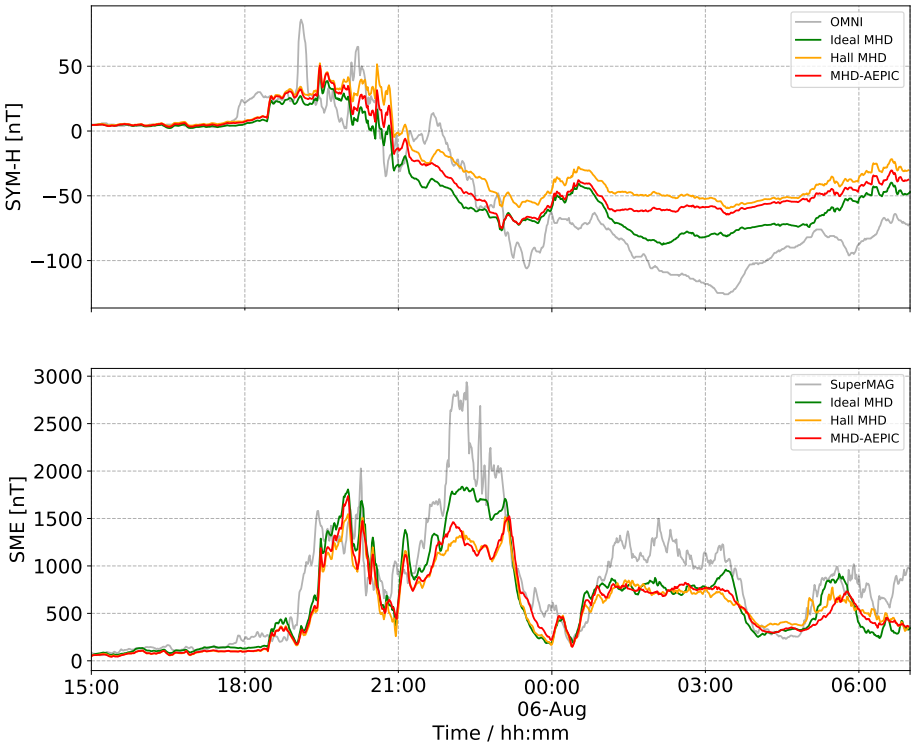

Figure 5. Aug. 6 2011 storm. Colored lines show the SYM-H and SuperMAG electrojet (SME) indexes from three different models and the gray line corresponsds to the observed indexes.

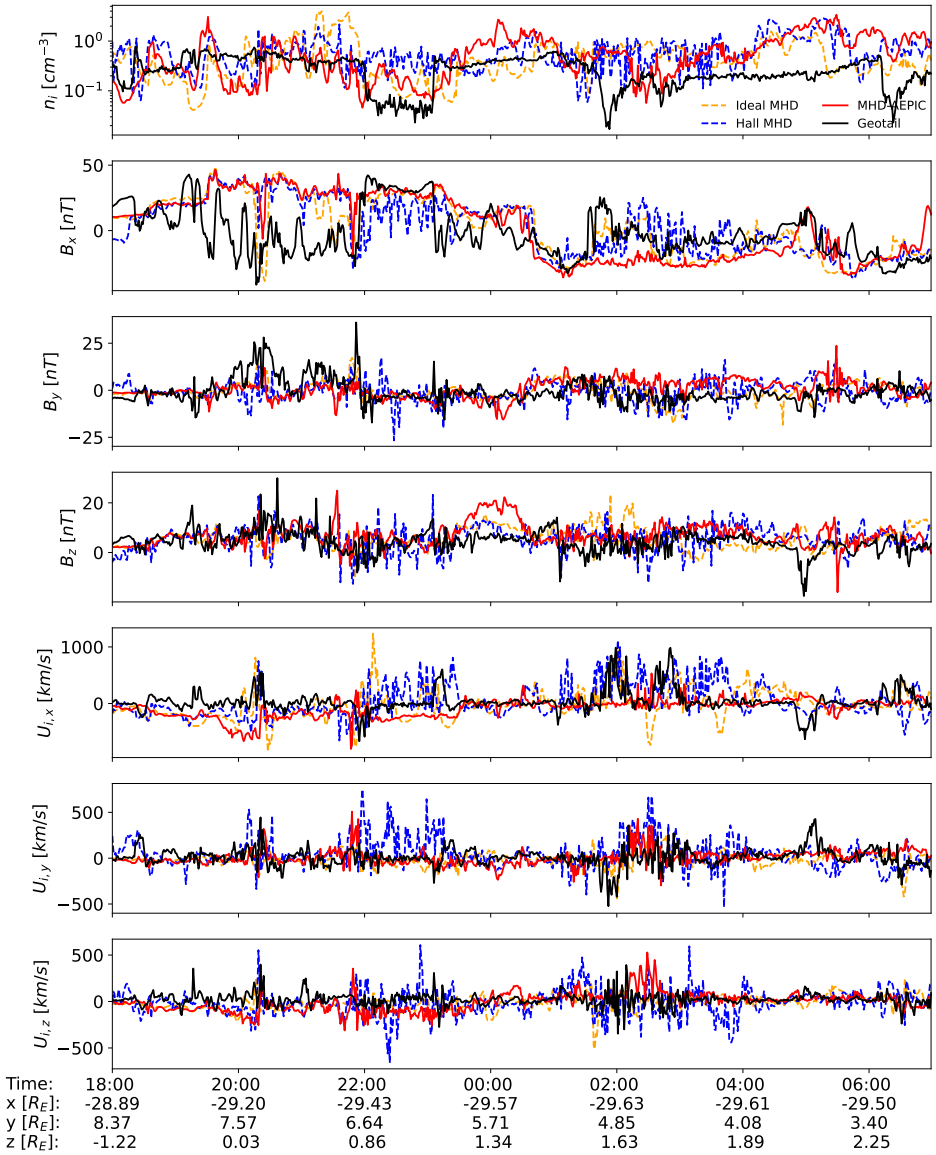

Figure 6. The ion density, magnetic field components and the ion velocity components observed by the Geotail spacecraft and the SWMF ideal MHD, Hall MHD and MHD-AEPIC simulations. The time interval shown starts from t = 2011-08-05 18:00:00 right before the sudden commencement to t = 2011-08-06 00:07:00 at the beginning of the recovery phase of the geomagnetic storm. The bottom X axis shows the GSE coordinates of the spacecraft at various times.

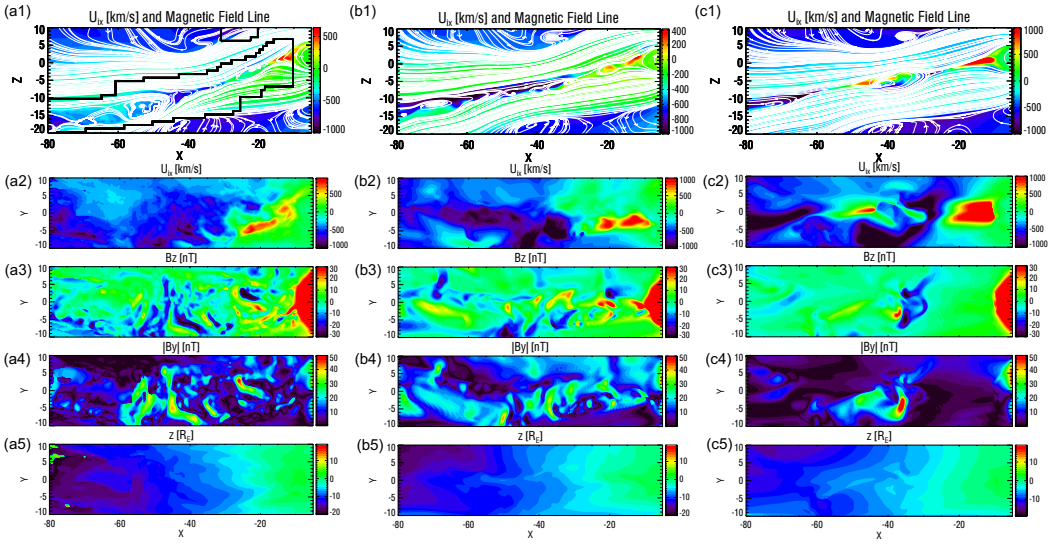

Figure 7. (a1) The x component of the ion bulk velocity $u_{i,x}$ and magnetic field lines on the meridional plane from the MHD-AEPIC simulation. The black line shows the boundary of the active PIC region. (a2) $u_{i,x}$ on the current sheet surface projected on the x-y plane. (a3) The contour plot of the B_z on the current sheet surface, color saturated at ± 30 nT. (a4) The absolute value of B_y on the current sheet surface. A pair of positive and negative B_z along with a core B_y indicates a flux rope structure. (a5) The z coordinate of the current sheet surface in the unit of R_E. (b1)-(b5) are same quantities from the Hall MHD and (c1)-(c5) are from the ideal MHD simulation. All snapshots are taken at the same time 2011-08-05 19:40:00.

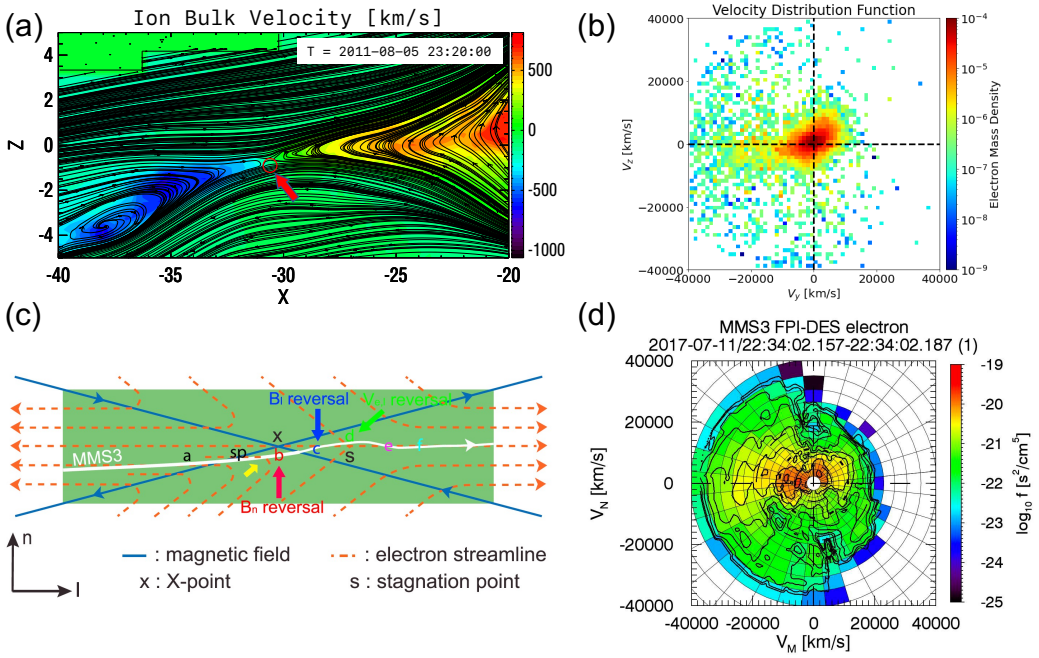

Figure 8. (a) The contour plot of the ion bulk velocity overplotted with magnetic field lines. The 2D cut is taken on the meridional plane. The red rectangle is the position where the electrons for the VDF are collected. Notice that some area at upper left is not covered by PIC which illustrates the AEPIC feature. (b) The electron VDF from the simulation, colored in electron mass density in log scale. (c) A sketch (Figure 1 (b) in Hwang et al. (2019)) demonstrating possible magnetic field geometries. The white curve represents a possible MMS3 trajectory. The electron VDF in (d) is taken at the position *b* pointed by a red arrow. (d) MMS3 observation (Figure 2 (c) in Hwang et al. (2019)).