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

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November 30, 2022

### Abstract

We perform a geomagnetic event simulation using a newly developed magnetohydrodynamic with adaptively embedded particlein-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. We also compare the ionospheric solver results and all three models generate similar polar cap potentials and field aligned currents. 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.

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

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# 8 Key Points:

9	• We perform a global simulation of a geomagnetic storm event with kinetic mod-
10	eling of the magnetotail reconnection
11	<ul> <li>The kinetic region is adaptively embedded to the MHD model and the reconnec-</li> </ul>
12	tion sites are identifed by physical criteria during the runtime
13	• The global scale, mesoscale and electron scale features are observed simultaneously
14	in one simulation

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### 15 Abstract

We perform a geomagnetic event simulation using a newly developed magnetohydrody-16 namic with adaptively embedded particle-in-cell (MHD-AEPIC) model. We have devel-17 oped efective criteria to identify reconnection sites in the magnetotail and cover them 18 with the PIC model. The MHD-AEPIC simulation results are compared with Hall MHD 19 and ideal MHD simulations to study the impacts of kinetic reconnection at multiple phys-20 ical scales. At the global scale, the three models produce very similar SYM-H and Su-21 perMag Electrojet (SME) indexes, which indicates that the global magnetic feld con-22 fgurations from the three models are very close to each other. We also compare the iono-23 spheric solver results and all three models generate similar polar cap potentials and feld 24 aligned currents. At the mesoscale we compare the simulations with in situ Geotail ob-25 servations in the tail. All three models produce reasonable agreement with the Geotail 26 observations. At the kinetic scales, the MHD-AEPIC simulation can produce a crescent 27 shape distribution of the electron velocity space at the electron difusion region which 28 agrees very well with MMS observations near a tail reconnection site. These electron scale 29 kinetic features are not available in either the Hall MHD or ideal MHD models. Over-30 all, the MHD-AEPIC model compares well with observations at all scales, it works ro-31 bustly, and the computational cost is acceptable due to the adaptive adjustment of the 32 PIC domain. It remains to be determined whether kinetic physics can play a more sig-33 nifcant role in other types of events, including but not limited to substorms. 34

# 35 1 Introduction

A geomagnetic storm is a major disturbance of Earth's magnetosphere that occurs 36 when a significant amount of energy is deposited into the geospace. The most widely used 37 and successful simulation tools to study the geomagnetic storms are based on the mag-38 netohydrodynamic (MHD) description, which is computationally feasible to solve. The 39 frst global MHD models were developed in the 1980s (LeBoeuf et al., 1981; Wu et al., 40 1981; Brecht et al., 1981, 1982). Later on, models with more advanced numerical algo-41 rithms have been developed, such as the Lyon-Fedder-Mobarry (LFM) (J. G. Lyon et 42 al., 1986; J. Lyon et al., 2004), the OpenGGCM (Raeder et al., 1995, 1996) and the GU-43 MICS (Grand Unifed Magnetosphere lonosphere Coupling Simulation) model (Janhunen, 44 1996). 45

In this paper, we use the University of Michigan's Space Weather Modeling Frame work (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 53 and in the tail. Despite all the successful applications MHD models have achieved, mag-54 netic reconnection in the global MHD models relies on either Hall resistivity, or ad hoc 55 anomalous resistivity, or simply numerical difusion. The numerical difusion plays an 56 important role in both ideal and Hall MHD models because it is required to break the 57 feld lines. As we show in Appendix A, the reconnection rate remains fnite when the grid 58 resolution becomes fner. The Hall resistivity, although does not break the feld lines that 59 are frozen into the electron fuid, changes the structure of the reconnection region, which 60 can lead to faster reconnection rate than ideal MHD (Birn et al., 2001). A current de-61 pendent anomalous resistivity has also been applied in MHD simulations (Raeder et al., 62 2001). However, none of these approximations truly describe the physical processes re-63 sponsible for collisionless reconnection. It is very important to properly represent kinetic 64 reconnection physics in a global simulation and check if it plays an important role in con-65

tributing to the larger scale processes that eventually produce geomagnetic disturbances
and space weather efects. 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 (Daldorf et al., 2014) 71 enables kinetic physics to be introduced into a global MHD model. The MHD-EPIC model 72 has been successfully used to study the interaction between the Jovian wind and Ganymede's 73 magnetopshere (Toth et al., 2016; Zhou et al., 2019, 2020); fux transfer events (FTEs) 74 at the Earth's dayside magnetopause (Y. Chen et al., 2017); Mars' magnetotail dynam-75 ics (Y. Ma et al., 2018) and the dawn-dusk asymmetries discovered at the Mercury's mag-76 netotail (Y. Chen et al., 2019). However, the iPIC3D (Markidis et al., 2010) code, which 77 is the PIC model used in the MHD-EPIC simulations, can only run on a fxed Cartesian 78 grid. The magnetotail (and the associated current sheet that contains the reconnection 79 sites) typically exhibits a fapping motion (Tsutomu & Teruki, 1976; Volwerk et al., 2013) 80 during a geomagnetic storms. Covering the whole domain of interest where reconnec-81 tion can occur in the magnetotail would require a very large PIC grid and would result 82 in a massive computational cost. This may be feasible for a short simulation time (up 83 to an hour or so) but geomagnetic storms that usually happen last for days, the com-84 putational cost would become prohibitive. 85

To tackle this problem, we have developed the MHD with Adaptively Embedded 86 PIC (MHD-AEPIC) algorithm that allows smaller PIC region than MHD-EPIC, which 87 saves computational resources. Shou et al. (2021) introduces this idea and verifes that 88 covering part of the simulation domain with a dynamically moving PIC box gives the 89 same solution as using alarger fxed PIC domain, while running significantly faster. This 90 justifes our efort to use an adaptive PIC region in the simulation. In this paper, we further improve this method and make it more fexible: 1. The size and shape of the ac-92 tive PIC regions can be adapted during the runtime; 2. The adaptation of the active PIC 93 region is fully automatic. To realize the frst feature, instead of iPIC3D, we use the FLex-94 ible Exascale Kinetic Simulator (FLEKS) (Y. Chen et al., 2021) as the PIC model. FLEKS 95 inherits all numerical algorithms from MHD-EPIC, and also accommodates an adaptive 96 PIC grid that allows PIC cells to be turned on and of during the simulation. In addi-97 tion, FLEKS employs a particle splitting and merging scheme to improve the simulation 98 efciency and accuracy. FLEKS is described in more detail in Section 2.2. 99

We have developed a reliable and efcient algorithm to identify potential recon-100 nection sites in the magnetotail using three local criteria. The criteria are easy to com-101 pute and provide the information to the FLEKS code to adapt its grid to cover the re-102 connection sites. This newly developed MHD-AEPIC model is applied to simulate a mag-103 netic storm. The SWMF simulation involves BATSRUS, FLEKS, the ionosphere elec-104 trodynamics model RIM (Ridley et al., 2004) and the inner magnetosphere model RCM 105 (Wolf et al., 1982; Tofoletto et al., 2003). This is the frst simulation of a real event with 106 kinetic reconnection physics in the magnetotail scaling from the global scales of the mag-107 netosphere to the electron scales near the reconnection sites. 108

In this paper, we employ the new model to simulate the magnetic storm of 2011-109 08-05. We cover the tail reconnection sites with the adaptive PIC model. We also per-110 form ideal MHD and Hall MHD simulations for comparison. All simulations are fully cou-111 pled with the inner magnetosphere and ionospheric electrodynamics models within the 112 Space Weather Modeling Framework. We focus on the impact of using ideal MHD, Hall 113 MHD and MHD-AEPIC physics on the dynamical processes in the magnetotail. To make 114 the comparison straightforward, we use the ideal MHD model at the dayside in all three 115 simulations. 116

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.

120 2 Methods

### 2.1 Global Magnetosphere Model: BATS-R-US

The Block-Adaptive Tree Solar-wind Roe-type Upwind Scheme (BATS-R-US) is 122 used as the Global Magnetosphere (GM) model in our simulation. In the Hall MHD and 123 MHD-AEPIC simulations in this paper, the Hall MHD equations (Toth et al., 2008) are 124 solved. The Hall term is handled with a semi-implicit scheme. The spatial discretiza-125 tion uses a 2nd order accurate TVD scheme with the Artifcial Wind Riemann solver (Sokolov 126 et al., 1999) and the Koren limiter (Koren, 1993) with1:2. The hyperbolic clean-127 ing (Dedner et al., 2003) and eight-wave scheme (Powell et al., 1999) are used to keep 128 the magnetic feld approximately divergence-free. 129

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The Hall MHD equations with a separate electron pressure equation are

$$\frac{@}{@t} = -r \cdot (u)$$
(1)

$$\frac{@(u)}{@t} = -r \cdot uu + (p + p_e)\bar{I} + \frac{B^2}{2\mu_0}\bar{I} - \frac{BB}{\mu_0}$$
(2)

$$\frac{@e}{@t} = -r \cdot (+p)u + p_e u_e + u_e \cdot \frac{B^2}{\mu_0} \overline{I} - \frac{BB}{\mu_0} + p_e r \cdot u_e$$
(3)

$$\frac{@B}{@t} = -r \times -u_e \times B - \frac{r p_e}{ne}$$
(4)

$$\frac{@p_e}{@t} = -r \cdot (p_e u_e) - (-1)p_e r \cdot u_e$$
(5)

where  $\bar{i}$  is the identity matrix, is the mass density, is the plasma bulk velocit

is the magnetic feldpe is the electron pressure is the ion pressure and  $r \times B = \mu_0$ 

is the current density. The Hall velocity and electron bulk velocity are defined as

$$v_{H} = -\frac{j}{ne} = -\frac{M_{i}j}{e}$$
(6)

$$u_e = u + v_H \tag{7}$$

where  $m = -M_i$  is the number densit  $M_i$  is the ion mass, and is the elementary charge. The total energy density is defined as

$$e = + \frac{B^2}{2\mu_0} = \frac{1}{2}u^2 + \frac{p}{-1} + \frac{B^2}{2\mu_0}$$
(8)

where =  $u^2=2 + p=(-1)$  is the hydrodynamic energy density of the ions and 5=3 is the adiabatic index. The thermal energy density of the electrons  $ig_e=(-$ 1). We note that the+  $_e$  is conserved both analytically and numerically as the nonconservative source terenger u in equations (3) and (5) cancel out. Apart from (B; p; p\_e), other variables are derived quantities.

The continuity equation (1), momentum equation (2), energy equation (3) and elec-141 tron pressure equation (5) are solved with an explicit time stepping scheme. In the in-142 duction equation (4), the convection term B and pressure gradient term  $p_e = ne$ 143 are solved using an explicit scheme, while the Hall term B is advanced with an 144 implicit scheme. The Hall MHD equations introduce whistler mode wave, which has a 145 characteristic wave speed inversely proportional to the wavelength. The shortest wave-146 length that exists in a numerical simulation is proportional to the cell size the 147 fastest whistler wave speed in a simulation is proportional to The time step in 148

a fully explicit scheme is limited by the Courant-Friedrichs-Lewy (CFL) condition:  $x=c_{max}$ , where  $c_{max}$  is the fastest wave speed, which leads to a time step proportional to 1=(x)<sup>2</sup>. We use a semi-implicit scheme (Tóth et al., 2012) to handle the stif 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 com-154 putational domain- $22R_{\rm E}$  < x <  $32R_{\rm E}$ , -1 $2R_{\rm E}$  < y; z < 1 $2R_{\rm E}$  in GSM coor-155 dinates. The Hall efect is restricted  $\mathbf{x}$  o2  $[-10 \Omega_{\rm E}; 2\Omega_{\rm E}]; jy < 3 \Omega_{\rm E}$  and jz  $j < 10 \Omega_{\rm E}$ 156  $2OR_E$  box region excluding a sphere of radiulize 3 centered at the Earth to speed up 157 the simulation. Outside this region the Hall efect is neglected by setting 0. In 158 the magnetosphere, the smallest ion inertial lendgthc= $!_{pi}$  is about  $\pm 2 CR_E$  in the 159 tail lobe region, which is already extremely difcult for a 3-D global MHD model to re-160 solve, let alone the PIC code. Tóth et al. (2017) introduced a scaling approach which 161 scales up the kinetic length by artificially increasing ion mass per charge by a scaling fac-162 tor. The scaling does not change the fuid variables, such as density, pressure, velocity, 163 IMF and dipole feld, and the global structure of the magnetosphere will not change sig-164 nifcantly as long as the scaled up ion inertial length is much smaller than the global scales. 165 In this paper, we use a factor of 16, which satisfes this condition. On the other hand, 166 with the ion inertial length scaled up by 16 times, we don't need an extremely fne grid 167 to resolve it. We set the grid cell size in the magnetotalkte  $1=4R_{\rm F}$ , which is about 168 4 times smaller than the scaled up ion inertial length. About fourteen million cells are 169 used in total. For MHD model simulations, we also  $app + \Re R_{\rm E}$  grid resolution in the 170 tail: x 2 [ $-6\Omega_E$ ;  $-1\Omega_E$ ] and jy; jzj <  $1\Omega_E$ . This increases the total number of cells 171 to about twenty three millions, which is still feasible to do (but would be too expensive 172 for MHD-AEPIC model). Comparing the simulation results with  $R_F$  and 1=8R<sub>F</sub> res-173 olutions in the tail allows us to look into the role of numerical resistivity. 174

At the inner boundary =  $2:5R_E$ , the density is calculated by the empirical for-175 mula  $_{inner} = (28 + 01CPCP)$  amu/cm<sup>3</sup>, where CPCP is the average of the northern 176 and southern cross polar cap potentials measured in keV. This boundary condition has 177 been used successfully in previous geomagnetic storm simulations (Pulkkinen et al., 2013). 178 The pressure and the magnetic felled (excluding dipole feld) have zero gradient at the 179 inner boundary, while the radial velocity is set to zero and the tangential velocity is cal-180 culated from the corotation and the B drift, where the electric feld is provided 181 by the Ridley lonosphere Model (RIM) (Ridley et al., 2004). 182

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# 2.2 Particle-in-cell Model: FLEKS

The FLexible Exascale Kinetic Simulator (FLEKS) (Y. Chen et al., 2021) is used 184 as the particle-in-cell (PIC) model (PC component in the SWMF) to resolve kinetic physics. 185 FLEKS uses the same two-way coupling method as MHD-EPIC (Daldorf et al., 2014) 186 and the Gauss's law satisfying energy-conserving semi-implicit method (GL-ECSIM) (Y. Chen 187 & Tóth, 2019) for the PIC solver. To enable the adaptation in MHD-AEPIC, FLEKS 188 introduces an adaptive grid that allows changing simulation region dynamically. Figure 189 1 shows a schematic plot of the adaptive grid. We choosse1=4 $R_F$  to be the PIC 190 grid resolution so that the scaled x 4. The ion inertial length inside the mag-191 netosphere is described in Subsection 2.1. The ion-electron mass ratio is set to 100 in 192 this simulation so that the electron skin ded the 0:1d<sub>i</sub>. Li et al. (2019) perform 2-193 D PIC simulations using different ion-electron mass ratios and conclude that features 10/ like reconnection rate and magnetic energy conversion are similar in simulations using 195 diferent ion-electron mass ratios. Although the grid is not refned to resolve the elec-196 tron scale, in the PIC model the electron particles can resolve sub-grid scale physics un-197 der the infuence of the electromagnetic feld that is resolved on the ion scale. Y. Chen 198 and Tóth (2019) show that the semi-implicit PIC model can reproduce the most impor-199 tant ion scale features of magnetic reconnectiond with 4. The selected reso-200

lution balances between the computational cost and the requirement of resolving kineticscales.

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 of 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 feld 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 densityj is strong and the magnetic fetblis weak. In particular, the felt  $\mathbf{B}_{\perp}$  that is perpendicular to the current be close to zero, while the guide feld parallel to the current can be non-zero. We define the following non-dimensional relation as our frst criterion

$$\frac{J}{B_{\perp} + "} = \frac{J^2}{jJ \times Bj + J"} > C_1$$
(9)

where  $J = \mu_0 j = r \times B$  and " is a small dimensional constant in units of the magnetic feld introduced to avoid dividing by zero. We use1 nT in our simulations presented here, which is much smaller than the typical magnetic feld intensity in the tail current sheet. x is the local cell size that is used in calculating the curl of the magnetic feld, so that x is the jump of the transverse magnetic feld between neighboring grid cells. We set J = 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 fnd that it selects the axis of fux ropes, or O-lines, in addition to X-lines, especiallyisfvery 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 feld curvature vector:

$$[r \cdot (b \cdot r b)](x)^2 > c_2$$
 (10)

where B = B = jBj is a unit vector along the magnetic feld. We  $w_2 = -0.1$  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 specifc 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 specifc entropy as the third criterion:

$$\frac{p}{c_3} > c_3 \tag{11}$$

where p is the plasma thermal pressure is the plasma density, and = 5=3 is the ra-

tio of the specifc heats (Birn et al., 2006, 2009). Diferent from the  $c_2$  introduced

 $_{245}$  above, this criterion is dimensional and we use the threshold  $\alpha_{24} = 0.02 \text{ nPa} \text{cm}^{-3}$ .

The three criteria combined can identify X-lines in the magnetotail well. To make 246 the active PIC region large enough around the X-lines, we fag all patches where all three 247 criteria are met, and then activate all patches within a distance  $L_z$  from these 248 fagged patches in the, y and z directions, respectively. The extension in each direc-249 tion enables the PIC model to cover a bufer area outside the reconnection sites. This 250 bufer ensures that the velocity distribution of ions and electrons at the boundary of the 251 PIC region can be well approximated with a drifting Maxwellian distribution, which re-252 sults in a consistent coupling between the MHD model. We  $\mu$ se4R<sub>F</sub> and L<sub>v</sub> = 253  $L_z = 2R_E$  in this work. 254

Each MPI process of BATS-R-US calculates the above criteria on their respective 255 sub-domains overlapping with the PIC grid and activate the patches of the PIC grid where 256 all 3 criteria are satisfed. Then the processors collect the information: a PIC patch is 257 activated if any of the BATS-R-US processes activated it. Since the status of all PIC patches 258 (on/of) is stored in each MPI processor of BATS-R-US, using the default logical array 259 would consume a lot of memory. To reduce the memory use, the status is stored by a 260 single bit, which is 32 times smaller than the size of the default logical variable in For-261 tran. The information is conveniently collected with the bitwise "or" opermetance 262 used in the MPI\_ALLREDUCE call. 263

264 2.4 Ionospheric Electrodynamics Model: RIM

The lonospheric Electrodynamics (IE) is simulated by the Ridley lonosphere 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 itoboth longitude and latitude directions. The lower latitude boundary is atwidere the electric potential is set to zero.

The BATS-R-US and RIM models are two-way coupled every 5 seconds. To cal-270 culate the Poisson-type equation, RIM obtains the feld-aligned currents (FAC) calcu-271 lated at  $\mathfrak{B}_{F}$  from the BATS-R-US model and maps them down to its grid. The F10.7 272 fux is also an input parameter of RIM that is used together with the FAC to calculate 273 the particle precipitation and conductances based on an empirical model. The electric 274 feld calculated by the RIM is mapped back to the inner boundary of BATS-R-US to ob-275 tain the  $E \times B = B^2$  velocity for its inner boundary condition. The cross polar cap po-276 tentials (CPCP, (the difference of the maximum and minimum potentials in the two hemi-277 spheres) are also sent to BATS-R-US to set the density at the inner boundary. 278

279 2.5 Inner Magnetosphere Model: RCM

The Inner Magnetosphere (IM) is modeled by the Rice Convection Model (RCM) (Wolf et al., 1982; Tofoletto 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. As a component of the SWMF geospace model, RCM is used in all simulations presented in this paper.

The RCM model is one-way coupled with RIM and two-way coupled with BATS-285 R-US every 10 seconds. RIM sends the electric potential to RCM, where it is used to 286 advect the feld lines with the  $B = B^2$  drift. In the two-way coupling between BATS-287 R-US and RCM, BATS-R-US identifes the closed feld line regions and calculates feld 288 volume integrals of pressure and density (De Zeeuw et al., 2004). The integrated pres-289 sure and density are applied to RCM as the outer boundary condition with the assump-290 tion of 90% Ħ and 10% O<sup>+</sup> number density composition. From RCM to BATS-R-US, 291 the GM grid cell centers are traced to the RCM boundary along the magnetic feld lines 292 (De Zeeuw et al., 2004) and the BATS-R-US pressure and density are pushed towards 293 the RCM values with a 20 relaxation time. 294

#### 3 3D Global Simulation with Kinetic Physics in the Magnetotail 295

#### 3.1 Simulation Setup 296

We apply the MHD-AEPIC method to the geomagnetic storm event of Aug. 6. 2011 297 with an observed minimum Dst126 nT. Previous modeling works show frequent fap-298 ping motion of the megnetotail current sheet during the storm (Tsutomu & Teruki, 1976; 299 Volwerk et al., 2013), so the adaptive embedding feature is perfect for only covering the 300 current sheet during the simulation. We start our simulation at 2011-08-05 15:00:00 and 301 end it at 2011-08-06 07:00:00. This time range covers the main phase and the early re-302 covering phase of the storm when the largest geomagnetic impact happens. The solar 303 wind inputs are shown in Figure 2. First the BATS-R-US and RIM models are run to 304 reach an quasi-steady state after 50k iteration steps using local time stepping. Figure 305 3 shows the plasma density along with the diferent refinement level boundaries of the 306 AMR grid in the meridional plane for the steady state solution. Then the SWMF is switched 307 to a time-accurate mode with FLEKS and RCM models turned on. Y. Chen et al. (2017) 308 and Zhou et al. (2020) study the dayside reconnection at Earth and Ganymede by putting 309 PIC regions at the magnetopause. They also compare the results with Hall MHD and 310 conclude that the two models generate similar global features, such as fux rope forma-311 tion and reconnection rate. In this paper, we only put PIC regions in the magnetotail, 312 in order to control variants. The dayside reconnection is modeled by the ideal MHD. The 313 computational domain of FLEKS is determined by the selection criteria introduced above. 314 For sake of comparison, we also conduct two other simulations without FLEKS: one with 315 Hall MHD model and the other with ideal MHD model. 316

#### 3.2 PIC Region Adaptation 317

In this subsection, we highlight the utility and efciency of the adaptive embed-318 ding scheme. Figure 4 illustrates how the PIC region is changing over the simulation. 319 Panels (a)-(f) are snapshots from six different times. The color contours showcome 320 ponent of the current density on the meridional plane to show the magnetospheric cur-321 rent system. Boundaries of the active PIC region are shown by the gray isosurface. Snap-322 shots 4 (a) and (b) are taken before the sudden commencement of the storm. At this time, 323 the IMF  $B_7$  is pointing northward and the solar wind speed is about 400 km/s. From 324 the isosurface plot, the PIC region is covering the tail current sheet tilting southward. 325 In Figure 4 (b), the tail current sheet is kinked and the PIC region adjusts its shape to 326 accommodate the tail current sheet. Snapshots 4 (c)-(f) are taken after the sudden com-327 mencement of the storm. Here we observe a much compressed magnetosphere as well as 328 an enhanced current density. In the last two snapshots, the tail current sheet is tilting 329 northward and it is well covered by the PIC region. From the snapshots, we can conclude 330 that the PIC region selection criteria work well in identifying the tail current sheet, which 331 can make the PIC region accommodate with the fapping motion of the magnetotail. The 332 translucent red line in Figure 4 (g) shows the volume of the active PIC region recorded 333 every second from the simulation, while the solid red line is the volume smoothed over 334 every minute. The Dst index is also presented in the background for reference. The vol-335 ume of the PIC region increases after the sudden commencement and starts dropping 336 in the recovering phase. This refects that the tail current system intensity is related to 337 the solar wind condition. Notice that the volume is less than 183000 the entire 338 storm simulation, which is only about 11.2% of the large PIC box extending-fit  $\Omega \sigma R_F$ 339 to  $-1\Omega R_E$  in the direction and  $2\Omega R_E$  to  $2\Omega R_E$  in the y and z directions. This con-340 frms that the MHD-AEPIC method saves substantial amount of computational resources. 341

### 342

3.3 Global Scale: Geomagnetic Indexes and Ionospheric Quantities

To evaluate the models' performance at the global scale, we use the SYM-H and 343 SME as evaluation metrics. The SYM-H index approximates the symmetric portion of 344

the northward component of the magnetic feld near the equator based on measurements 345 at six ground magnetometer stations. This index characterizes the strength of the ring 346 current (Ganushkina et al., 2017) and it is an indicator of storm activity. The SYM-H 347 data with a 1-minute cadence is downloaded from NASA OMNIWeb Data Service. The 348 SuperMAG electrojet (SME) index is an indicator of substorms and auroral power (Newell 349 & Gjerloev, 2011). SME utilizes more than 100 ground magnetometer stations at geo-350 magnetic latitudes between 4400d + 80, which resolves the large and extreme events 351 more efectively than the traditional Auroral Electrojets (AE) index (Davis & Sugiura, 352 1966; Bergin et al., 2020). 353

In our model, the simulated SYM-H is calculated by evaluating the Biot-Savart in-354 tegral at the center of the Earth from all currents in the simulation domain. Calculat-355 ing SME is more complicated: the magnetic feld disturbances are calculated at the po-356 sitions of the 100+ ground magnetometer stations and the simulated SME is obtained 357 following the SuperMAG procedure. From Figure 5, the MHD-AEPIC produces geomag-358 netic indexes close to the other two MHD models. The SYM-H plot shows that the ini-359 tial, main and recovery phases of the storm event are reproduced by all three models rea-360 sonably well. However, the models cannot reproduce the lowest SYM-H values that cor-361 respond to the strongest observed geomagnetic perturbations. This feature can also be 362 observed in the SME plots: all three models produce increased auroral electrojets, how-363 ever the second and third enhancements are weaker than the observed values. For MHD model simulations, the root mean square errors (RMSE) of SYM-H and SME are not 365 changing much from= $4R_E$  to  $1=8R_E$  grid resolutions as shown in the fgure 5. This 366 means that the numerical difusion is not the major reason for the similarity of global 367 indexes generated from the three models, which demonstrates that the numerical difu-368 sion efect is converged to some extent #R1 grid resolution in the tail. Fine grid 369 resolution towards 10 R<sub>F</sub> is also applied in simulations using the LFM model (Wiltberger 370 et al., 2015; Merkin et al., 2019) and the authors demonstrate that the reconnection will 371 not be significantly suppressed if the grid resolution is further increased. 372

Apart from the global indexes such as SYM-H and SME, it is also important to com-373 pare the amount of energy that the solar wind and interplanetary magnetic feld (IMF) 374 transfer to Earth's magnetosphere-ionosphere system through direct driving. The cross 375 polar cap potential (CPCP) is an indicator of this energy transfer process (Troshichev 376 et al., 1988, 1996). The CPCP is not directly measured but can be derived from obser-377 vations using the Assimilative Mapping of Ionospheric Electrodynamics (AMIE) (Richmond 378 & Kamide, 1988) technique or from the Defense Meteorological Satellite Program (DMSP) 379 measurements (Hairston et al., 1998). Another approach based on the Super Dual Au-380 roral Radar Network (SuperDARN) observations (Ruohoniemi & Greenwald, 1998) usu-381 ally underestimates the CPCP significantly. We opt to use the readily available Polar 382 Cap Index (PCI) from the OMNIWeb website and convert it into CPCP using the em-383 pirical relationship derived by Ridley and Kihn (2004): 384

$$CPCP_{North} = 29.28 - 3.31 \sin(1 + 1.49) + 1781PCI_N$$
(12)

where T is the month of the year normalized to 2 he storm event in this paper is in August, so T = (8 – 1) 2 = 12. Gao (2012) showed that this formula provides good agreement with AMIE and DMSP based approaches. For the southern hemisphere, since there is no published empirical relationship between southern CPCP and PCI, we change the sign in front of the sTn(1:49) term (expressing the seasonal dependence) in the formula:

$$CPCP_{South} = 29.28 + 331 \sin(1 + 1.49) + 1781PCLS$$
(13)

The simulated CPCP is defined as the diference between the maximum and the minimum of the electric potential obtained from the RIM model for both hemispheres.

Figure 6 (a) shows the northern and southern cross polar cap potentials from the three models together with the CPCP derived from the PCI. In general, the results from

the three models are very close to each other and have good agreements with the PCI 395 derived CPCP for both hemispheres. Notice that the PCI is derived from a single sta-396 tion for each hemisphere while the model calculates CPCP using the entire electric po-397 tential. The diferences between the model output and CPCP could because the PCI is 398 not measuring the ionospheric dynamics for the entire polar region. We observe that the 399 three models generate the most diferent CPCP results during the main phase of the storm 400 event at around = 2011-08-05 22:00:00. Figure 6 (b) shows the polar cap potential and 401 radial component of the feld aligned currents for both hemispheres. The structure of the 402 electric potentials as well as the feld aligned currents are very similar among the three 403 models. 404

The geomagnetic indexes and ionospheric quantities demonstrate that introducing kinetic physics in the magnetotail does not change the global confguration of the simulated magnetosphere and ionosphere 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-a29R E 410 crossing the equatorial plane and approaching to the meridional plane. Figure 7 shows 411 the magnetic feld and ion moments observed by Geotail and compares them with the ideal-MHD, Hall-MHD and MHD-AEPIC simulations. The MHD-AEPIC model shows 413 a reasonable agreement with the Geotail number density observation the f20041-414 08-06 00:00, including the current sheet crossing event bet@001-08-05 22:00 and 415 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 ob-417 served aftet =  $2011-08-06\ 00:00$ . None of the three models show perfect agreement with 418 the magnetic feld observations. The component gives us information about which 419 side of the current sheet the satellite is. The comparison plot shows that the virtual satel-420 lites in the simulations are all on the opposite side of the current sheet than Geotail be-421 foret = 2011-08-05 22:00. Betwteen2011-08-05 23:00 and 2011-08-06 01:00, 422 Geotail is crossing the current sheet from the north side to the south side, and this is 423 captured by all three models. However, the next current sheet crossing attaround 424 2011-08-06 01:30 is not captured by MHD-AEPIC and ideal-MHD. The Hall-MHD sim-425 ulations produces a similar structure but with a 30-minute time shift  $\sqrt{2}$  the  $B_{\gamma}$ 426 components give information about fux rope structures. All three models provide good 427 agreement with the observation in terms of overall feld magnitude, while it is difcult 428 to tell which one is better in capturing fne details. Geotail obserted draversal along 429 with a relatively strong  $coB_{e}$  at around t = 2011-08-06 05:00, which indicates a fux 430 rope. A similar structure is produced by MHD-AEPIC with a 30-minute delay, while there 431 is no similar signal from the ideal-MHD and Hall-MHD simulations. Geotail observed 432 high ion speed around 1000 km/stat 2011-08-06 02:00 and 2011-08-06 03:00. 433 The MHD-AEPIC model only generates around 500 km/s ion speeds. Although the ideal-434 MHD and Hall-MHD models can produce maximum ion speeds around 1000 km/s, they 435 also generate large scale oscillations that are not present in the observations. Overall, 436 introducing kinetic physics in the magnetotail did not improve plasma and magnetic fea-437 tures compared to the ideal MHD simulation at the mesoscale. The Hall MHD simula-438 tion, on the other hand, produces significantly more oscillations than observed in mul-439 tiple time periods. 440

Since Geotail only observes along a single trajectory, it cannot provide insight into the full dynamics of the magnetotail. To compare the diferent models, we plot results on 2-D surfaces. Figure 8 shows the magnetosphere simulation results from three models at the same time 2011-08-05 19:40:00. Figure 8 (a1), (b1) and (c1) **shcom**the ponent of the ion bulk velocity and magnetic feld lines in the meridional pla8eR( $_{E}$  <  $x < -5R_{E}$  and  $-20R_{E} < z < 10R_{E}$ ) 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 diferences as well. All three models give a southward tilted magnetotail that is compressed most inz the ection at around  $= -4 \Omega R_E$ 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  $= -2 \Omega R_E$  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 quanti-453 ties along a surface where e = 0 and project this surface to the y plane for plot-454 ting. The bottom row in Figure 8 shows the coordinate of the center of the current sheet. 455 The structure is similar as in the meridional plane plots: the current sheetszare at 456 O near Earth and at  $-15R_E$  at far tail for MHD-AEPIC and Hall MHD models, 457 while  $z = 12R_E$  for ideal MHD. Figure 8 (a2)-(c2) show the ion bulk fow speed on 458 the current sheet surface. There are significant differences among the three models in 459 the earthward ion fow structures. For ideal MHD, the earthward ion fow is distributed 460 roughly symmetrically at  $3R_F < y < 3R_F$ . The earthward ion jet generated by Hall 461 MHD can only be observed on the dawn side- $atra R_E < y < 0$ . The MHD-AEPIC 462 simulation produces earthward ion jet both on the dawn and dusk sides. However, the 463 ion jet on the dawn side is further away from the earth than the jets on the dusk side. 464 Also, the earthward ion jets can be observed  $f \neq GR_F$  to  $\mathcal{R}_F$  in the y direction, which 465 agrees with the observations that earthward fows are observed at a wide yarade of 466 ues (Angelopoulos et al., 1994). 467

Although the earthward ion fow from MHD-AEPIC is diferent from pure MHD 468 models, the similar magnetic feld structure and current sheet position indicate that these 469 snapshots from different models represent the same physical state of the magnetosphere. 470 Hence, it is valid to examine the fux rope features based on these results. As frst pro-171 posed to be formed in the Earth's magnetotail (Schindler, 1974), magnetic fux ropes are 472 reported to be closely related to magnetic reconnection by various observations and sim-473 ulations (Hones Jr et al., 1984; Slavin et al., 1989; Daughton et al., 2006; Markidis et 474 al., 2013). The observational characteristics of the fux ropes are a pair of positive and 475 negative  $B_7$  signatures with a core magnetic f Bld in between. Hence, we plot t Be 476 and  $jB_{y}j$  components on the current sheet surface in Figure 8(a-c)(2-3). Panels (c3) and 477 (c4) show only one fux rope  $at4OR_F$  and there is no evidence indicating fux rope ex-478 ists at the near earth plasma sheet  $f_{FO}$  to the Earth based on the ideal MHD 479 model results. The Hall MHD and MHD-AEPIC give very diferent fux rope occurrence 480 (Figure 8 (a-b)(3-4)) from ideal MHD. In addition to the moving directions of the fux 481 ropes, the diameter of the fux ropes also varies: the earthward fux ropes are observed 482 as smaller ones. This diference has been reported in a thorough analysis of Geotail ob-483 servations (Slavin et al., 2003). By examining the fux ropes as a mesoscale feature, we 484 can conclude that by modeling the reconnection physics better, the MHD-AEPIC and 485 Hall MHD simulations produce more fux ropes in the magnetotail than ideal MHD as 486 well as distinguish two types of the fux ropes. However, there is no evidence supporting that MHD-AEPIC can produce better mesoscale features than Hall MHD. This could 488 be the case because the spatial scale of the fux ropes is much larger than the kinetic scale 489 which PIC model is resolving. 490

491 Figure 9 shows different physical quantities near the reconnection X-line at the same time as Figure 8. Panel (a) shows the current density of the current shows the current density of the current shows the current density of the current density o 492 of-plane magnetic fel $\mathbf{B}_{v}$  and the ion bulk velocit  $\psi_{ix}$  from the ideal MHD model. The 493 current sheet is smooth and narrow around the X-line. The simullation produces diverg-494 ing ion outfow as expected. There is no signifcant the reconnection site due 495 to the lack of Hall physics in the ideal MHD model. Panel (b) shows the same quanti-496 ties as Panel (a) for the Hall MHD model. In addition, the bottom plot shows the elec-497 tron velocity in the x direction calculated from the ion bulk velocity and the Hall veloc-498 ity as  $u_{ex} = u_{ix} - j_x = (ne)$ . Diferent from the current sheet in the ideal MHD model, 499

the current sheet in the Hall MHD simulation breaks up at multiple locations. There are 500 strong  $B_{v}$  signatures in the Hall MHD simulation as expected from Hall physics, although 501 the presence of the non-uniform guide feld somewhat distorts the classical quadrupo-502 lar structure. The diverging ion bulk fow is very similar to the diverging electron fow, 503 because the component of the current is weak. Panel (c) shows the same quantities 504 as Panel (b) from the MHD-AEPIC model with an extra ion nongyrotropy meaburg. 505 The current sheet in the MHD-AEPIC simulation also forms multiple fux ropes simi-506 lar to the Hall MHD results. The MHD-AEPIC model also generates the Hall magnetic 507 feld B<sub>y</sub>. The ion and electron velocities from the MHD-AEPIC show very clear infow 508 and outfow features that are quite different from the Hall MHD solution. While both 509 ideal and Hall MHD assume isotropic pressures, the PIC simulation allows a general pres-510 sure tensor with anisotropy and even nongyrotropy (non-zero of-diagonal terms). Aunai 511 et al. (2013) defines the nongyrotropy measure as 512

$$D_{ng} = 2 \frac{\rho \frac{P_{12} + P_{23}^2 + P_{13}^2}{P_{11} + P_{22} + P_{33}}}{P_{11} + P_{22} + P_{33}}$$
(14)

Here P<sub>ij</sub> are the pressure tensor components in the local magnetic feld aligned coordinate system. Th<sup>D</sup><sub>ng</sub> quantity produced by the MHD-AEPIC model shows that the ion nongyrotropy increases near the X-line. In conclusion, both Hall MHD and MHD-AEPIC generate more features than the ideal MHD model. The MHD-AEPIC and the Hall MHD models generate similar Hall magnetic feld structures and current sheet features. The MHD-AEPIC model generates distinct ion and electron bulk fows, as well as the nongy-rotropic pressure distribution near the X-line.

### 3.5 Kinetic Scale: Electron Velocity Distribution Function

In this subsection, we will demonstrate that the kinetic physics at the reconnec-521 tion site is also properly captured by the MHD-AEPIC model. The magnetic reconnec-522 tion is regarded as one of the most fundamental physical processes to transfer energy from 523 magnetic feld to plasma. Since the launch of the Magnetospheric Multiscale (MMS) mis-524 sion (Burch et al., 2016), magnetic reconnection has been observed at the electron scale 525 during multiple satellite crossings of the electron difusion region (EDR) (Webster et al., 526 2018). The EDR encounters exhibit electron nongyrotropy, which can be recognized by 527 a crescent-shaped electron distributions (Torbert et al., 2018). 528

Figure 10 compares the MHD-AEPIC simulation with MMS observations (Hwang 529 et al., 2019). Panel (a) is a contour plot of ion bulk velocity in the meridional plane at 530 t = 2011-08-05 23:20:00. The ion jets, a clear signature of magnetic reconnection, are 531 shown by the blue and red colors. The dashed white line near the X-line, which is ro-532 tated about 1:3°, is theL direction of the local reconnetion coordinate system. We also 533 found that the axis is aligned with the axis in GSM. So the LMN coordinate vec-534 tors for this reconnection event lare(0.9720, 0.233)M = (0, 1, 0) and N = (-0.2330, 0.972). 535 The electron velocities are shown in the LMN coordinate system to allow a direct com-536 parison with the MMS observations. Panels (b) and (d) show the electron velocity dis-537 tribution functions (VDF) from the model and the MMS observation. The simulation 538 VDF of the electrons is collected inside an ellipsoid region centered  $\mathfrak{B}\mathfrak{B}(0.5 - 0.9)$  R<sub>E</sub> 539 with principle semi-axes:  $(\mathfrak{Q}25, \mathfrak{Q}3) \mathbb{R}_{\mathsf{F}}$  in the  $(\mathfrak{x}; \mathfrak{y}; \mathfrak{z})$  directions, respectively. The red 540 circle in panel (a) labeled by B is the cross section of the ellipsoid with the meridional 541 plane. The choice of the ellipsoid shape is based on panel (c) that shows where the MMS 542 observations were taken with respect to the reconnection site according to Figure 2 by 543 Hwang et al. (2019). The MMS3 observations of the electron VDF (Hwang et al., 2019) 544 at the location -(181; 7:300.66) R<sub>F</sub> are shown in panel (d). Although the simulation 545 and observation are not from the same event and the EDR is not at the same position 546 in GSM coordinates, the electron data is collected at a similar location relative to the 547 X-line and the velocity components are all projected to the LMN coordinates (see pan-548 els (a) and (c)). 549

This suggests that we can directly compare the two VDF plots in panels (b) and 550 (d), and they indeed agree very well. The agreement is not only gualitative, but in fact 551 quantitative. since the ion-electron mass ratio is 100, the simulated electron velocity is552  $\frac{m_{i;real}}{m_{e;real}} = \frac{m_{i;simulation}}{m_{e;simulation}}$ multiplied by 1836 4:28 to be comparable with the obser-553 vations. In both panels the velocity distribution extends 40000 km/s in the di-554 rection and (40,000+20,000) km/s in the direction. A non-Maxwellian core dis-555 tribution can also be clearly identifed in both panels-at0000 kms <  $v_v$  < 10000 kms) 556 and  $|v_z| < 10,000$  km/s. In addition to the electron difusion region, we also collected electrons inside two other ellipsoids at the infow (labeled by A) and outfow (labeled by 558 C) regions. The semi-axes of these two ellipsoids are the same as before while the cen-559 ters of the ellipsoids are 285; 1:5; 0.5) R<sub>E</sub> and (- 330, 1:5; - 1:0) R<sub>E</sub> in the (x; y; z) 560 directions, respectively. Panels (e) and (f) shows the electron VDF iN and L -561 M coordinates, the distribution can be characterized as a bidirectional beam distribu-562 563 tion (Asano et al., 2008). The distribution functions at outfow region in panels (g) and (h) are almost circles with shifted centers indicating the direction of the bulk velocities. 564 The distribution functions from the infow and outfow also agree very well with the ex-565 isting theories (Pritchett, 2006; Egedal et al., 2010). Hence, we can conclude that an MHD-566 AEPIC global simulation can generate electron phase space distributions that are very 567 close to the MMS observations, and reproduces the main features of reconnection physics 568 even at the electron scales. 569

# 570 4 Conclusions and Discussions

In this paper, we introduced a newly developed magnetohydrodynamic with adap-571 tively embedded particle-in-cell (MHD-AEPIC) model. The MHD-AEPIC allows PIC 572 grid cells to be turned on and of during the simulation based on the physical criteria 573 provided. Diferent from the previous MHD-EPIC model, which requires a fxed Carte-574 sian box to cover the PIC region, the MHD-AEPIC model enables PIC regions moving 575 with the reconnection sites to save computational resources substantially. During the main 576 phase of the storm, from ≥ 2011-08-06 00:05:00 = 2011-08-06 02:54:00, when the 577 volume of the PIC domain is about  $12,000^{\circ}$ . The relative timings are the following: 578 7272% of CPU time is used on FLEKS, 1:26% is for BATS-R-US and 1035% is taken 579 by the coupling between FLEKS and BATS-R-US. The rest: 87% of CPU time is con-580 sumed by RIM, RCM and the overhead of the SWMF. For the entire 16-hour geomag-581 netic storm simulation, the total wall time is 256.29 hours on 5600 CPU cores. 582

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 frst time. It remains to be determined whether kinetic physics can play a more important role in other events, including but not limited to substorms. The fapping 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 590 and compared the three models at multiple physical scales. We examined the global scale 591 features by comparing the SYM-H and SME indexes which refect the equatorial and au-592 roral region disturbances, respectively. All three models properly capture the global scale 593 disturbances such as the main phase of the storm or the increase of the auroral electro-594 jet. However, all three models fail to produce the strongest intensity for the geoindices. 595 Hence no significant difference is found among the three different models at the global 596 scale for this event. This indicates that the global magnetosphere configuration from the 597 three models are very close, the kinetic model embedded in the magnetotail does not im-598 prove the global scale feature for this geomagnetic storm. If this trend persists for other 599 storms, especially extreme events, is still to be investigated. 600

We analyze the mesoscale features by comparing the magnetic feld components and ion profles 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 fux 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 fux rope structures in the current sheet. Only one major fux rope can be observed from the ideal MHD simulation at the selected time, while Hall MHD and MHD-AEPIC can produce fux ropes at a wider range in the dawn-dusk direction. The diference of two types of the fux 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. 615 We collect electron macro-particle velocities at the same side of the electron difusion re-616 gion as the MMS3 satellite did (Hwang et al., 2019). The velocity distribution functions 617 show excellent agreement between the simulation and the MMS3 observation. This demon-618 strates that MHD-AEPIC can properly produce the electron scale features within a sin-619 gle self-consistent global model while simulating a complete geomagnetic storm event. 620 In this particular simulation, including the kinetic reconnection physics does not improve 621 agreement with observations at meso- and global scales. This suggests that in this storm 622 event, the magnetosphere is mostly driven by the external solar wind and interplanetary 623 magnetic feld and not by the internal reconnection dynamics. 624

It is to be investigated if the kinetic physics can have a more pronounced infuence
 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 numer ical reconnection during extreme events. In addition to studying the Earth's magneto sphere, we also expect the novel MHD-AEPIC model will fnd its applications in vari ous collisionless plasma systems that form small regions where kinetic efects are important inside a large spatial domain.

# Data Availability Statement

The Geotail data is publicly available at Data ARchives and Transmission System 633 (DARTS) of Institute of Space and Astronautical Science (ISAS) (https://darts.isas.jaxa.jp). 634 The MMS observation plot is acquired with consent from Dr. K.-J. Hwang (jhwang@swri.edu). 635 The SWMF code (including BATS-R-US and FLEKS) is publicly available through the 636 csem.engin.umich.edu/tools/swmf web site after registration. The simulation output and 637 scripts used for generating fgures in this paper can be obtained online (https://doi.org/10.7302/xtvh-638 tq17) through the University of Michigan's Deep Blue Data repository, which is specif-639 ically designed for U-M researchers to share their research data and to ensure its long-640 term viability. 641

# Acknowledgments

We thank Dr. Qusai Al Shidi at the University of Michigan for the script calculating the SME index using interpolated virtual magnetometer data from BATS-R-US. This work was primarily supported by NSF PRE-EVENTS grant No. 1663800. We also acknowledge support from the NASA DRIVE Center at the University of Michigan under grant NASA 80NSSC20K0600. We acknowledge the use of computational resources provided by an NSF LRAC allocation at the Texas Advanced Computing Center (TACC) at The University of Texas at Austin.



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

# <sup>650</sup> Appendix A Reconnection due to numerical resistivity

It is a common practice to rely on numerical resistivity to mimic reconnection physics
 in global ideal and Hall MHD simulations. Analytic solutions of ideal MHD obey the frozen in condition: the magnetic fux through a surface co-moving with the plasma (i.e. the
 ion fuid) does not change. For Hall MHD the magnetic fux is frozen into the motion
 of the electron fuid. A consequence of the frozen-in condition is that if two plasma el ements are connected by a feld line, then they remain connected forever, which means
 that magnetic reconnection cannot take place.

In reality, and also in the kinetic PIC model, the electrons and ions can "detach" from the magnetic feld lines in the ion and electron difusion regions, respectively. In efect, this allows the magnetic feld lines to reconnect inside the electron difusion region where the frozen in condition does not apply. The simplest mathematical description of this process is adding an Ohmic resistive termeto the induction equation:

$$\frac{@B}{@t} = -r \times [-u_e \times B + j]$$
(A1)

For magnetic difusivity  $' = = \mu_0$  one can write this as

$$\frac{@B}{@t} = -r \times [-u_e \times B] - r \times ('r \times B)$$
(A2)

where we use  $d = (1 = \mu_0)r \times B$  and assumed that is not constant in space in gen-664 eral. The usual argument in favor of using the ideal MHD model is that numerical re-665 sistivity will behave similarly to the difusive terma ( 'rx B) and indeed, numeri-666 cal experiments show that magnetic reconnection remains a robust feature of ideal MHD 667 simulations. On the other hand, one would expect numerical difusion to go to zero with 668 increased grid resolution, which implies that reconnection should disappear from a well-669 resolved solution. In this appendix, we take a closer look at resolving this contradiction 670 for 1D geometry and provide arguments for 3D geometry. 671



Figure 2. The solar wind bulk plasma and interplanetary magnetic feld input in Geocentric Solar Magnetospheric coordinates (from top panel to the bottom: plasma density, plasma temperature,x; y and z components of the plasma fow velocityand z components of the magnetic feld) for the simulation in this paper. The x-component of the magnetic feld 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).

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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 di erent re nement levels. The re nement ratio between two adjacent levels is 2. The grid resolution near Earth is  $1 = 8R_E$  it is  $1 = 4R_E$  on the dayside and the magnetotail out to  $x > 80R_E$ .

Figure 11. (a) The  $B_x$  pro les across the current sheet from two simulations with di erent grid resolutions in the magnetotail. The pro les are taken along the  $x = 20R_E$  and y = 0 line from  $z = 5R_E$  to  $5R_E$ . The symbols show the discrete values at the grid cell centers. (b) The  $J_y$  current pro les taken at the same position as  $B_x$  in panel (a). (c) The meridional cut of the simulation domain with  $J_y$  and magnetic eld lines for  $1 = 4R_E$  grid resolution in the magnetotail. (d) Same physical quantities as panel (c) but with  $1 = 8R_E$  grid resolution in the magnetotail. Two snapshots are taken at the same time 2011-08-05 15:30:00.

The main argument is that an ideal MHD reconnecting current sheet behaves like 672 a discontinuity and therefore the derivatives of the solution across the current sheet do 673 not converge to a nite value. In particular, the current density, obtained from the deriva-674 tive of the magnetic eld, goes to in nity as the grid resolution is increased, while the 675 numerical di usion goes to zero. Their product, which determines the reconnection rate, 676 remains nite. Although it is still an open question, the Axford Conjecture (Axford, 1984; 677 Gonzalez et al., 2016) suggests that the global time averaged reconnection rate is pre-678 dominantly set by the external solar wind and IMF driver. On the dayside, the solar wind 679 brings in magnetic ux at a rate of  $ju_x jB_z$ . A fraction of this ux will reconnect at the 680 dayside magnetopause fo $B_z < 0$ . For a time period that is much longer than substorms, 681 since the magnetic ux attached to Earth cannot grow without bound, there has to be 682 a matching reconnection rate in the magnetotail. 683

We now look into more detail, how the numerical scheme actually achieves this. For nite volume methods solving the

$$\frac{@U}{@t} + r \quad F = 0 \tag{A3}$$

equation, the numerical ux is calculated at the cell interfaces, and it depends on the right and left states U<sup>R</sup> and U<sup>L</sup> extrapolated from the right and left directions, respectively, and the characteristic wave speeds. The Lax-Friedrichs ux is the simplest example:

$$F^{LF} = \frac{F(U^{R}) + F(U^{L})}{2} - \frac{1}{2} \max(U^{R} - U^{L})$$
 (A4)

where F is the physical ux function. The rst term contains the physical ux as the average of  $F(U^R)$  and  $F(U^L)$ . The second term introduces numerical di usion to preserve