MHD with embedded particle-in-cell model and its applications

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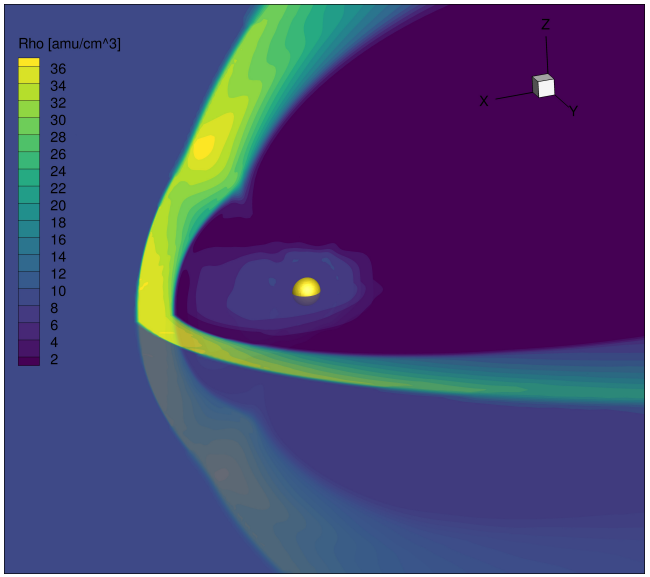
Outline

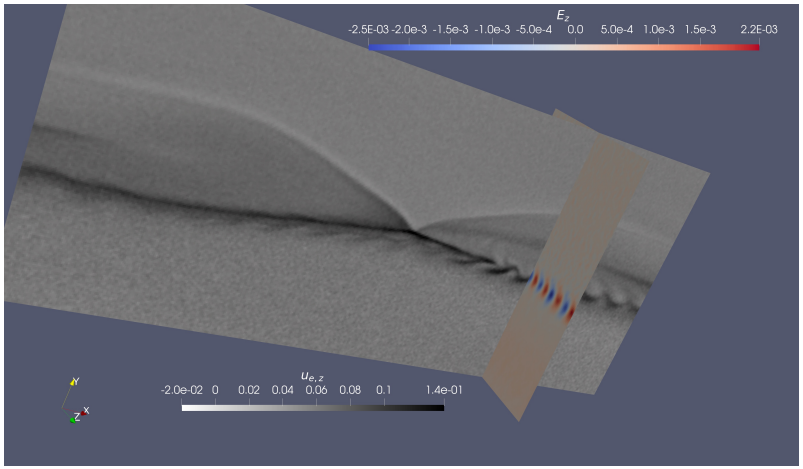
- **Introduction**
  - Background of developing MHD with embedded particle-in-cell (MHD-EPIC) model
- **Coupling between MHD and PIC**
- **Improvement of the PIC component**
  - Gauss's Law satisfying Energy Conserving Semi-Implicit Method (GL-ECSIM)
  - FLexible Exascale Kinetic Simulator (FLEKS)
- **Applications**
  - Mercury's magnetotail
  - Earth's dayside magnetopause

Introduction: MHD vs. Kinetic

- **Ideal MHD**
  - Efficient for 3D global simulations.
  - Does not contain kinetic physics.



- **Kinetic models** of collisionless plasma: Vlasov-Maxwell solver, PIC
  - Solve the evolution of the velocity space (Vlasov equation)
  - Computationally expensive



- Why it is difficult to capture kinetic processes in global simulations?
  - Orders of difference between the kinetic scales and the global scale
  - Example of Earth's magnetosphere:

$\lambda_D \sim 100$ m; $d_e \sim 5$ km; $d_i \sim 100$ km; Magnetosphere size $\sim 10R_E \sim 10^5$ km

Introduction: Incorporate Kinetic Physics into Global Simulations

- **Hybrid models**
  - Fluid massless electrons + kinetic (PIC or Vlasov solver) ions
  - Local kinetic + global fluid -> MHD-EPIC
- **Extended MHD**
  - Five-moment (isotropic pressure), six-moment (anisotropic pressures), and ten-moment (pressure tensors)

Earth's magnetosphere:
$\lambda_D \sim 100$ m; $d_e \sim 5$ km; $d_i \sim 100$ km;
Magnetosphere size $\sim 10R_E \sim 10^5$ km

- **Multi-scale simulations: reduce the separation between scales**
  - Reduce speed of light: reduce separation between λ_D and d_e
  - Reduce the m_i/m_e ratio: reduce separation between d_e and d_i

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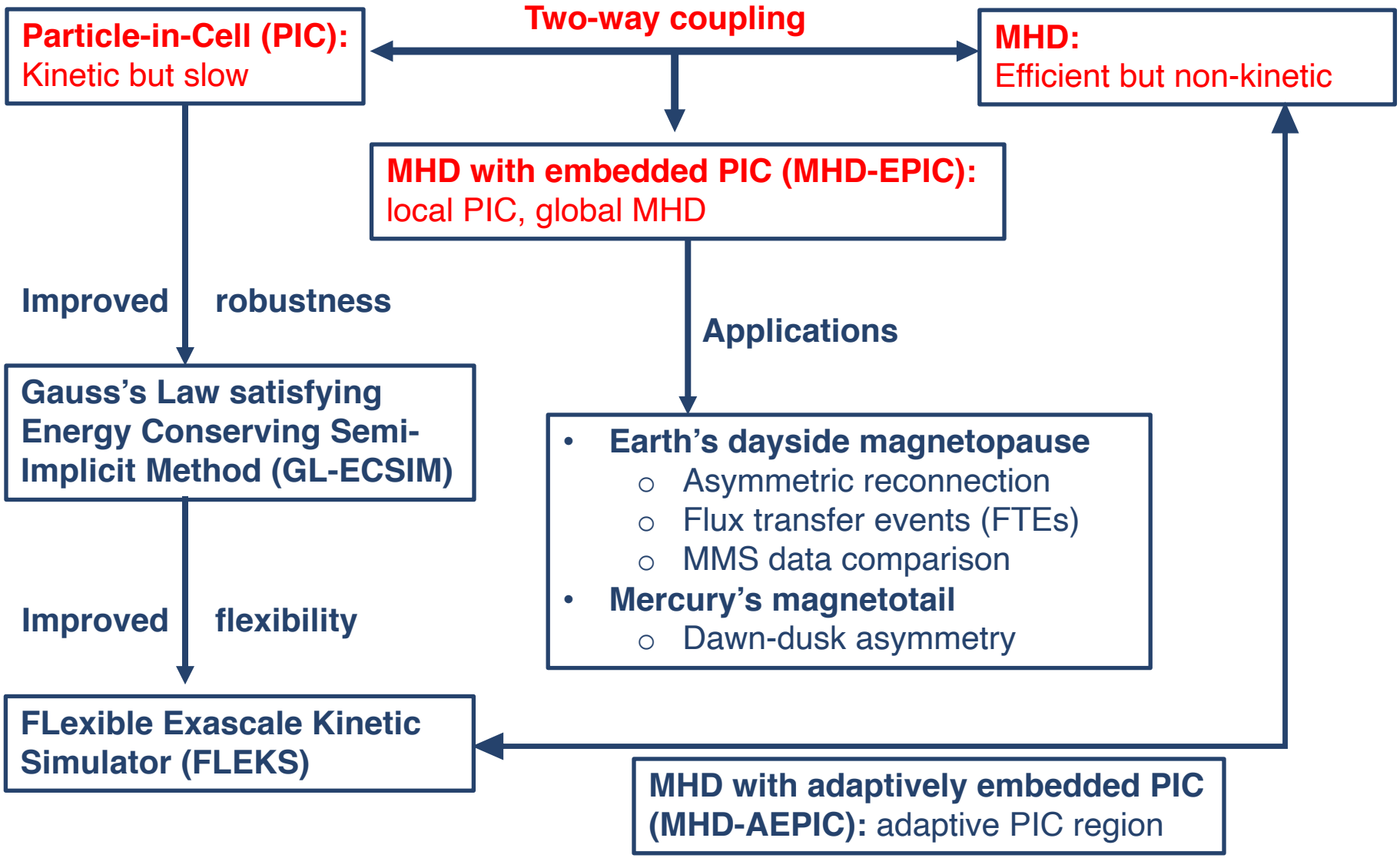
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Kinetic but slow
Two-way coupling
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MHD-EPIC Algorithm

The goal is to combine the efficiency of the global fluid code with the physics capabilities of the local PIC code!

- **MHD code - BATS-R-US**
  - Solves the ideal, Hall, two-fluid, multi-ion, anisotropic MHD equations on 1, 2 or 3D block-adaptive Cartesian and non-Cartesian grids
  - Five- and six-moment multi-fluid equations
  - Explicit and implicit time stepping, up to 5th order accurate schemes
  - Complicated initial and boundary conditions, variety of source terms
- **PIC code - IPIC3D & FLEKS**
  - Solves full set of Maxwell's Equations implicitly on 2D or 3D Cartesian grid
  - Relaxed stability constrains compared to explicit PIC
- **Framework – SWMF**
  - Executes and couples multiple models on massively parallel machines
  - Efficient parallel coupler developed for MHD-EPIC

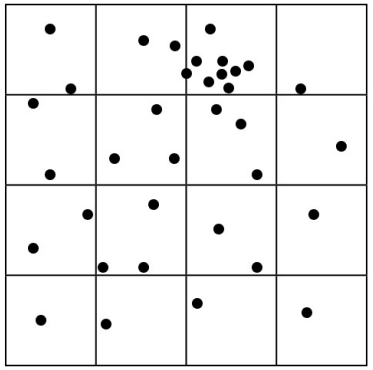
Particle-in-Cell Method

$$\frac{\partial \mathbf{B}}{\partial t} = -c\nabla \times \mathbf{E}$$

$$\frac{\partial \mathbf{E}}{\partial t} = c\nabla \times \mathbf{B} - 4\pi \mathbf{J}$$

$$\frac{d\mathbf{p}}{dt} = q(\mathbf{E} + \frac{\mathbf{V} \times \mathbf{B}}{c})$$

- **Physics**
  - Collisionless plasma
  - Solves Maxwell's Equations
  - Equations of motion for electrons and ion macro-particles
- **Calculation steps**
  - Loop through all the particles once to calculate the current at each grid cell
  - Solve the Maxwell equations on the grid
  - Interpolate the EM field from the grid to the particles
  - Move the particles



Explicit PIC vs. Semi-Implicit PIC

- **Explicit PIC**
  - Updates EM fields with known E, B and current
  - Cell size needs to resolve Debye length to suppress finite grid instability
  - Conditional stable: time step needs to resolve plasma oscillation and propagation of light wave

$$\frac{\mathbf{B}^{n+1}-\mathbf{B}^{n}}{\Delta t} = -c\nabla\times\mathbf{E}^{n}$$

$$\frac{\mathbf{E}^{n+1}-\mathbf{E}^{n}}{\Delta t} = c\nabla\times\mathbf{B}^{n} - 4\pi\mathbf{J}^{n}$$

- **Semi-Implicit PIC**
  - $0.5 \le \theta \le 1$
  - Updates fields with E, B and J in the future.
  - Semi-implicit: $J^{n+1/2}$ linearly depends on $E^{n+\theta}$. $J^{n+1/2} \sim J^{n} + \mathbf{M}\cdot E^{n+\theta}$
  - Solves linear system with an iterative solver
  - No need to resolve Debye length
  - Linearly unconditional stable: time step is not limited by plasma oscillation and propagation of light wave

$$\frac{\mathbf{B}^{n+1}-\mathbf{B}^{n}}{\Delta t} = -c\nabla\times\mathbf{E}^{n+\theta}$$

$$\frac{\mathbf{E}^{n+1}-\mathbf{E}^{n}}{\Delta t} = c\nabla\times\mathbf{B}^{n+\theta} - 4\pi\mathbf{J}^{n+1/2}$$

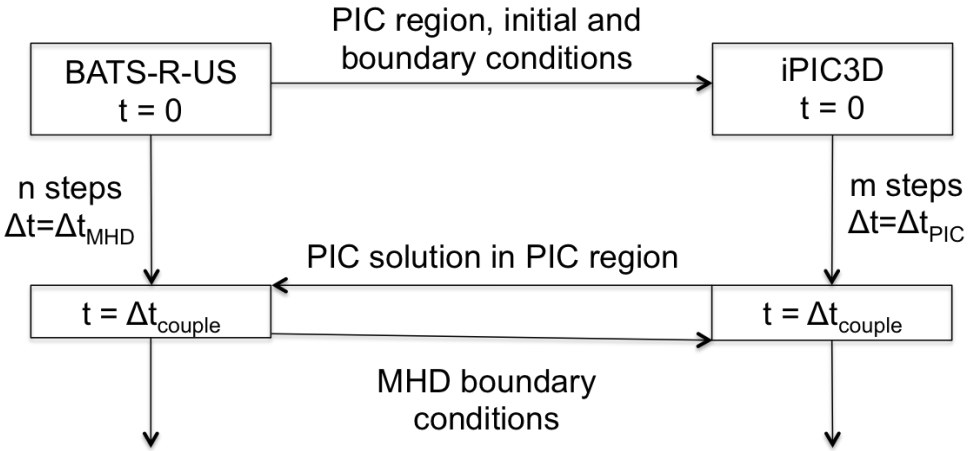
Explicit PIC vs. Semi-Implicit PIC

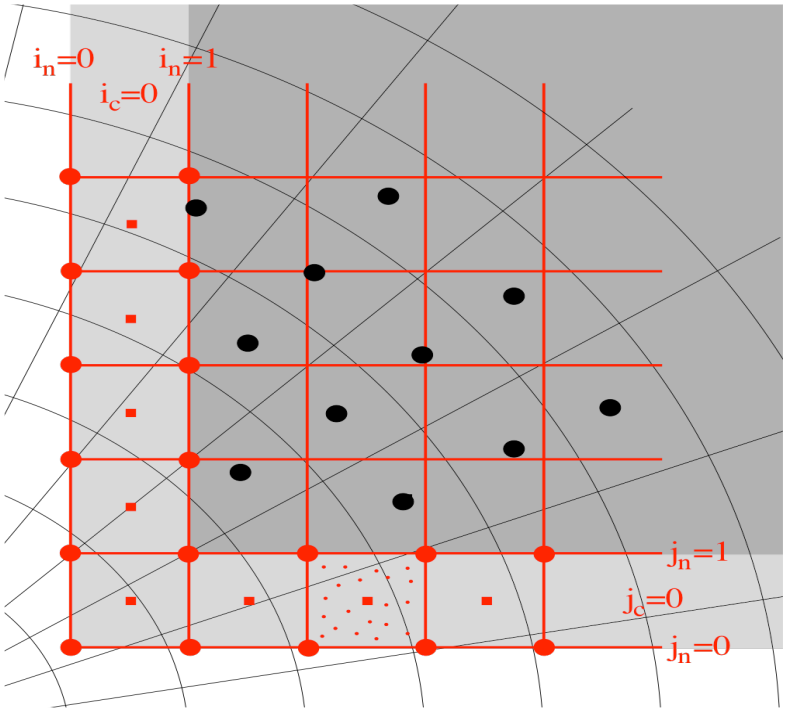
- **Explicit PIC vs. Semi-implicit PIC**
  - Both solve the same set of equations, but with different discretization
  - Converge to the same solution
  - With the same cell size and number of macro-particles, explicit PIC is ~10 times faster than semi-implicit PIC
  - Explicit PIC needs to resolve Debye length and plasma oscillations for stability reason
  - Semi-implicit PIC only needs to resolve the scales of interest

- **Unresolved scales**
  - When Δt is large, the unresolved waves are strongly damped (Brackbill et al., 1982, JCP)

Coupling between MHD and PIC

- **Capabilities**
  - Ideal, Hall and multi-ion MHD. Separate electron pressure.
  - Different PIC and MHD grids including non-Cartesian AMR MHD grids.
  - Different PIC and MHD time steps.
  - Efficient coupling through the SWMF.
  - Multiple PIC domains.
  - Works in 2D and 3D.
- **For the PIC code, MHD-EPIC is a method of setting initial and boundary conditions**





PIC Initialization

MHD equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \left[\rho \mathbf{u}\mathbf{u} + p_\perp \mathbf{I} + (p_\parallel - p_\perp)\mathbf{b}\mathbf{b} - \frac{1}{\mu_0}\left(\mathbf{B}\mathbf{B} - \frac{B^2}{2}\mathbf{I} \right) \right] = 0$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times (-\mathbf{u}_e \times \mathbf{B}) = 0$$

$$\frac{\partial e}{\partial t} + \nabla \cdot \left[\mathbf{u}\left(e + p_\perp + \frac{\mathbf{B}^2}{2\mu_0} \right) + \mathbf{u} \cdot \left((p_\parallel - p_\perp)\mathbf{b}\mathbf{b} - \frac{\mathbf{B}\mathbf{B}}{2\mu_0} \right) \right] = 0$$

Particle-in-Cell:

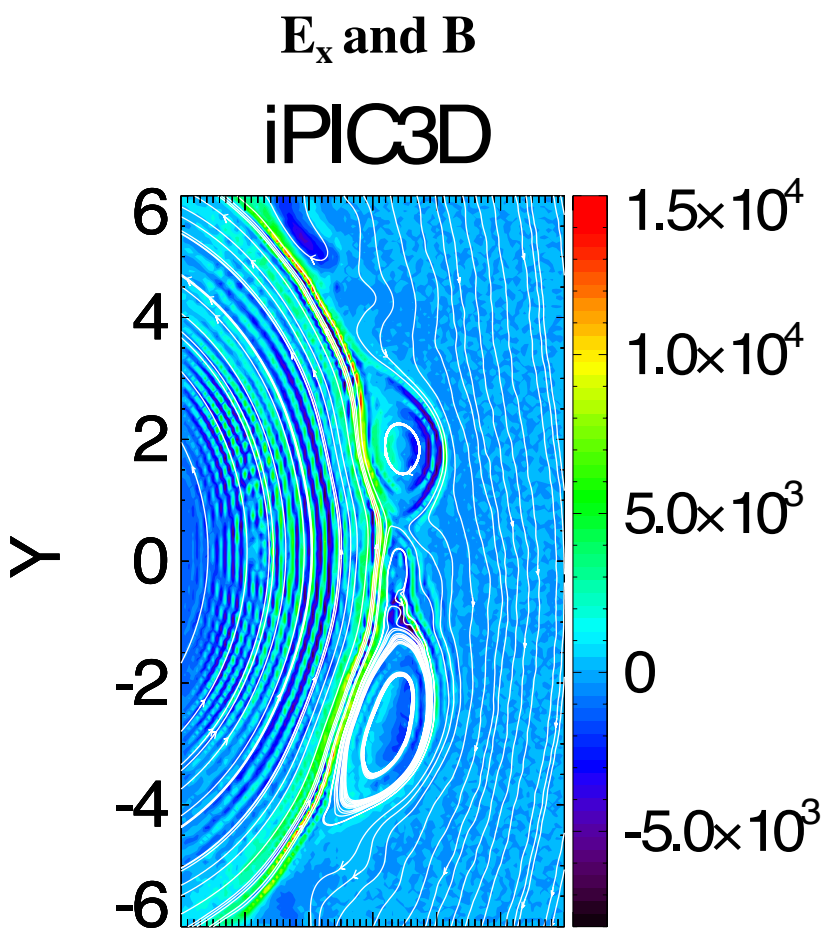
$$\frac{\partial \mathbf{B}}{\partial t} = -c\nabla \times \mathbf{E}$$

$$\frac{\partial \mathbf{E}}{\partial t} = c\nabla \times \mathbf{B} - 4\pi \mathbf{J}$$

$$\frac{d\mathbf{p}}{dt} = q(\mathbf{E} + \frac{\mathbf{V} \times \mathbf{B}}{c})$$

- **Initialize PIC from MHD**
  - Calculate Electric field from Ohm's law: $\mathbf{E} = -\mathbf{u} \times \mathbf{B} + \frac{\mathbf{J} \times \mathbf{B}}{q_e n_e}$
  - Assume charge neutral: $n_i = n_e$
  - Ion and electron velocities can be obtained from the fluid momentum and current $n(m_i \mathbf{u}_i + m_e \mathbf{u}_e) = \rho \mathbf{u}_{\mathrm{MHD}}$ $n(q_i \mathbf{u}_i + q_e \mathbf{u}_e) = \mathbf{J}_{\mathrm{MHD}}$
  - Pressure
    Solve the electron pressure equation: $\frac{\partial p_e}{\partial t} + \nabla \cdot (p_e \mathbf{u}_e) = (\gamma - 1)(-p_e \nabla \cdot \mathbf{u}_e)$
  - Generate macro-particles from Maxwellian distribution

Numerical Oscillations in iPIC3D



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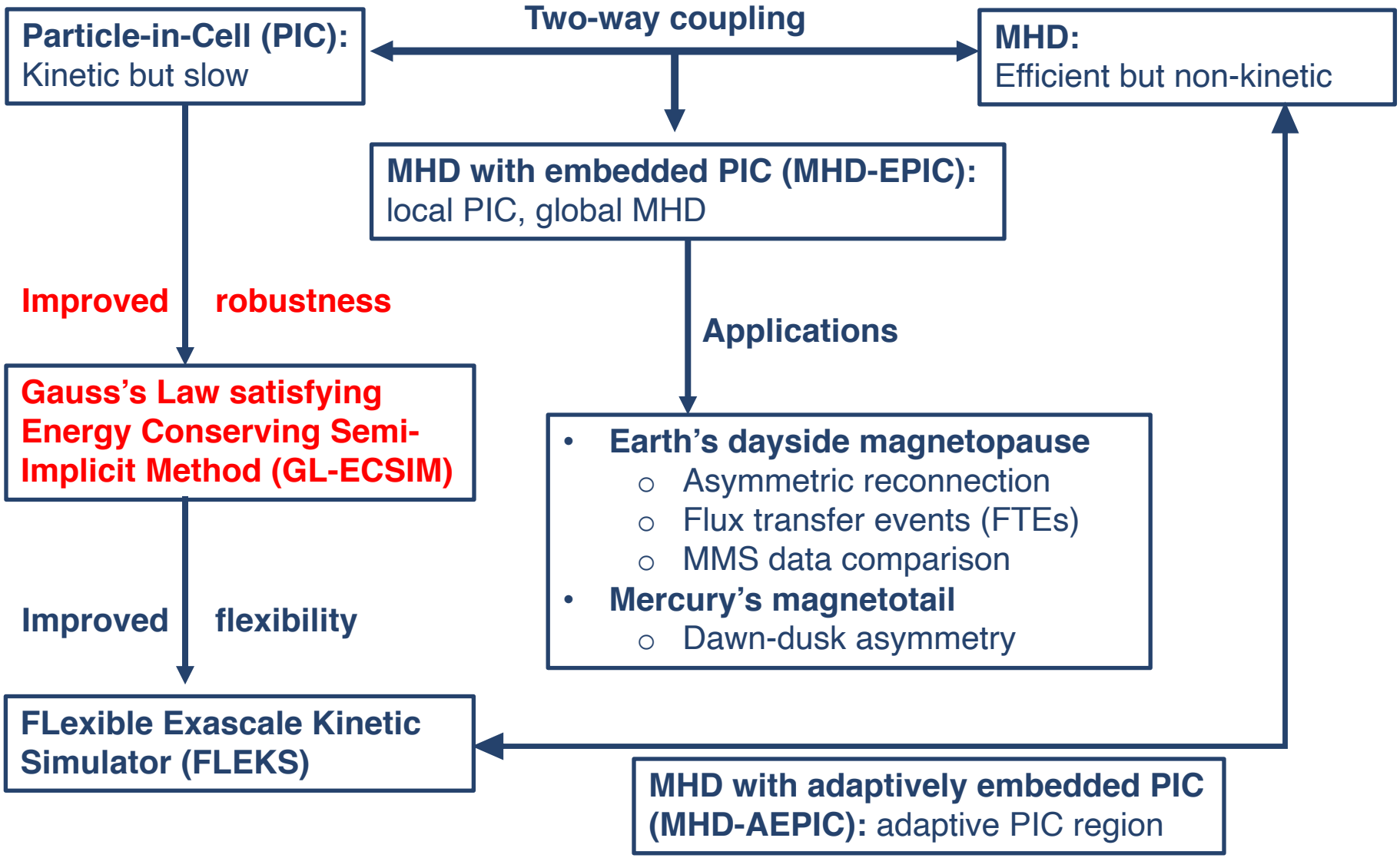
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General Idea of ECSIM (Lapenta 2017)

Maxwell equations are solved implicitly on the grid:

$$\nabla \times \mathbf{E}^{n+\theta} + \frac{1}{c}\frac{\mathbf{B}^{n+1} - \mathbf{B}^{n}}{\Delta t} = 0$$

$$\nabla \times \mathbf{B}^{n+\theta} - \frac{1}{c}\frac{\mathbf{E}^{n+1} - \mathbf{E}^{n}}{\Delta t} = \frac{4\pi}{c}\bar{\mathbf{J}}$$

$$\mathbf{E}^{n+\theta} = (1-\theta)\mathbf{E}^{n} + \theta\mathbf{E}^{n+1}$$

$$\mathbf{B}^{n+\theta} = (1-\theta)\mathbf{B}^{n} + \theta\mathbf{B}^{n+1}$$

The unknowns are at time level n+θ. The current $\bar{J}$ at time level n+1/2 is also calculated implicitly using $E^{n+\theta}$ and a mass matrix.

The particle velocity update uses $\bar{J}$.

For θ=1/2 the total energy (particles+fields) is exactly conserved

This means that instabilities requiring energy cannot grow.

Improving efficiency (borrowing idea from iPIC3D)

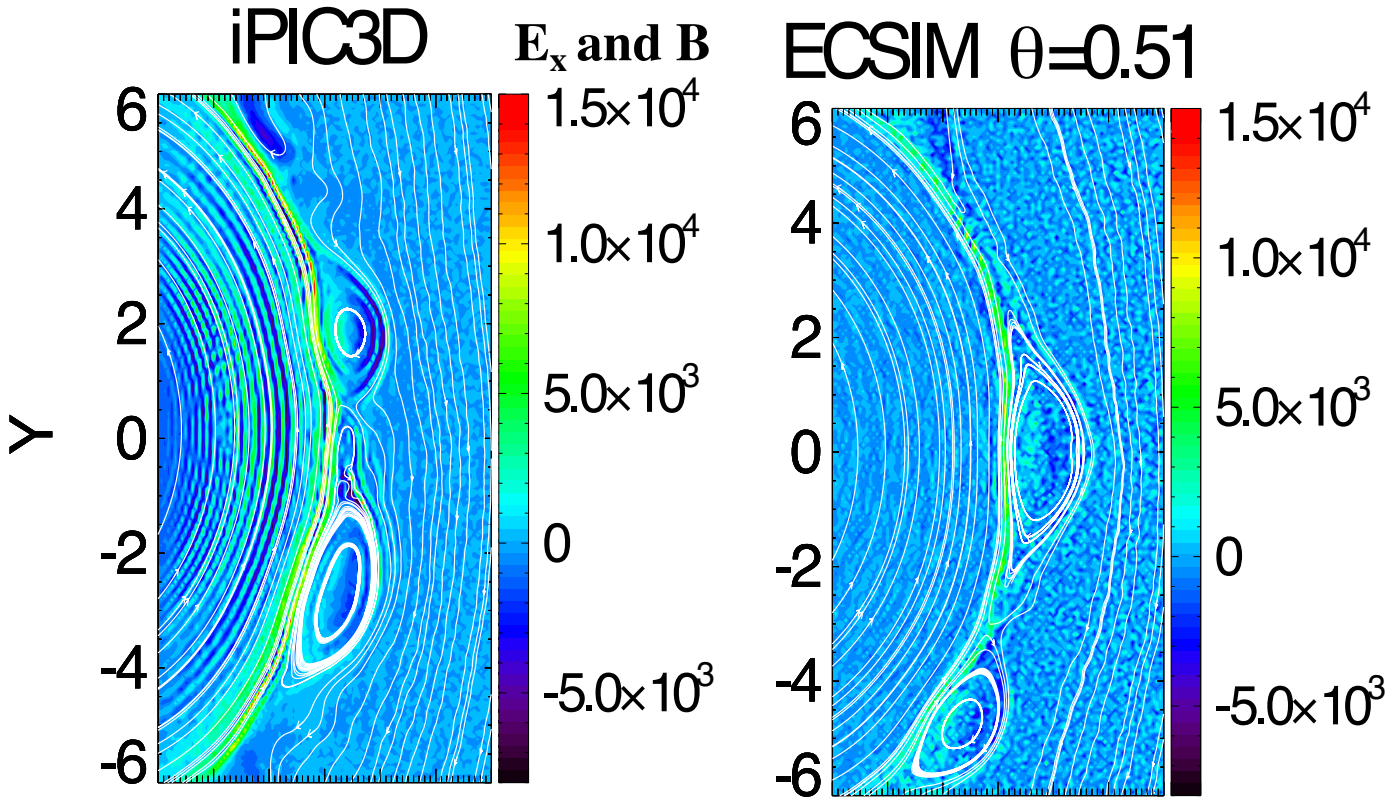
The above system can be combined into a numerically identical equation for $E^{n+\theta}$:

$$\mathbf{E}^{n+\theta} + \delta^2\left[\nabla(\nabla\cdot\mathbf{E}^{n+\theta}) - \nabla^2\mathbf{E}^{n+\theta}\right] = \mathbf{E}^{n} + \delta(\nabla\times\mathbf{B}^{n} - \frac{4\pi}{c}\bar{\mathbf{J}})$$

where $\delta = c\theta\Delta t$. This is faster to solve than the original system of equations.

B^{n+1} is obtained from the induction equation explicitly.

Comparison between iPIC3D and ECSIM



- **2D magnetopause simulation**
  - ECSIM with θ=0.51 produces good results. Small energy dissipation.

Gauss's Law in ECSIM

- **There is no mechanism to make the solution obey Gauss's law $\rho_c = \nabla.E/4\pi$**
- **Remedies**
  - iPIC3D uses Marder's scheme to diffuse away the error, but using similar approach in ECSIM destroys energy conservation and improvements compared to iPIC3D.
  - Poisson solver to project the electric field

$$\nabla^2\phi = \nabla \cdot \mathbf{E}^{n+1} - 4\pi\rho_c^{n+1}$$

$$\mathbf{E}_{new}^{n+1} = \mathbf{E}^{n+1} - \nabla\phi$$

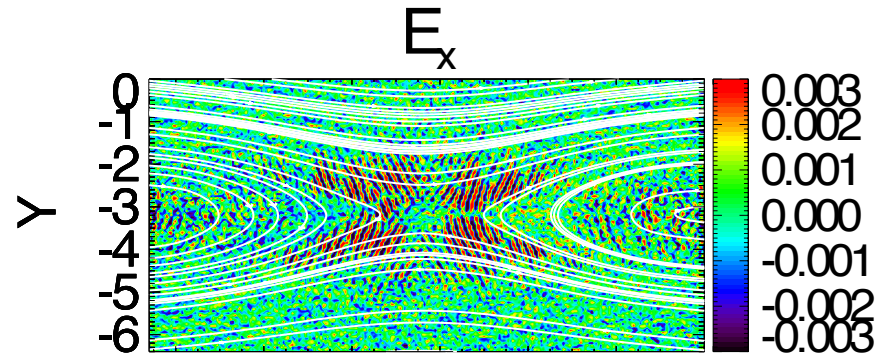
eliminates the error in Gauss's law, but energy is not conserved and results look similar to iPIC3D.

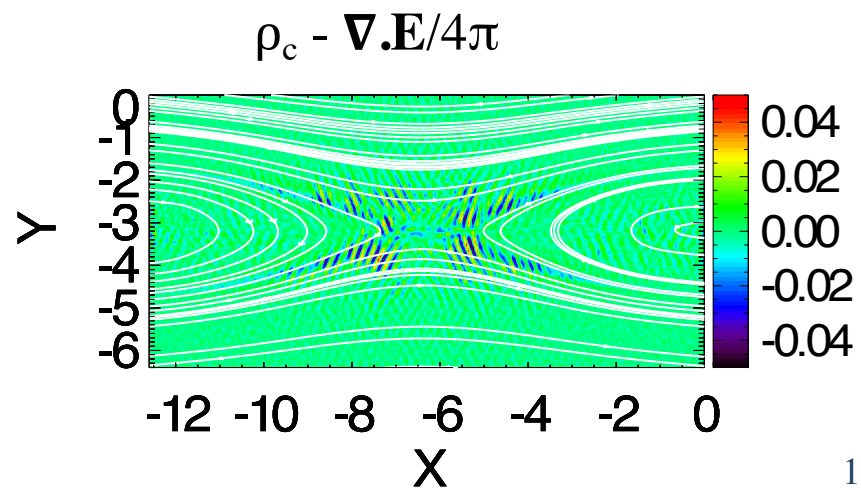
- **What to do?**

$$\frac{\partial \mathbf{B}}{\partial t} = -c\nabla \times \mathbf{E}$$

$$\frac{\partial \mathbf{E}}{\partial t} = c\nabla \times \mathbf{B} - 4\pi\mathbf{J}$$

ECSIM θ=0.51





Move Particles to Satisfy Gauss's Law

- **Why?**
  - Energy is still conserved: fields and velocity are unchanged, only particle positions are modified.
  - Integration of particle trajectories is approximate, so why not?
- **How?**
  - After completing the ECSIM update adjust particle positions to satisfy Gauss's law while minimizing the total displacement: Lagrange multiplier method. (Chen and Toth, 2019, JCP)
- **Our goal is to make the error zero at time level n+1**
  - Time staggering (fields are at integer levels, particles at half levels) we need to interpolate:

$$\rho_c^{n+\frac{1}{2}} = \sum_p q_p W(\mathbf{x}_p^{n+\frac{1}{2}} - \mathbf{x}_c)$$

$$\rho_c^{n+1} = \gamma \sum_p q_p W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} + \Delta\mathbf{x}_p - \mathbf{x}_c) + (1-\gamma)\rho_c^{n+\frac{1}{2}} = \frac{1}{4\pi}\nabla \cdot \mathbf{E}^{n+1}$$

  - γ=0.5 gives second order, but γ=0.51 works better.

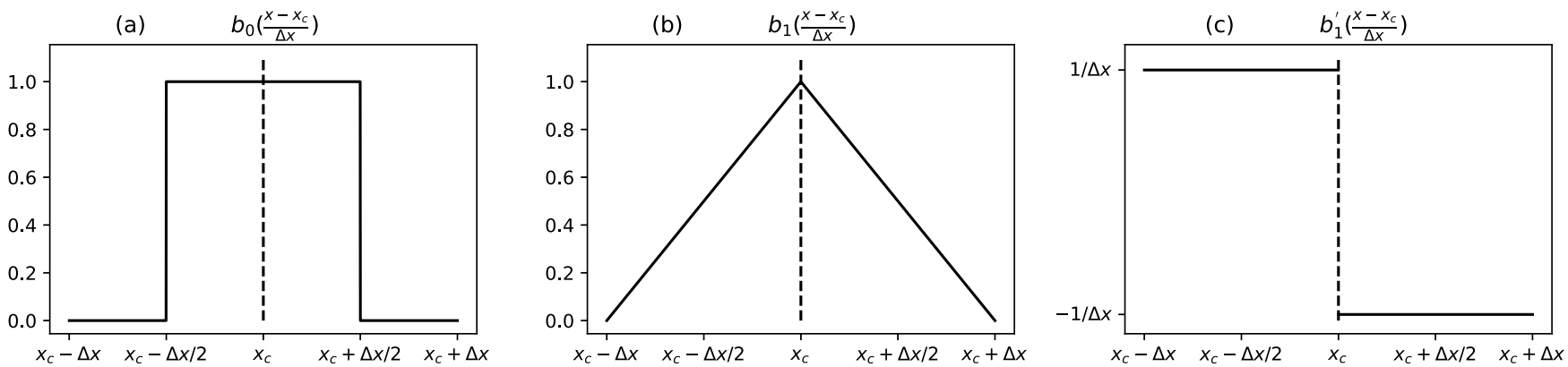
Linearization

Linearization of charge density in Δx_p is necessary for efficient solver:

$$\rho_c^{n+1} = \gamma \sum_p q_p W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} + \Delta \mathbf{x}_p - \mathbf{x}_c) + (1-\gamma)\rho_c^{n+\frac{1}{2}} = \frac{1}{4\pi}\nabla \cdot \mathbf{E}^{n+1}$$

$$W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} + \Delta \mathbf{x}_p - \mathbf{x}_c) = W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} - \mathbf{x}_c) + \nabla W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} - \mathbf{x}_c) \cdot \Delta \mathbf{x}_p + O((\Delta x)^2)$$

ECSIM uses b_1 spline weight functions, but there is a singularity and non-linearity in 2D and 3D, so the linearization is approximate



Solving with Lagrange Multipliers

Minimize $f(\Delta\mathbf{x}_p) = \sum_p \frac{1}{2}(\Delta\mathbf{x}_p)^2 |q_p|^\alpha$ (we will use $\boldsymbol{\alpha}$=1) with the constraints

$$g_c(\Delta\mathbf{x}_p) \triangleq \sum_p q_p \nabla W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} - \mathbf{x}_c) \cdot \Delta\mathbf{x}_p - S_c = 0$$

Construct Lagrange function with Lagrange multipliers λ_c:

$$L(\Delta\mathbf{x}_p, \lambda_c) = f(\Delta\mathbf{x}_p) - \sum_c \lambda_c g(\Delta\mathbf{x}_p)$$

Take derivatives of L with respect to Δx_p:

$$\frac{\partial L}{\partial \Delta\mathbf{x}_p} = \Delta\mathbf{x}_p |q_p|^\alpha - \sum_c \lambda_c q_p \nabla W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} - \mathbf{x}_c) = 0$$

Thanks to the linearization of g_c, this can be solved for Δx_p. Substitute into g_c=0:

$$\frac{\partial L}{\partial \lambda_c} = \sum_p q_p \nabla W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} - \mathbf{x}_c) \cdot \left[|q_p|^{-\alpha} \sum_{c'} \lambda_{c'} q_p \nabla W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} - \mathbf{x}_{c'}) \right] - S_c = 0$$

Swap the sums for p and c' to obtain a linear system for λ_c with a "mass matrix":

$$\sum_{c'} \lambda_{c'} M_{cc'} = S_c \qquad M_{cc'} = \sum_p |q_p|^{2-\alpha} \nabla W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} - \mathbf{x}_c) \cdot \nabla W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} - \mathbf{x}_{c'})$$

Non-linear and Alternative Schemes

- **Iterate over the linear solver (~3 times):**
  - Solve the linear system

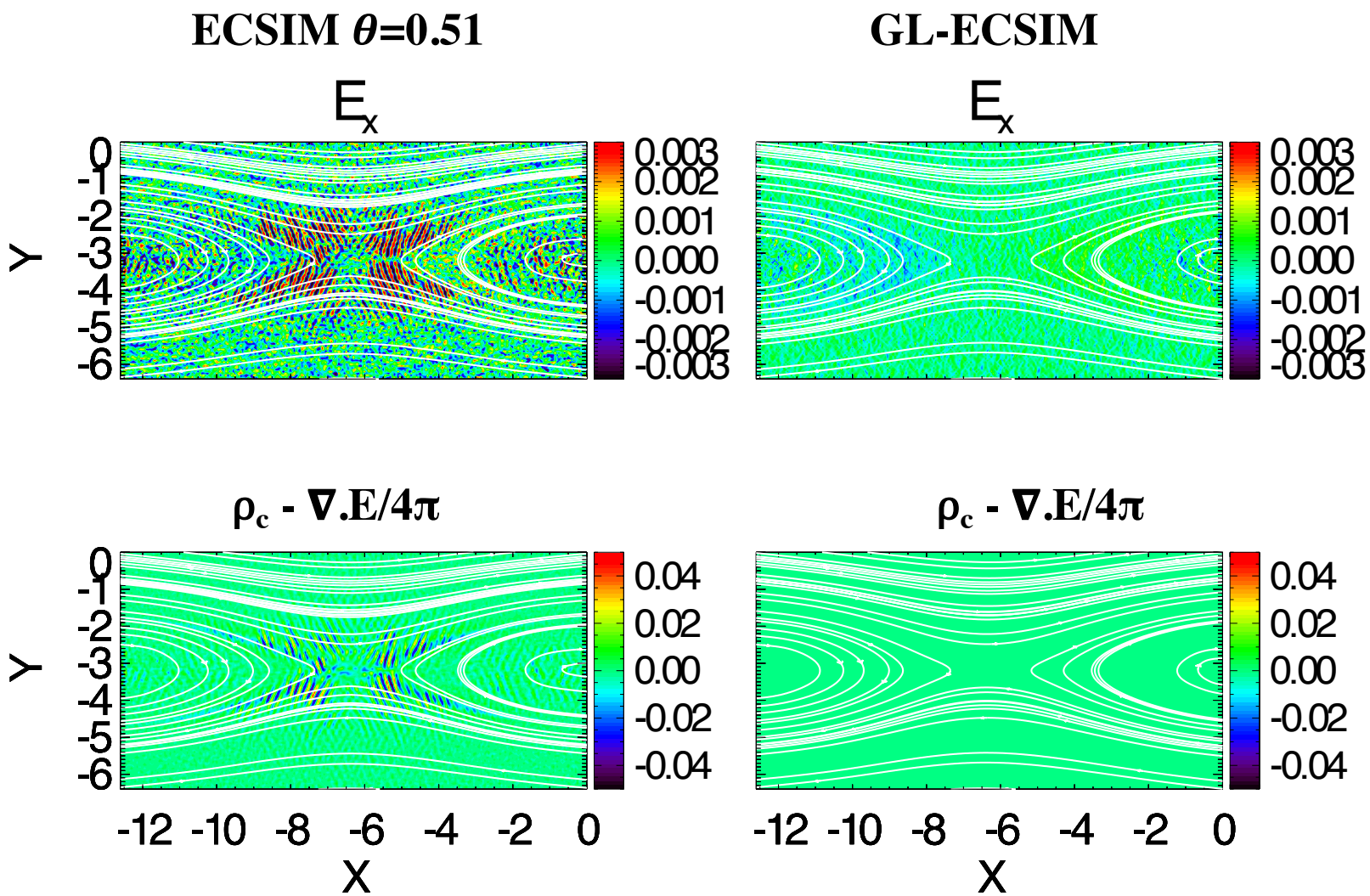
$$\sum_{c'} \lambda_{c'} M_{cc'} = S_c$$

  - for λc, then calculate

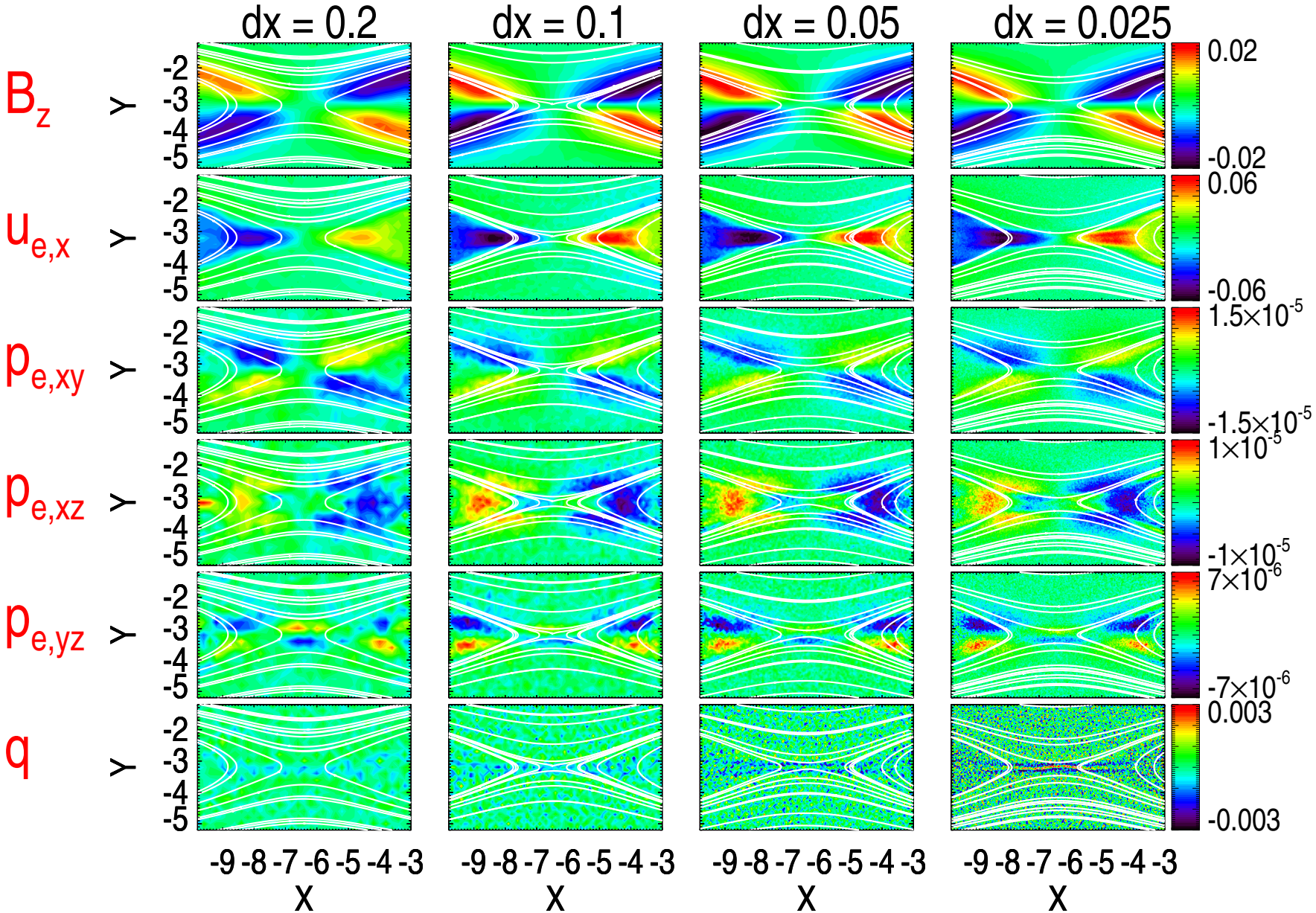
$$\Delta \mathbf{x}_p = \sum_c \lambda_c |q_p|^{1-\alpha} \frac{q_p}{|q_p|} \nabla W(\tilde{\mathbf{x}}_p^{n+\frac{3}{2}} - \mathbf{x}_c)$$

  - Update particle positions, recalculate $M_{cc'}$ and S_c and repeat
- **Alternatives**
  - Approximate solver that does not use a mass matrix
  - Local "push" of particles to reduce error in Gauss's law

GEM Reconnection



Grid Convergence (d_i=1, d_e=0.1)



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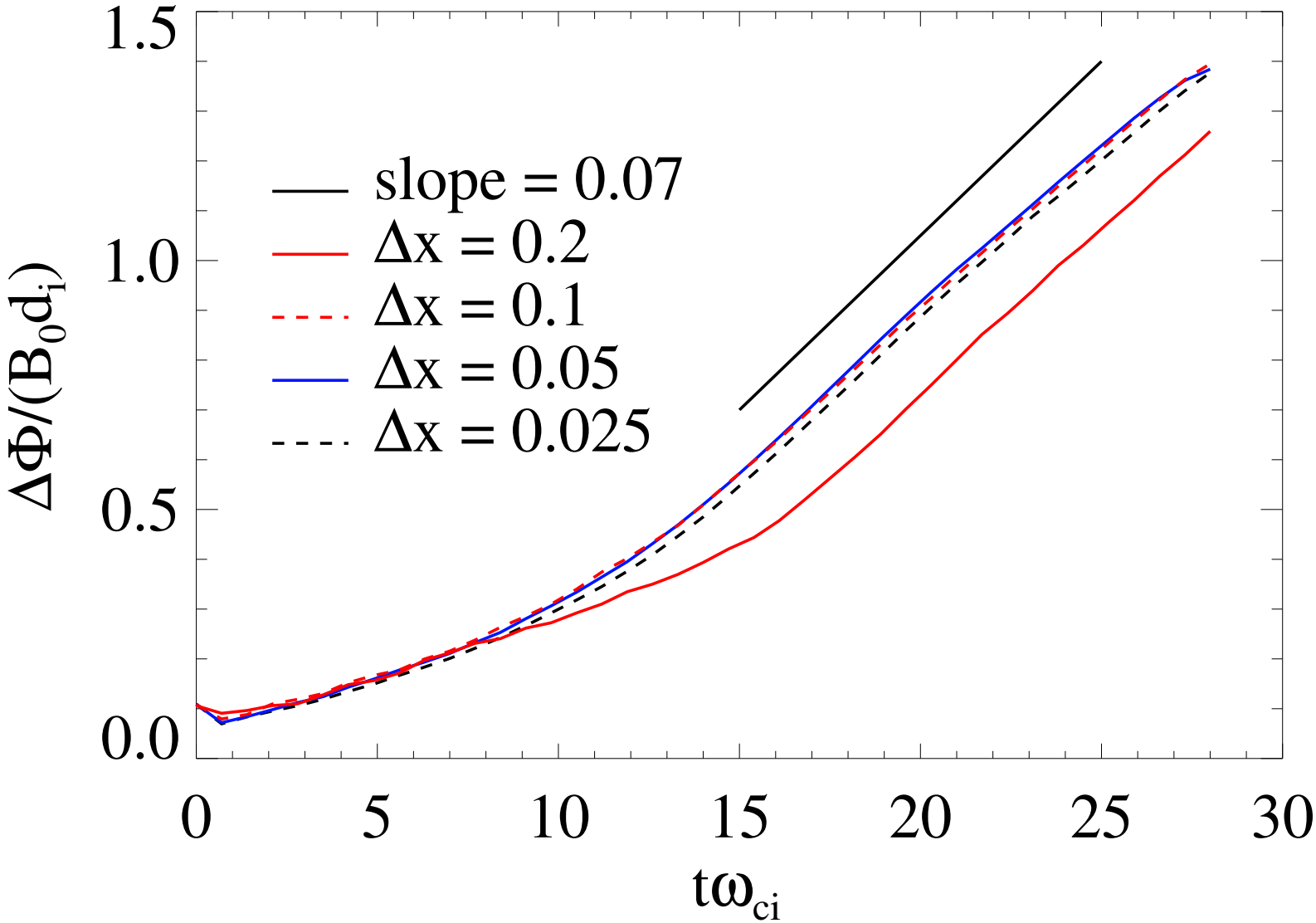
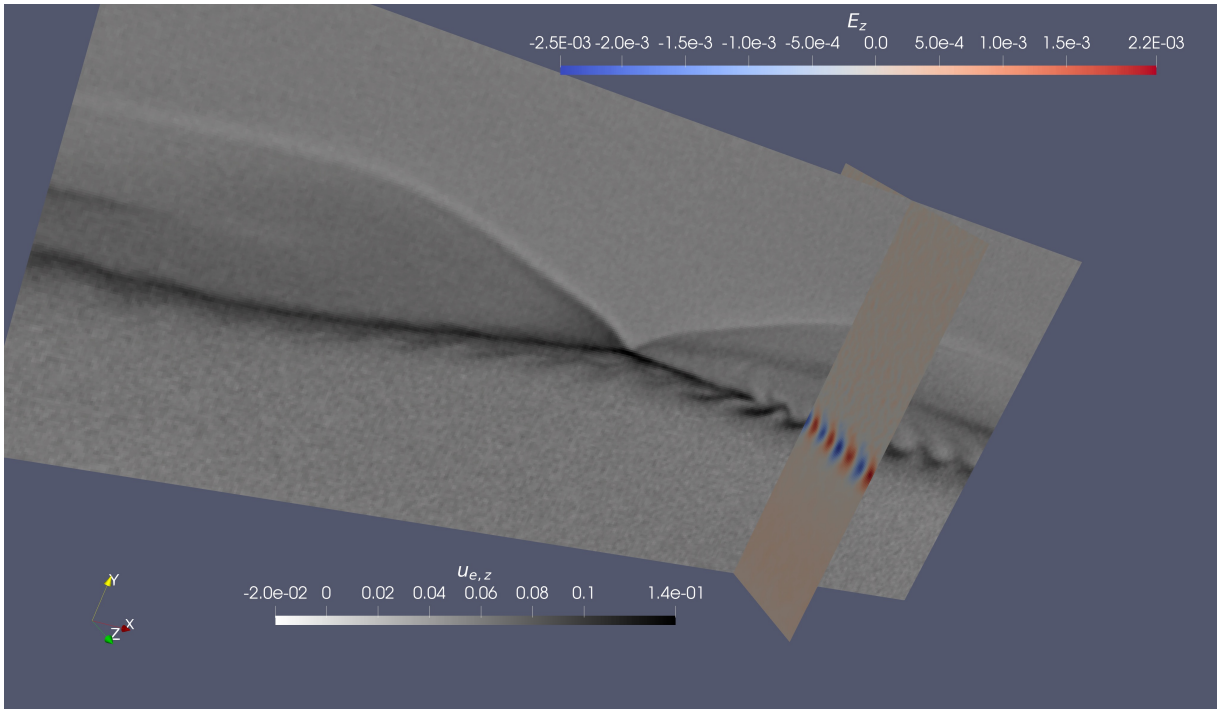
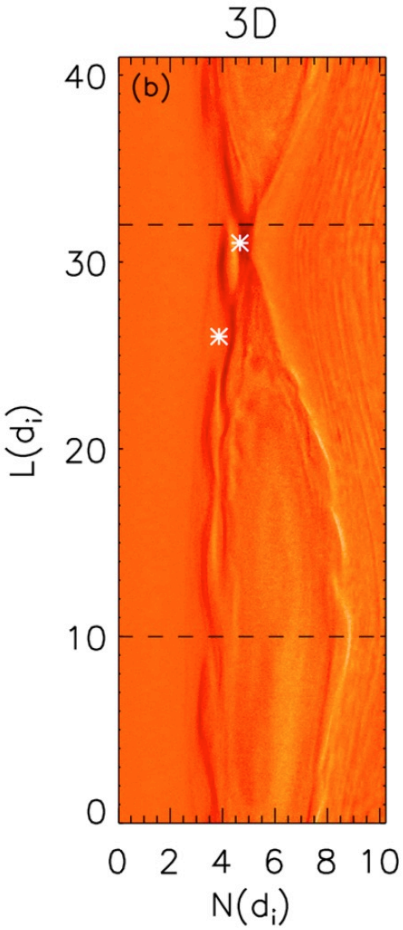


GL-ECSIM vs. Explicit PIC



GL-ECSIM
$\Delta x = 1/16\ \mathrm{d_i} \approx 0.06\ \mathrm{d_i}$

Electron current density



Explicit PIC (p3d).
$\Delta x \approx 0.02\ \mathrm{d_i}$

(Price et al., 2016, GRL)

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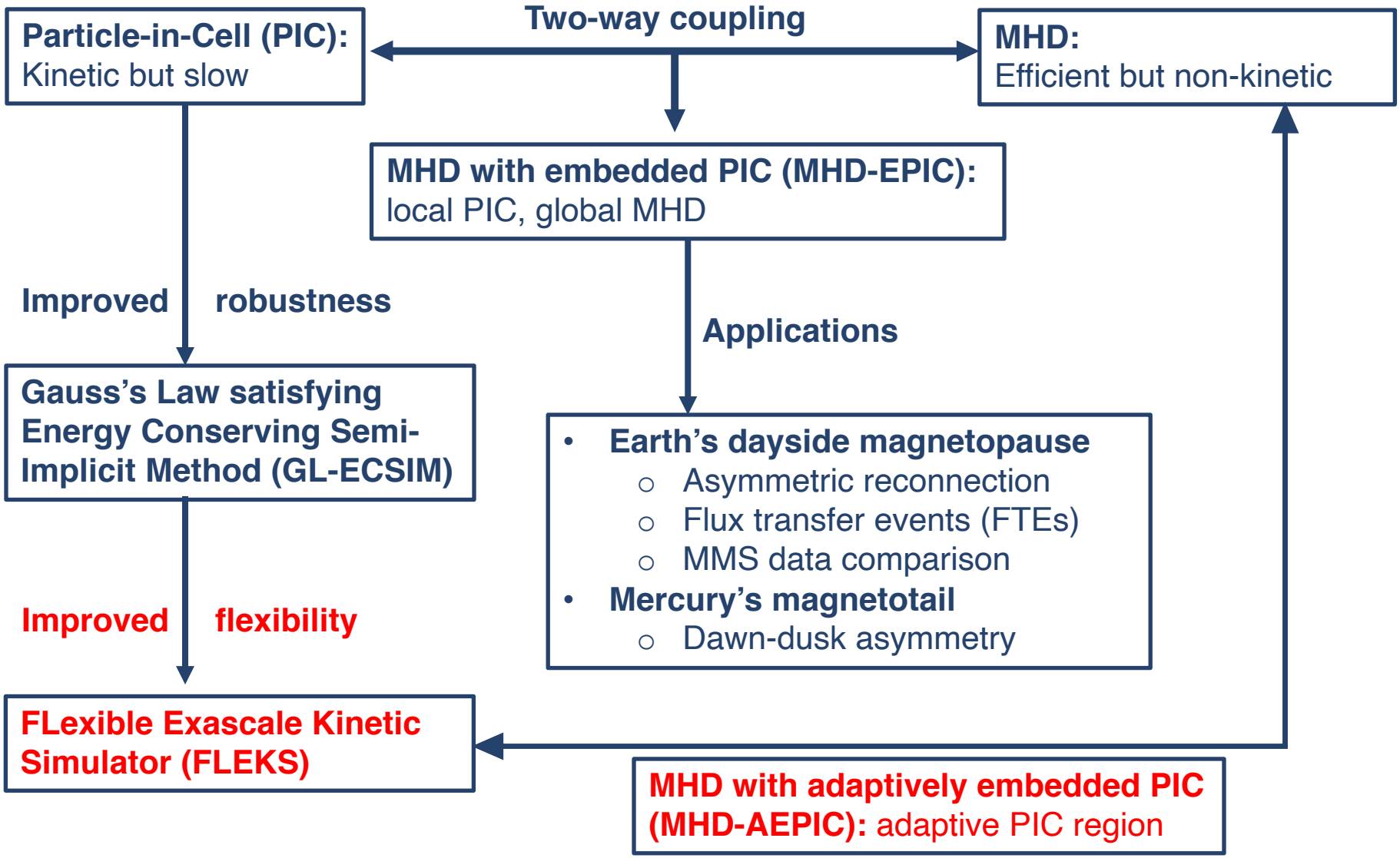
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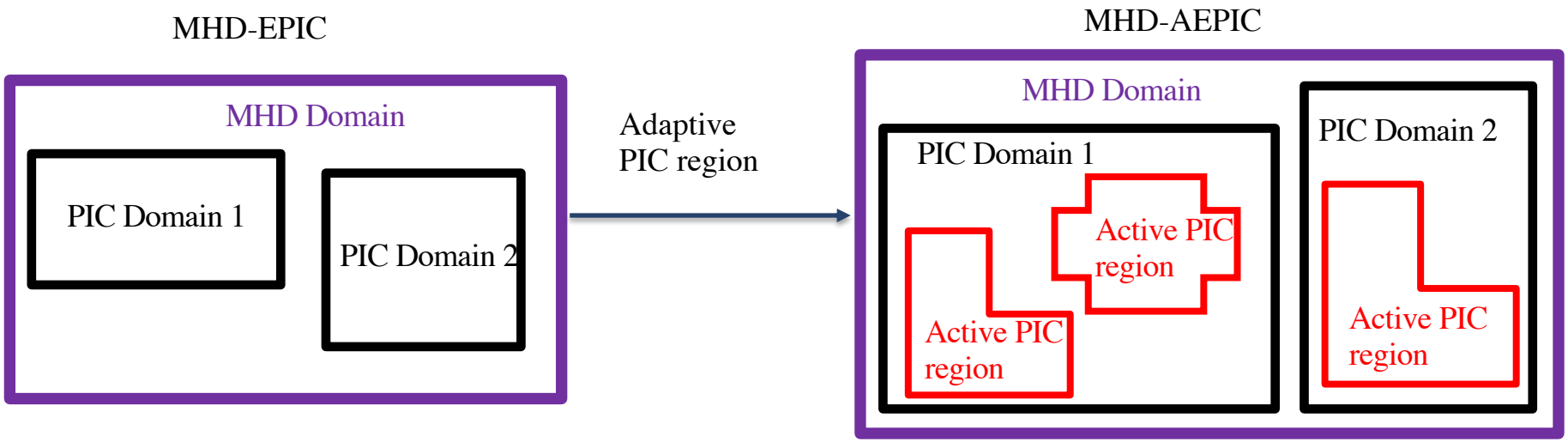
From MHD-EPIC to MHD-AEPIC



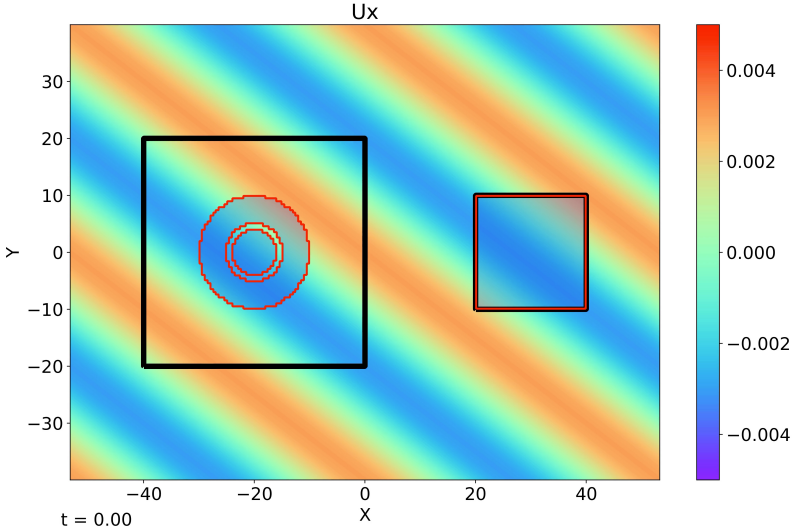
MHD with embedded particle-in-cell (MHD-EPIC)
- Coupled with iPIC3D
- PIC domains are fixed boxes

MHD with adaptively embedded particle-in-cell (MHD-AEPIC)
- Arbitrarily shaped PIC region
- Allows dynamic adaptation

FLexible Exascale Kinetic Simulator (FLEKS)

FLexible Exascale Kinetic Simulator (FLEKS)

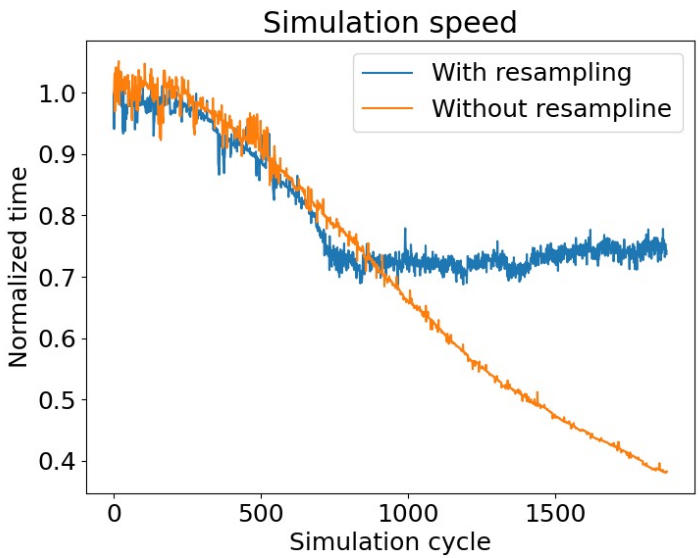
- **FLEKS is a brand new semi-implicit PIC code**
- **PIC algorithm**
  - Gauss's law satisfying energy-conserving semi-implicit particle-in-cell method (GL-ECSIM)
  - Particle resampling: splitting and merging
- **PIC grid**
  - Multiple independent PIC domains
  - Cartesian grid
  - Adaptation: PIC cells can be switched on/off
- **Implementation**
  - A third-party library AMReX provides high-performance parallel data structure
  - Parallelized with MPI. No OpenMP/GPU so far



- PIC domains: black squares
- Active PIC regions: shadowed areas, enclosed by red lines

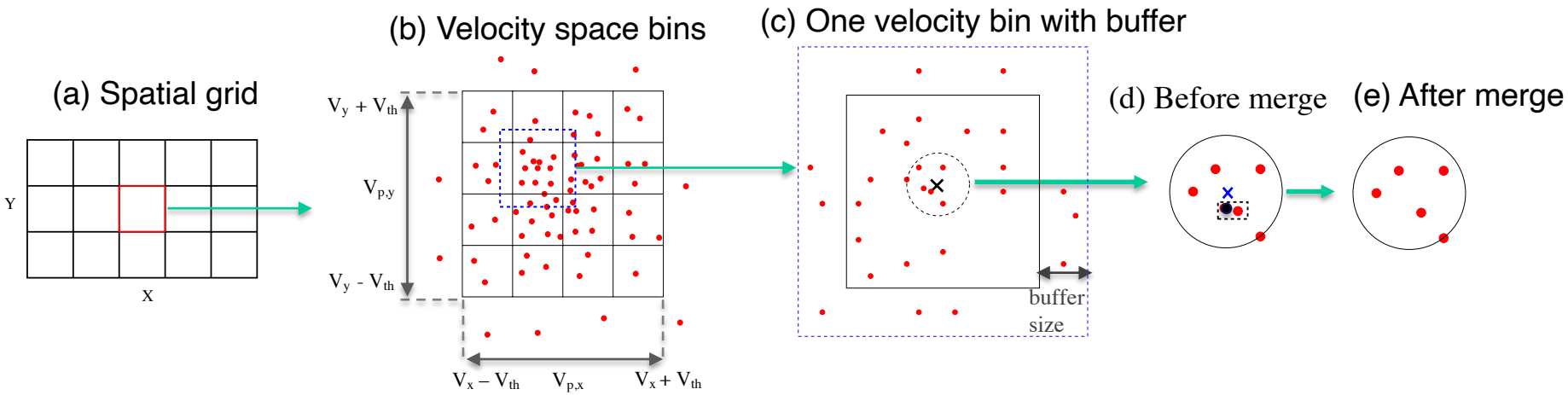
Particle Resampling: Splitting and Merging

- **Problem**
  - Concentration of mass (macro-particles)
    -> load imbalance
    -> slows down the simulation
  - Decreasing mass density (macro-particles)
    -> zero macro-particles in some cells
    -> reduces the simulation accuracy



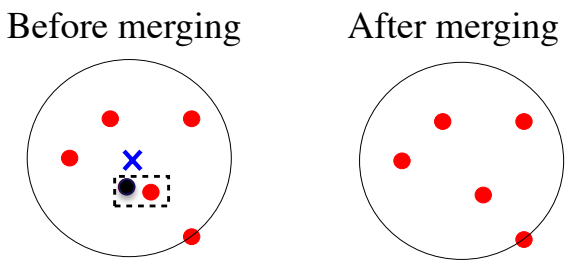
- **Solution**
  - Number of macro-particles per cell < N_{low} : split 1 particle into 2
  - Number of macro-particles per cell > N_{high} : merge 6 particles into 5
    - Find 6 particles that are close to each other in the 6D phase space.
    - Merge 6 particles into 5. Conserve mass, momentum and energy.

Particle Merging (1)



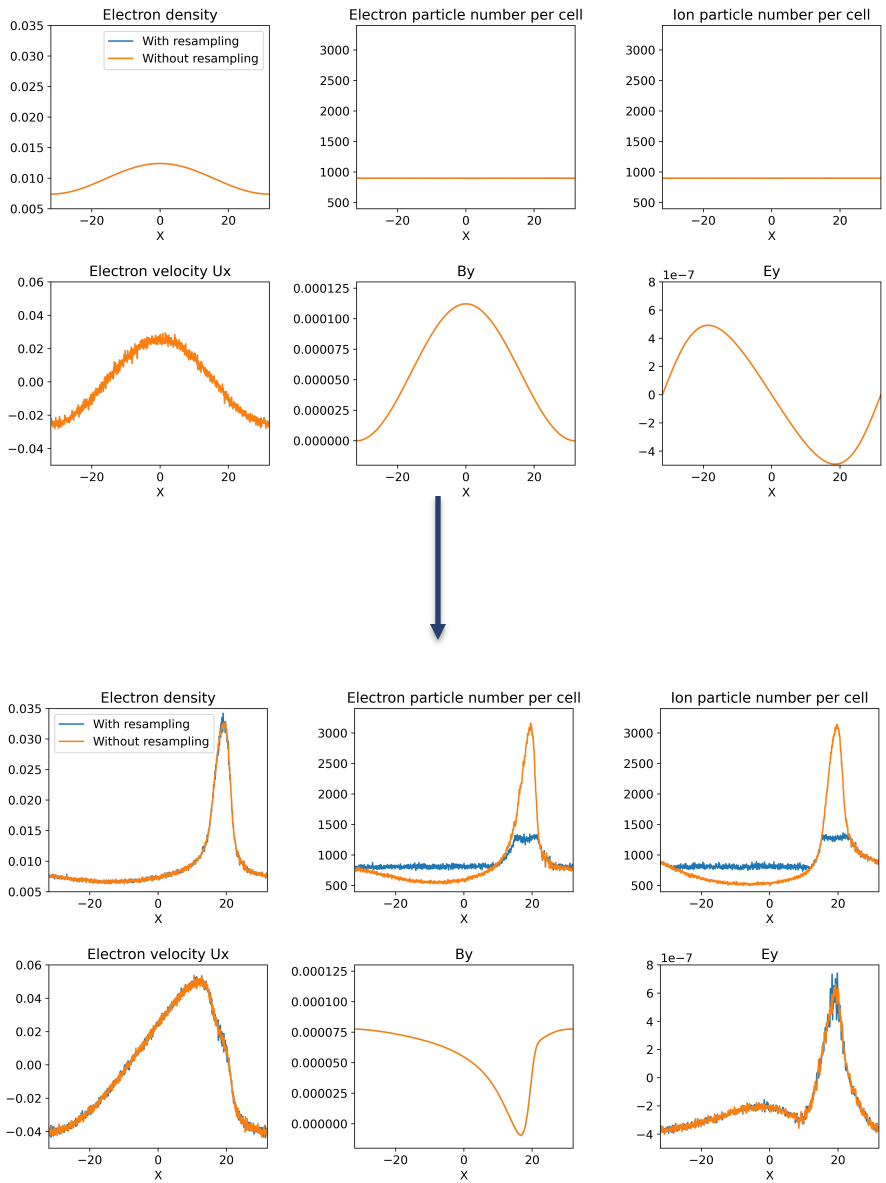
- **Step 1**: For each spatial cell (a) create a grid in the velocity space ranging from $V-V_{th}$ to $V+V_{th}$ and assign particles to velocity bins (b).
- **Step 2**: For each velocity bin, calculate the center of all the particles (black cross in panel c), and find the 6 particles closest to the center.
- **Step 3**: Find the 6D center (blue cross in panel d) of these 6 particles, the 6D distance of a particle to the center should NOT exceed a threshold value.
- **Step 4**: Merge 6 particles into 5

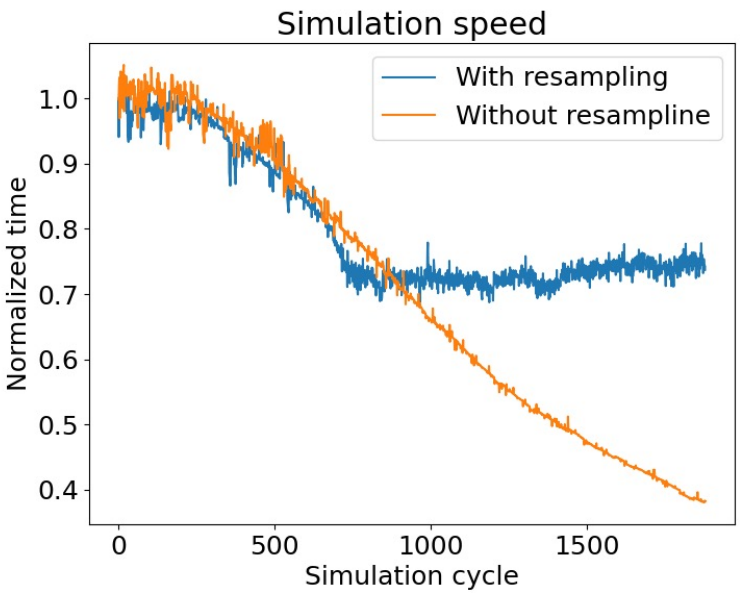
Particle Merging (2)



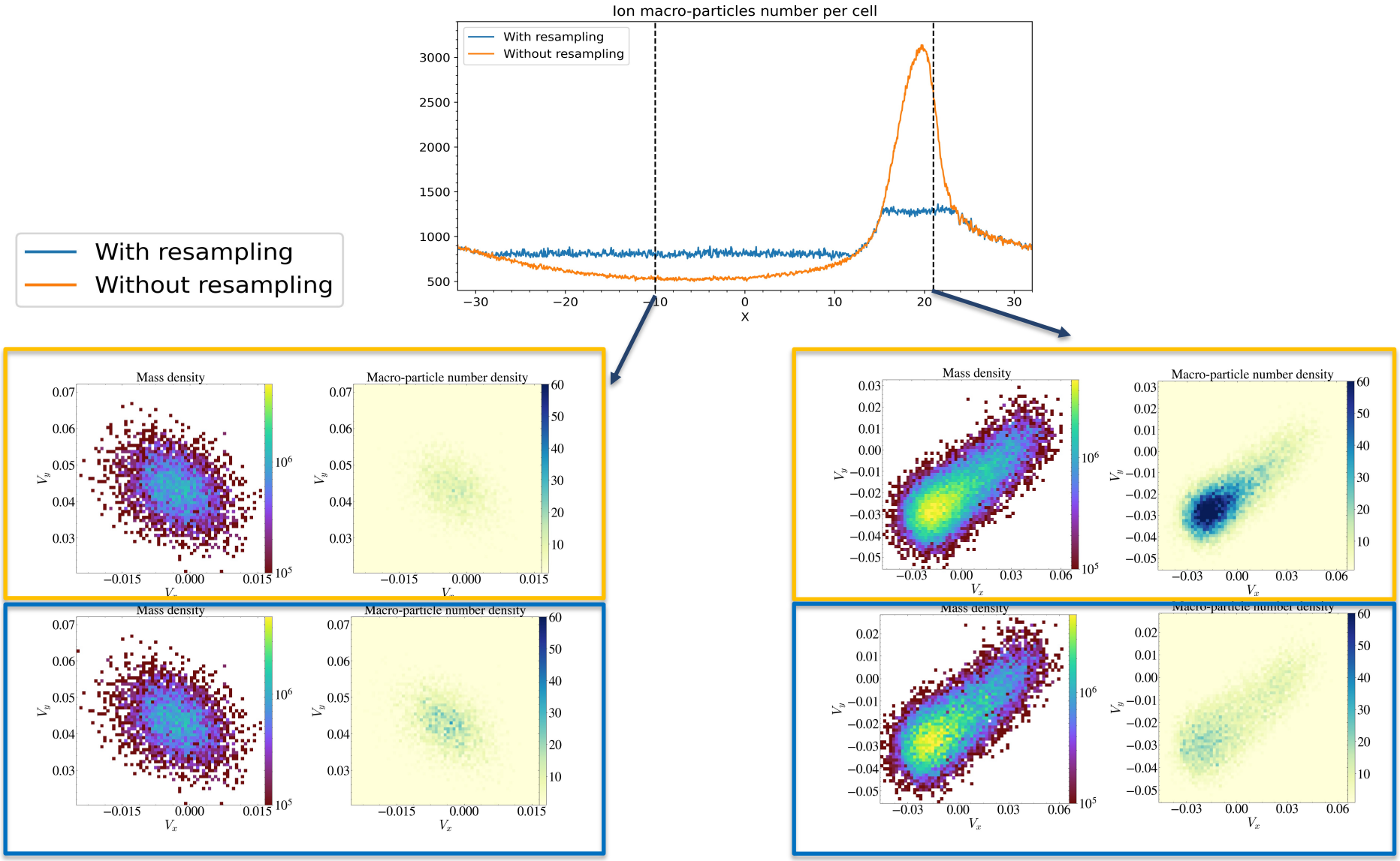
- From these 6 particles, find a pair that is closest to each other. Remove the lighter one and re-distribute its mass to the other 5 particles by changing their weights. These 5 particles keep their original positions and velocities. The total mass, momentum, and energy are conserved after merging by properly adjusting the weights:
  - 5 conserved quantities, needs 5 new particles.
  - A physical meaningful solution may not always exist.
  - This algorithm allows merging N particles into 5, where N >=6
- Why not change velocities and merge into fewer particles?
  The distribution function could change drastically.

Particle Resampling Test: 1D Magnetosonic Wave

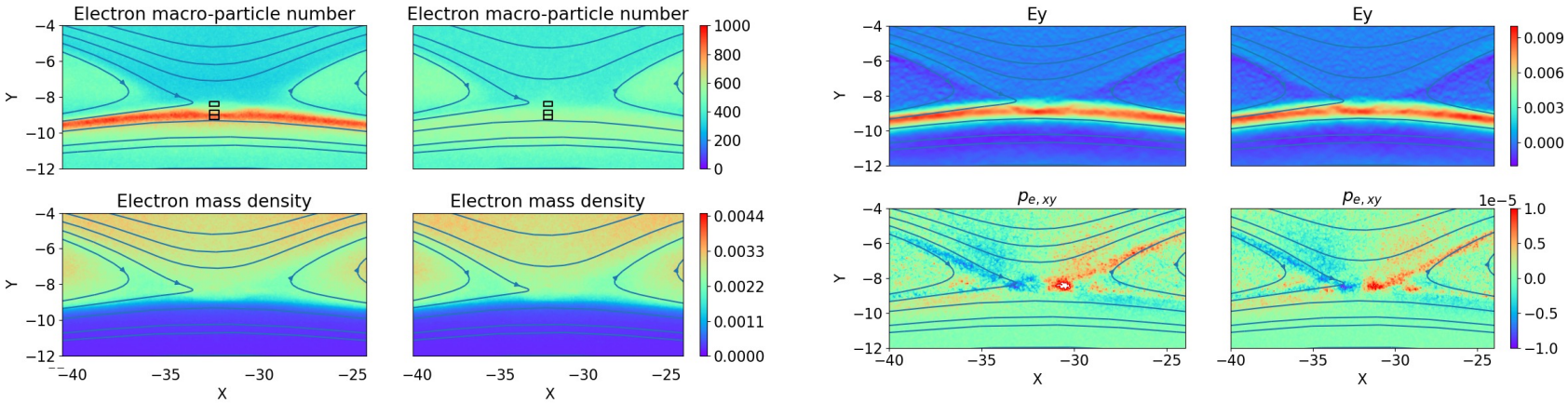




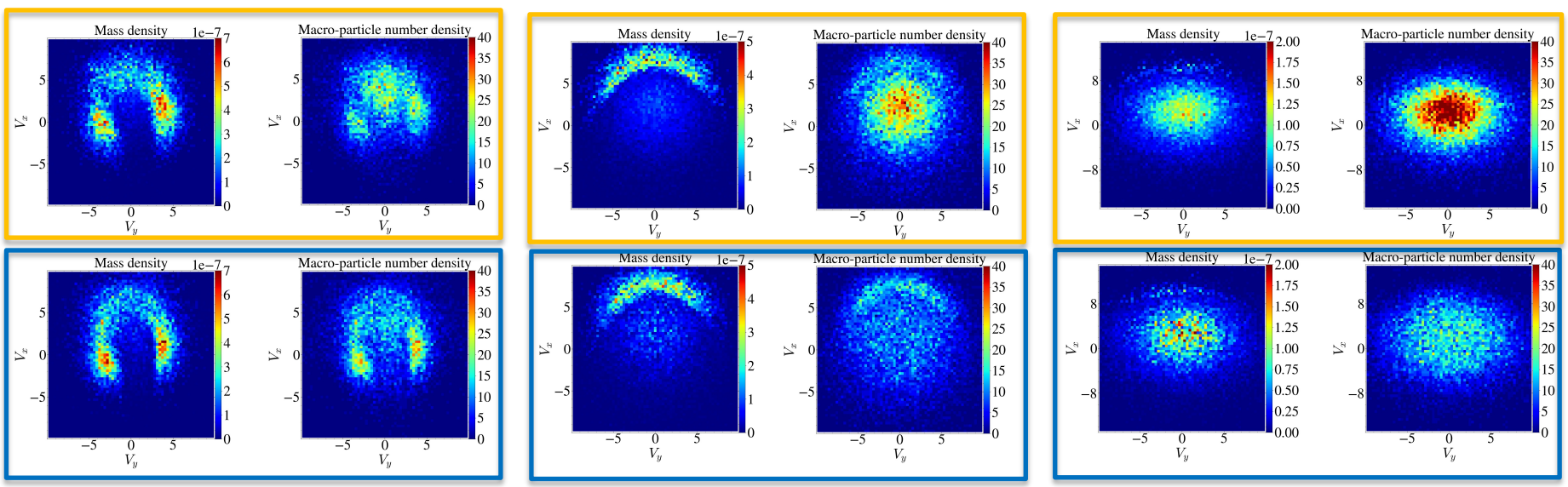
Magnetosonic Wave Test Particle Distributions



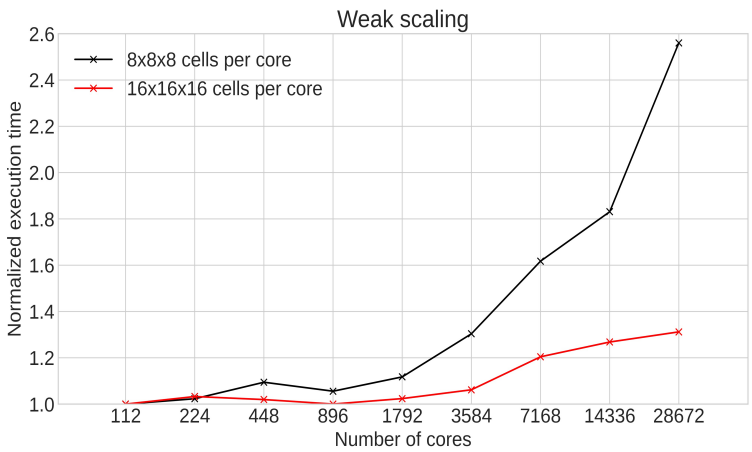
Particle Resampling Test: 2D Asymmetric Magnetic Reconnection



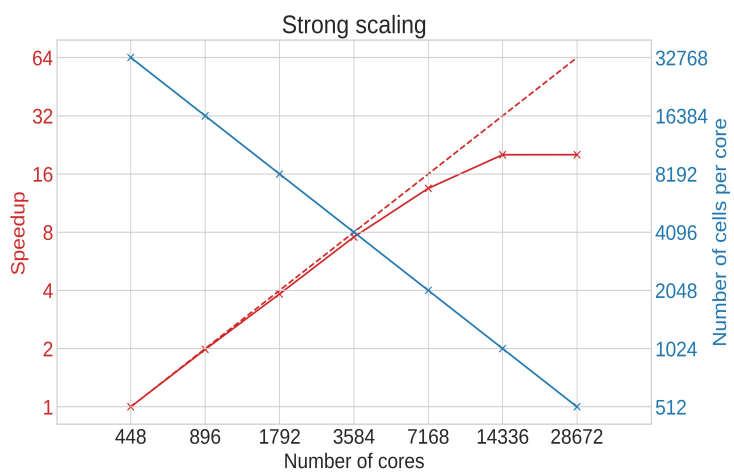
With resampling
Without resampling

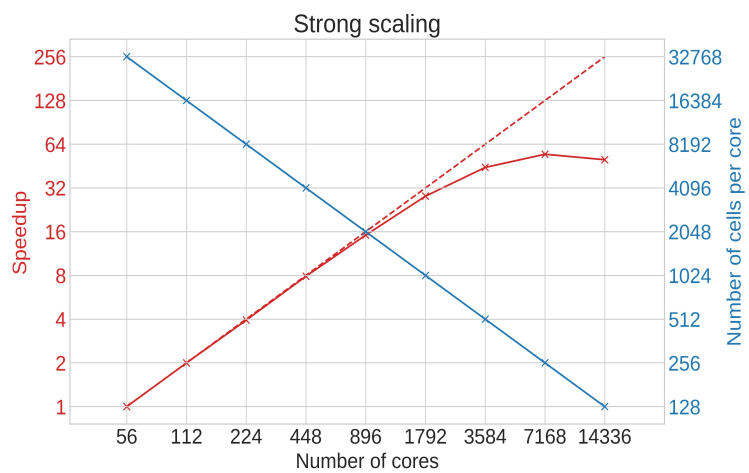


Performance of FLEKS

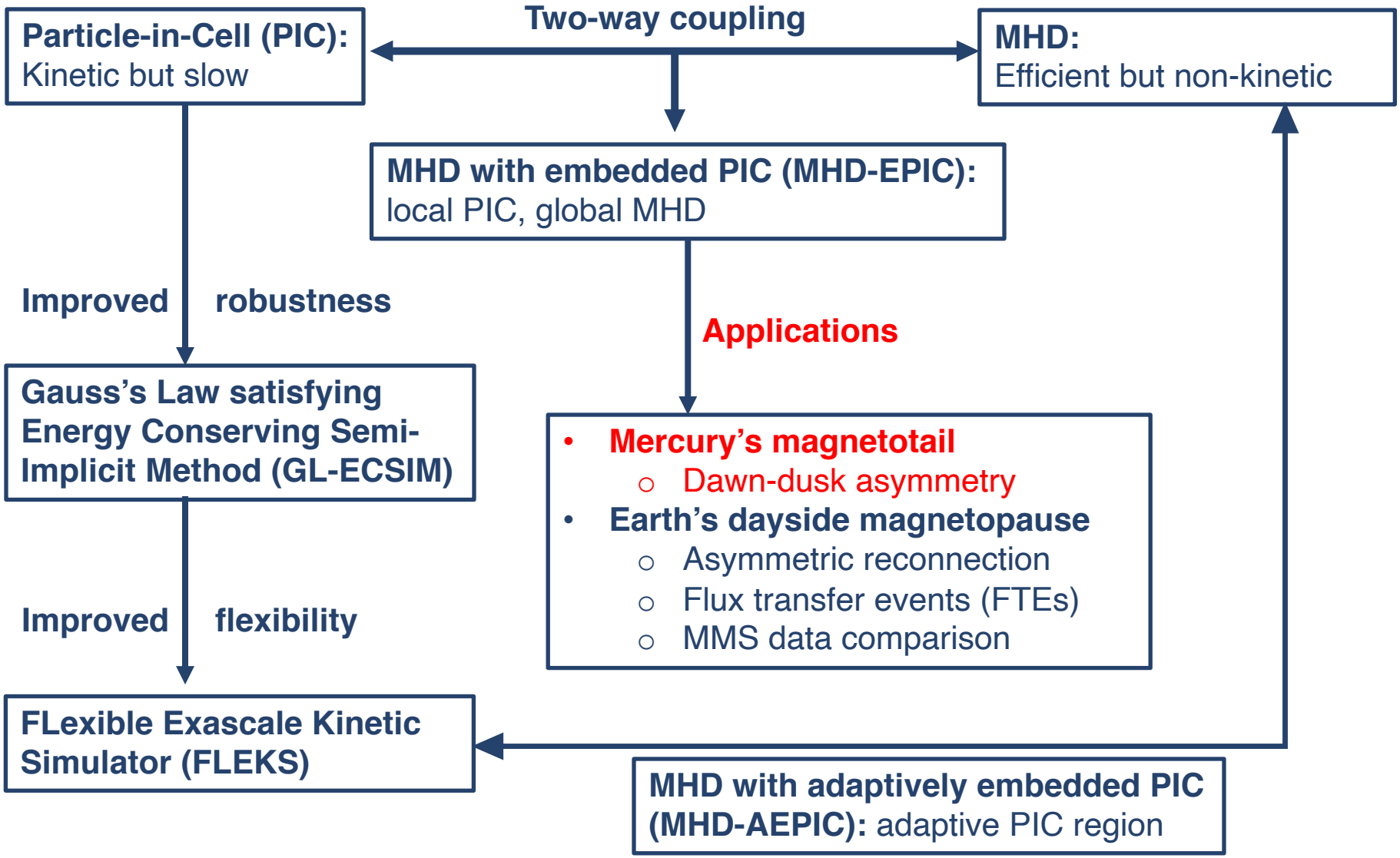


- Run on Frontera, which ranks 8th on Top 500. 23.5 PetaFLOPS peak performance
- In general, FLEKS can efficiently use ~30k cores, which is about 7% of the whole machine
- Exascale? OpenMP or/and GPU are needed





Outline


Particle-in-Cell (PIC): Kinetic but slow
Two-way coupling
MHD: Efficient but non-kinetic
MHD with embedded PIC (MHD-EPIC): local PIC, global MHD
Improved robustness
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Gauss's Law satisfying Energy Conserving Semi-Implicit Method (GL-ECSIM)
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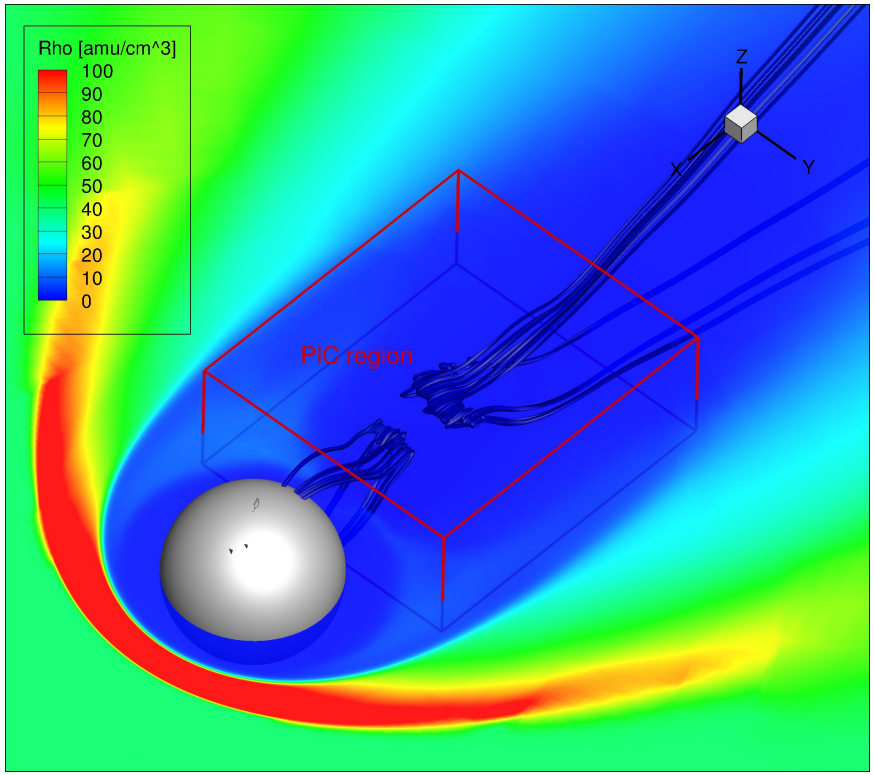
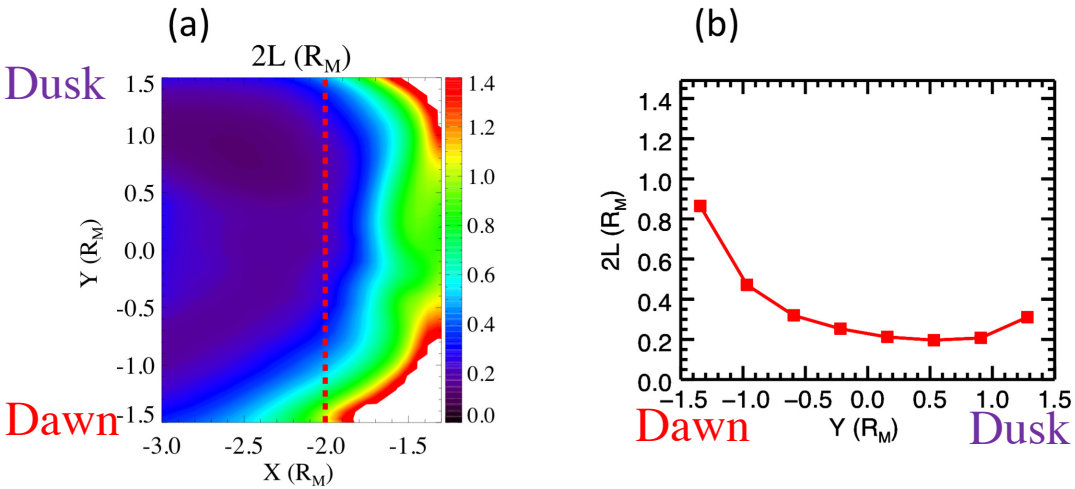
MHD-EPIC Simulation of Mercury's Magnetotail

- **Why Mercury?**
  - Mercury's magnetosphere is smaller than that of Earth
  - Magnetotail ion scale can be resolved without scaling
  - The kinetic effects may have global effects: dawn-dusk asymmetries
- **Simulation**
  (Chen et al., 2019, JGR)
  - PIC covers magnetotail
  - $dx = 1/32\ R_m \sim 1/5\ d_i$
  - 300 s long ~ 2 Dungey cycles
  - $B_y = 0$ and $u_y = 0$ in the solar wind
  - IMF condition:
    B = [-17.4, 0, -8.5] nT



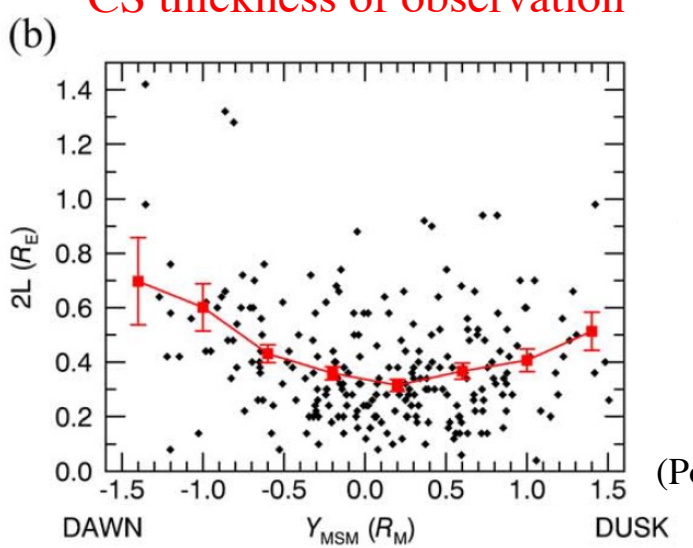
Current-Sheet (CS) Thickness

CS thickness of MHD-EPIC simulations



- **Cross-tail current-sheet is thicker on the dawnside (-Y) than the duskside (+Y)**

CS thickness of observation



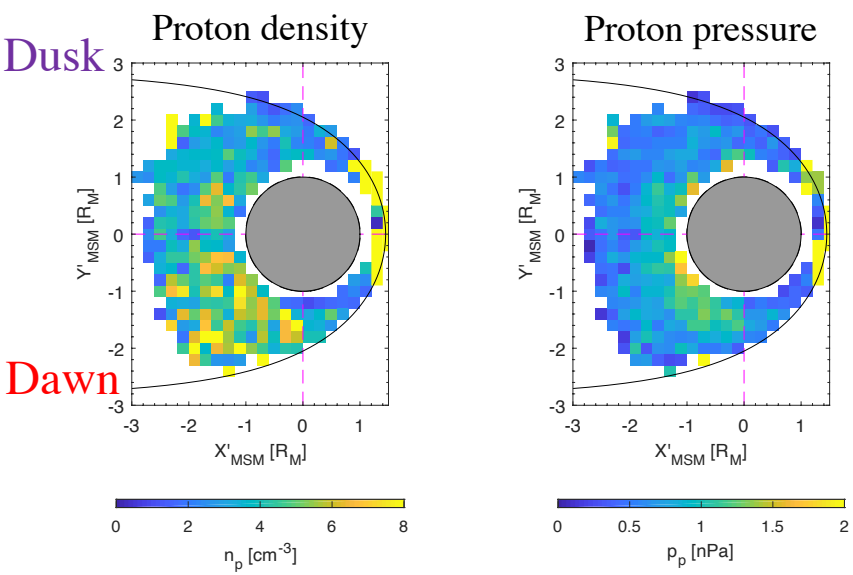
(Poh, 2017)

- **Potential explanation: Hall effect transport magnetic flux and plasma from duskside to dawnside (Lu, 2016)**

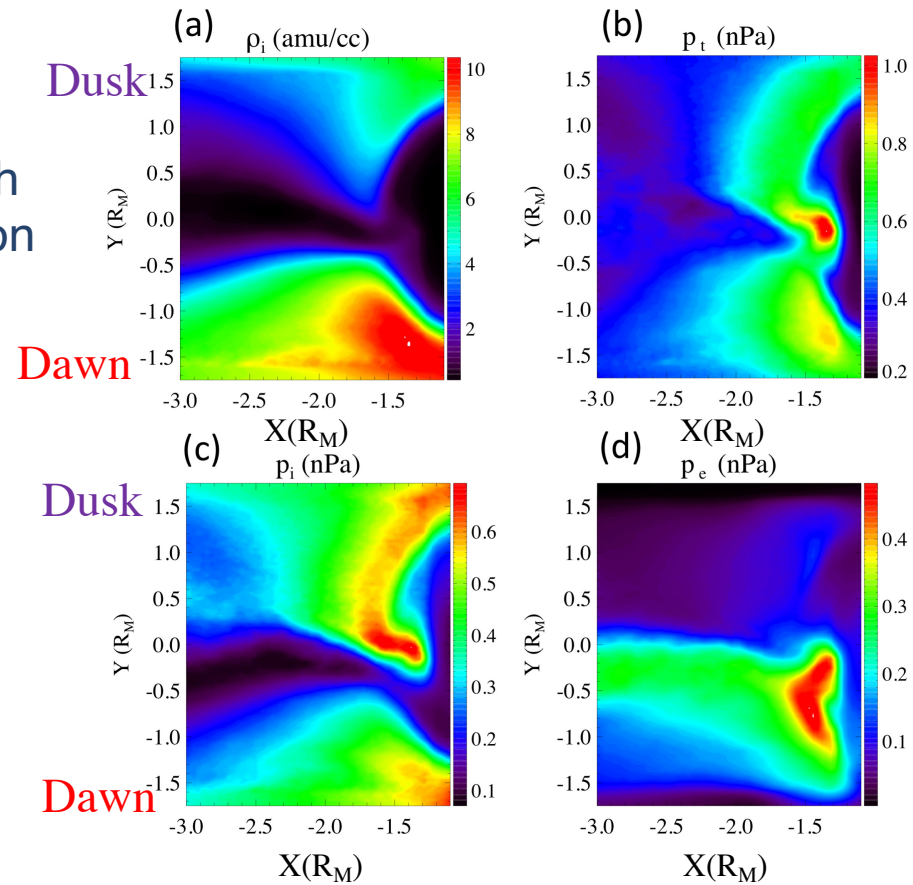
Plasma Inside Current-Sheet

- **Inside the current-sheet:**
  - Dawnside density is about twice of the duskside density
  - Simulation ion pressure does not show significant dawn-dusk asymmetry
  - Dawnside electron pressure is much higher than the duskside (no electron pressure observation)

MESSENGER observation

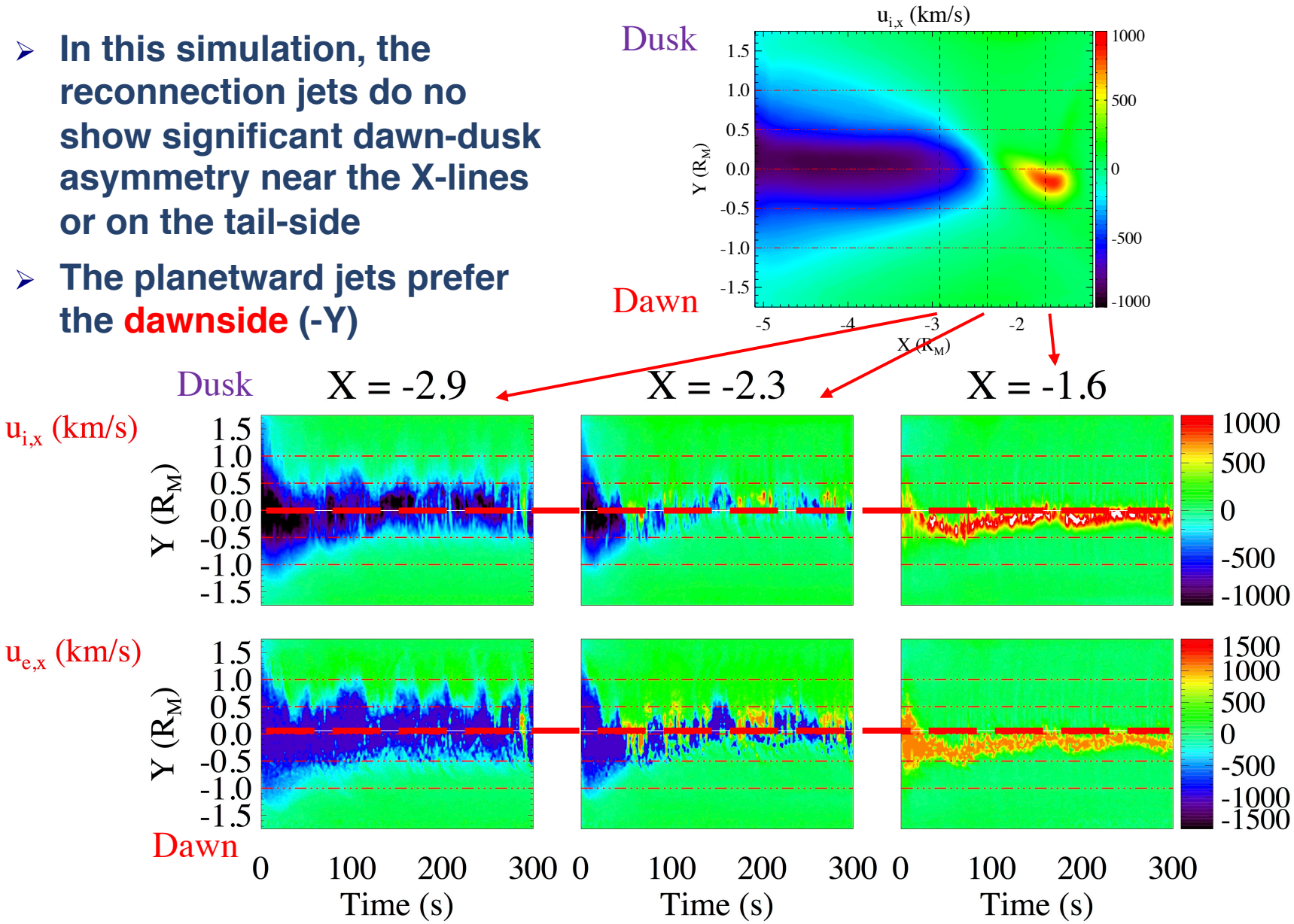


MHD-EPIC simulation

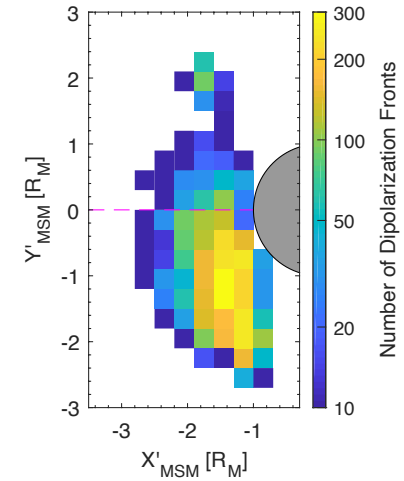


Dawn-dusk Asymmetry of Reconnection Jets

- In this simulation, the reconnection jets do no show significant dawn-dusk asymmetry near the X-lines or on the tail-side
- The planetward jets prefer the **dawnside** (-Y)

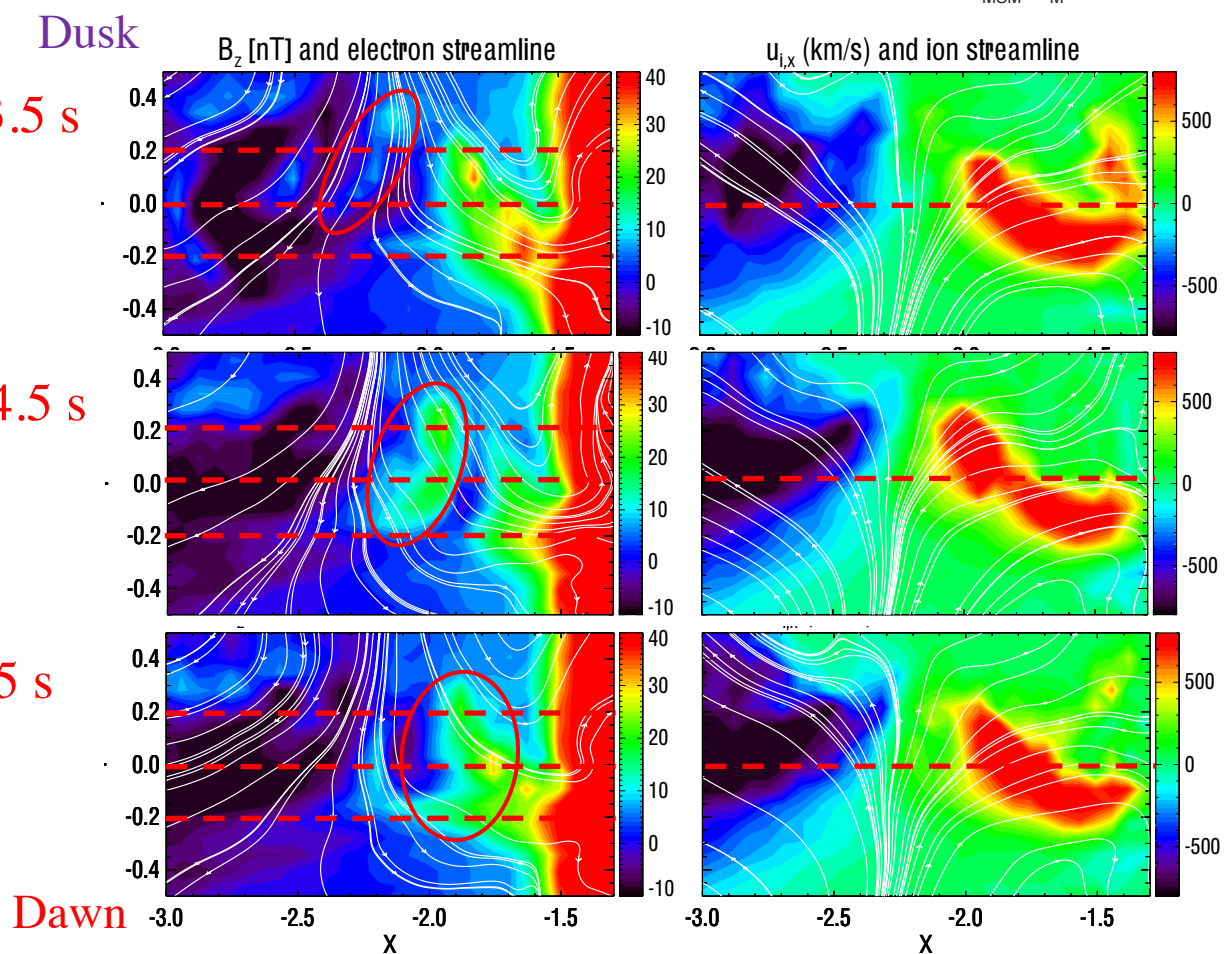


Dawnward Motion of Dipolarization Event

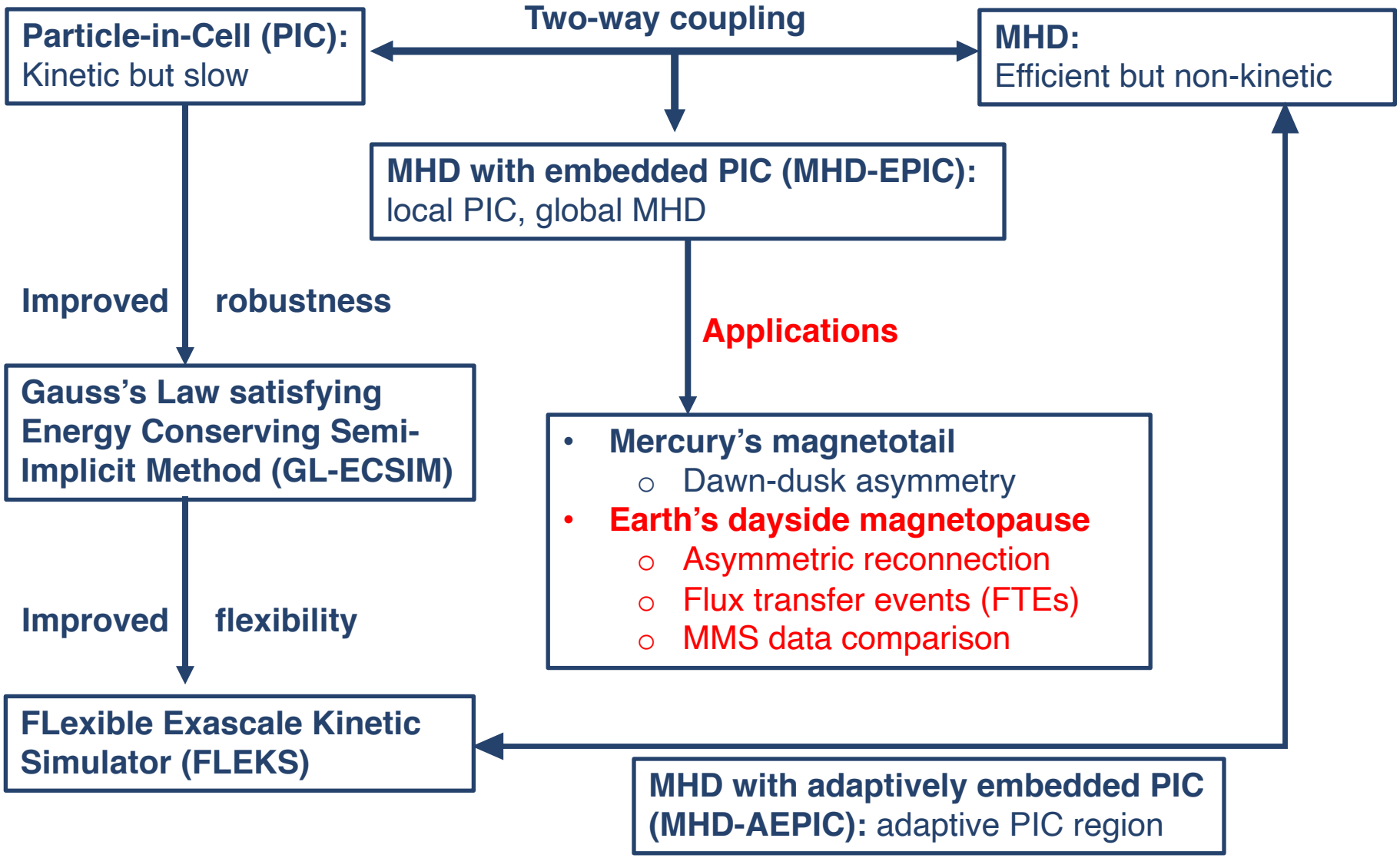


- Inside CS, electrons move **dawnward** (-Y)
- DF is also moving **dawnward** (-Y)

- Inside the current-sheet, ions move **duskward**, but fast ion flows still prefer **dawnside**. Maybe because fast ion flows are accelerated by dipolarization events



Outline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Introduction: Incorporate Kinetic Physics into Global Simulations

- **Hybrid models**
  - Fluid massless electrons + kinetic (PIC or Vlasov solver) ions
  - Local kinetic + global fluid -> MHD-EPIC
- **Extend MHD**
  - Five-moment (isotropic pressure), six-moment (anisotropic pressures), and ten-moment (pressure tensors)

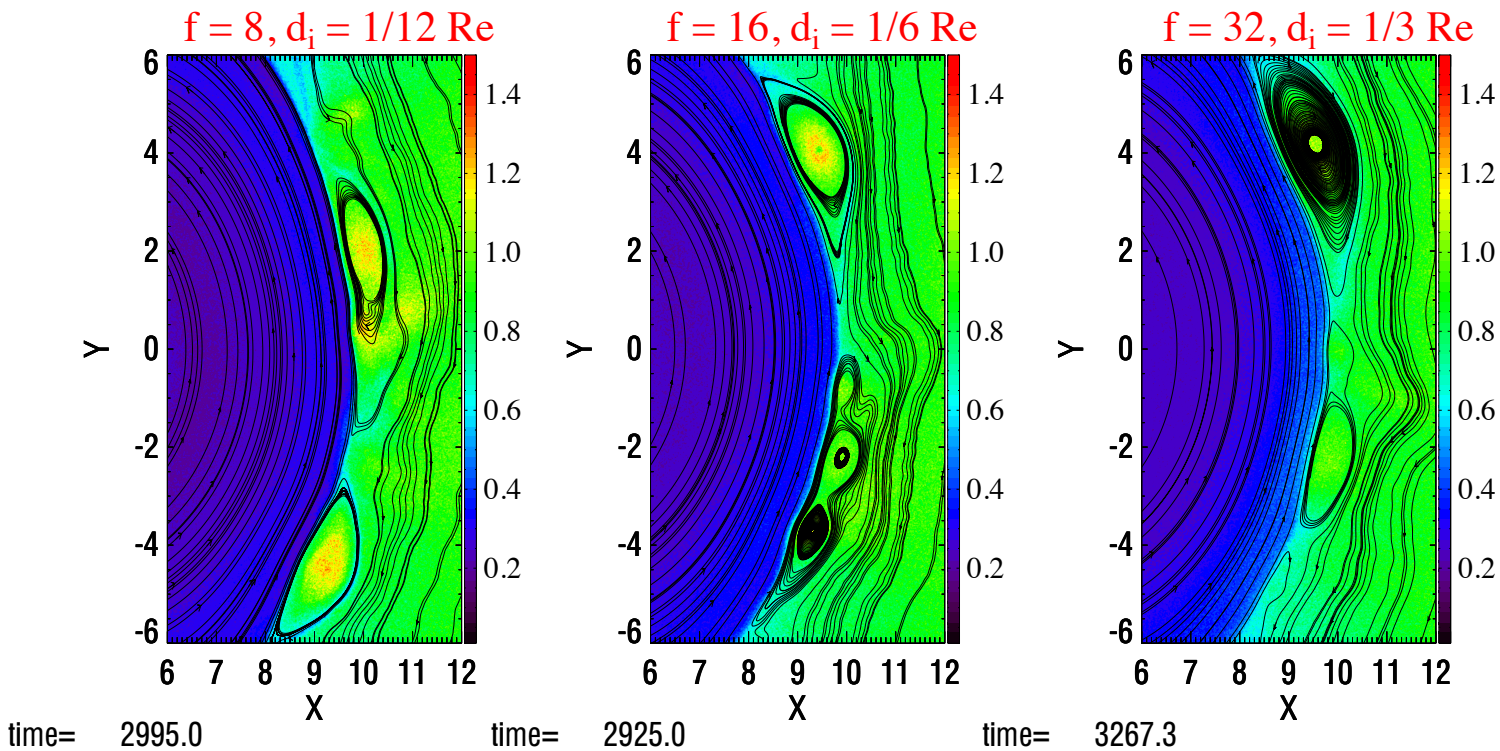
Earth's magnetosphere:
$\lambda_D \sim 100$ m; $d_e \sim 5$ km; $d_i \sim 100$ km;
Magnetosphere size $\sim 10 R_E \sim 10^5$ km

- **Reduce the separation between scales**
  - Reduce speed of light: reduce separation between λ_D and d_e
  - Reduce the m_i/m_e ratio: reduce separation between d_e and d_i
  - Reduce q_i/M_i to increase d_i

$$d_i = c\sqrt{\frac{M_i}{4\pi n q_i}}$$

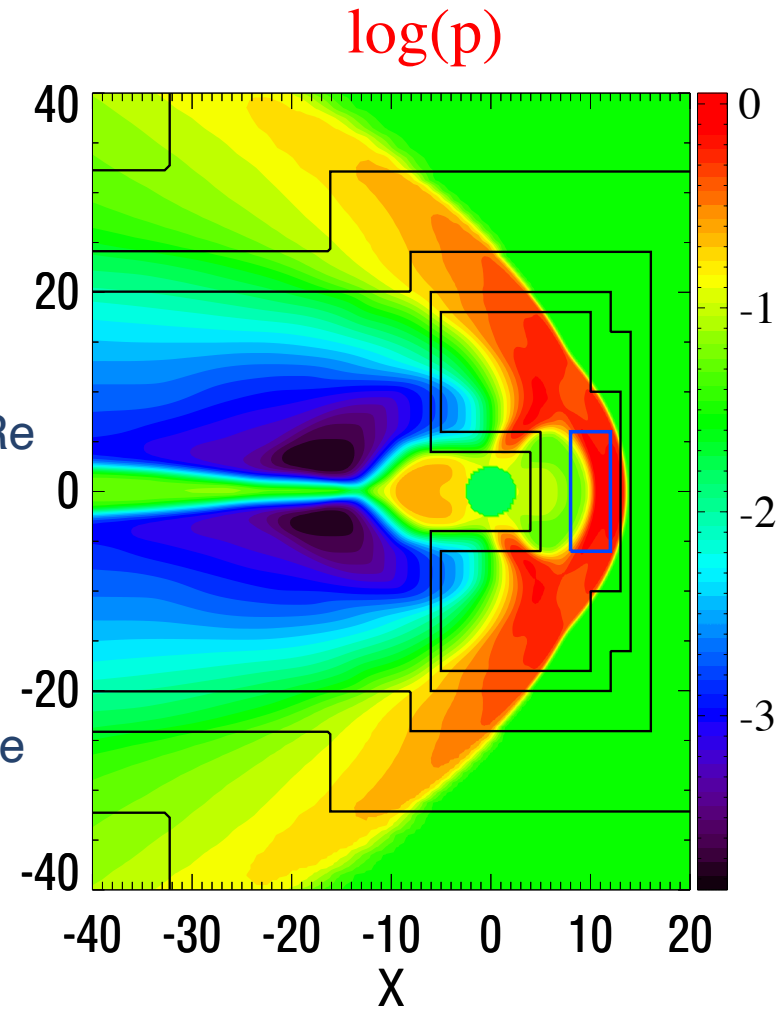
Changing the Kinetic Scales

- Reduce q_i/M_i by a scaling factor f to increase d_i, while the number density, pressure, thermal velocity do not change. (Toth et al., 2017, JGR)



3D MHD-EPIC Simulation Set Up

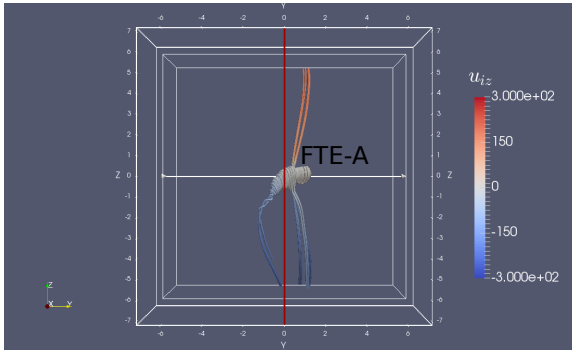
- **Physical parameters**
  - Use f =16 so d_i ~ 1/6 Re: doable
  - Typical solar wind conditions:
    ρ= 5 amu/cm^3, U_X = -400km/s, B = [0,0,-5] nT
- **Hall MHD with separate electron pressure equation**
  - MHD domain: -224 < x < 32, -128 < y, z < 128Re
  - At the magnetopause Δx=1/16Re (~400km)
  - MHD uses ~20% CPU time
- **PIC**
  - PIC domain: 8 < x < 12, -6 < y < 6, -6 < z < 6Re
  - Δx = 1/32Re: 5 cells per d_i (for f = 16)
  - 216 particles per cell per species: 8B total
  - Consuming ~80% simulation time
- **~18000 core hours modeling 1min**



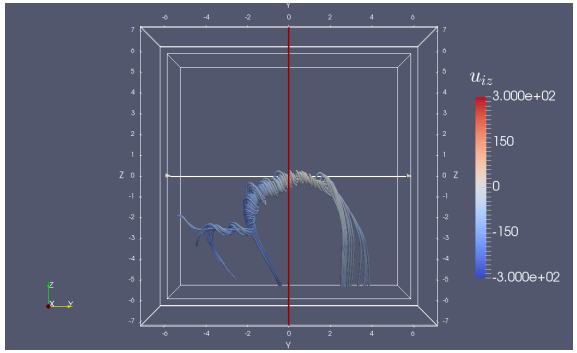
Evolution of FTEs

- **FTEs colored u_{iz}**
  - IMF is purely southward
  - FTEs grow in the dawn-dusk direction
  - u_{iz} varies along the FTE, and the FTE becomes tilted
  - Two FTEs can merge into one

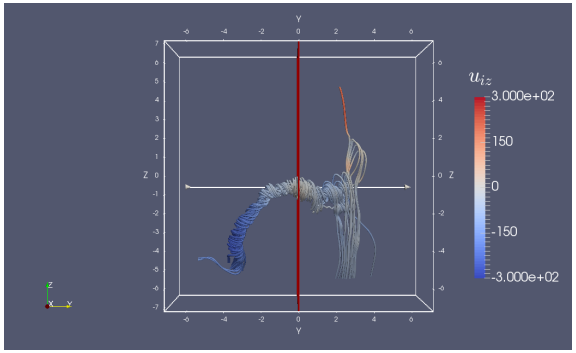
t=100s



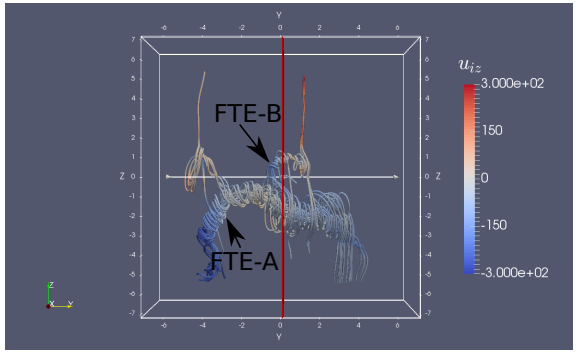
t=150s



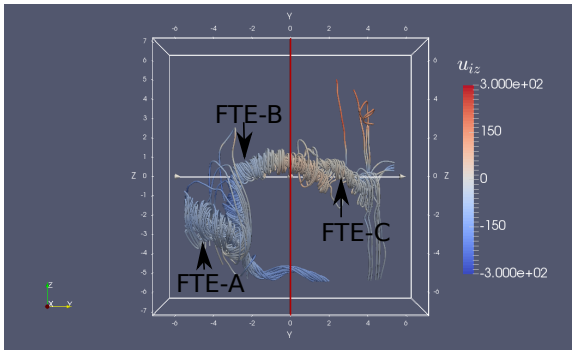
t=240s



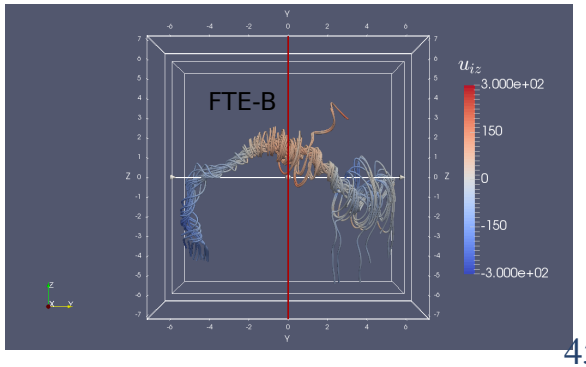
t=320s



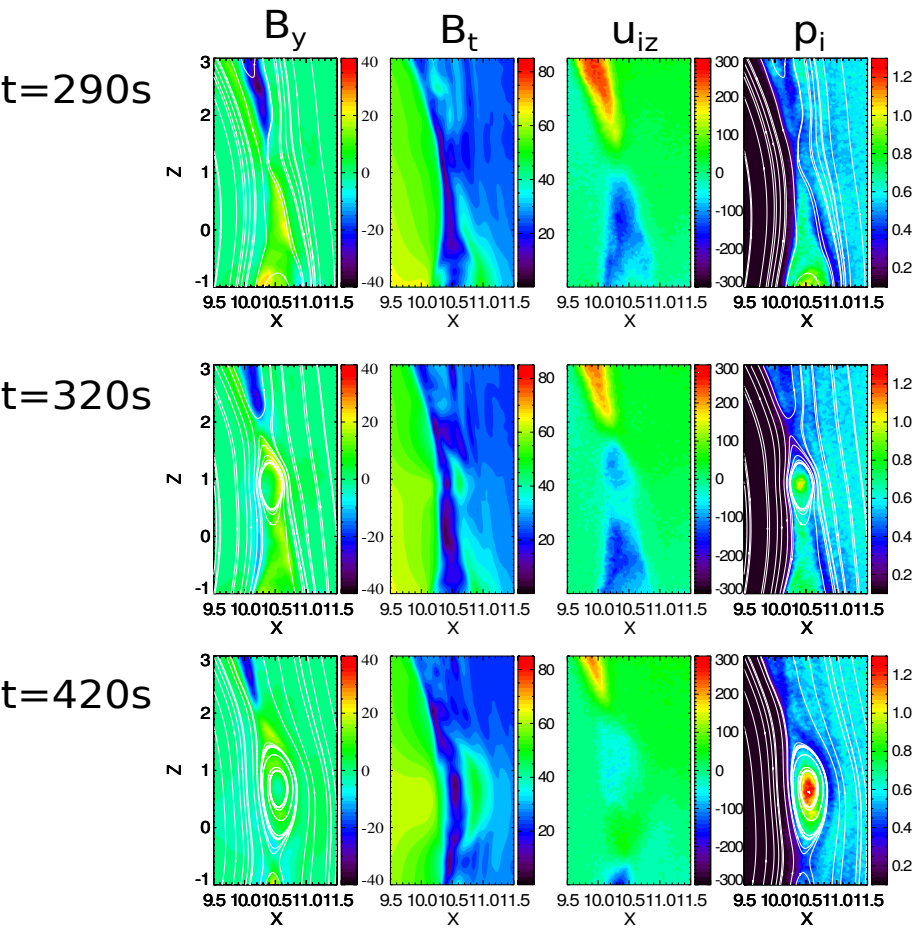
t=540s

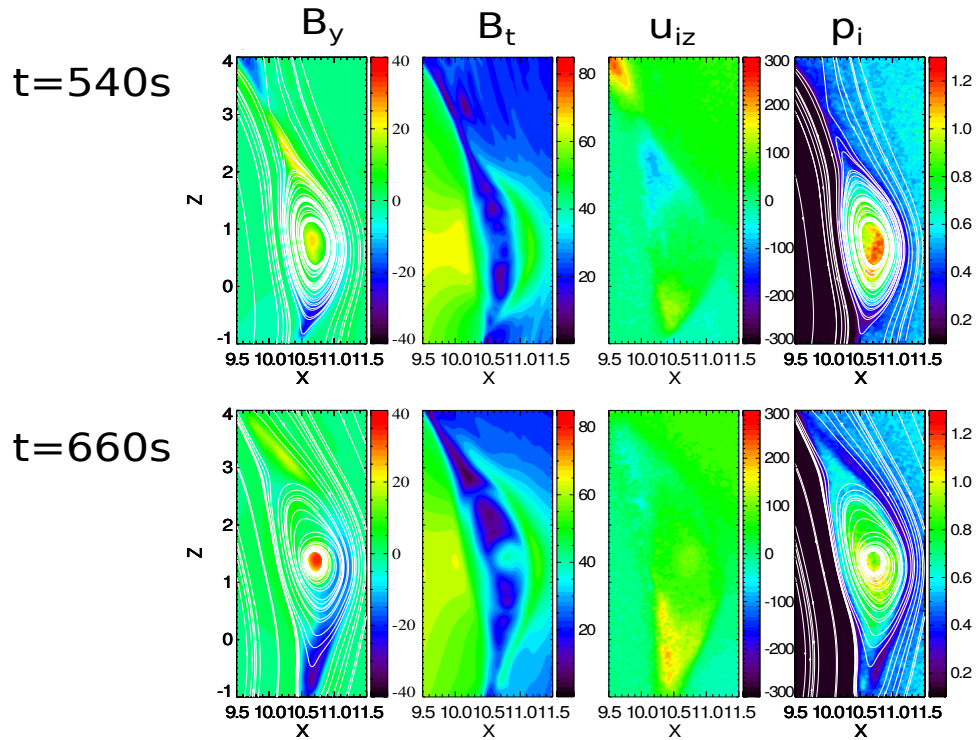


t=660s



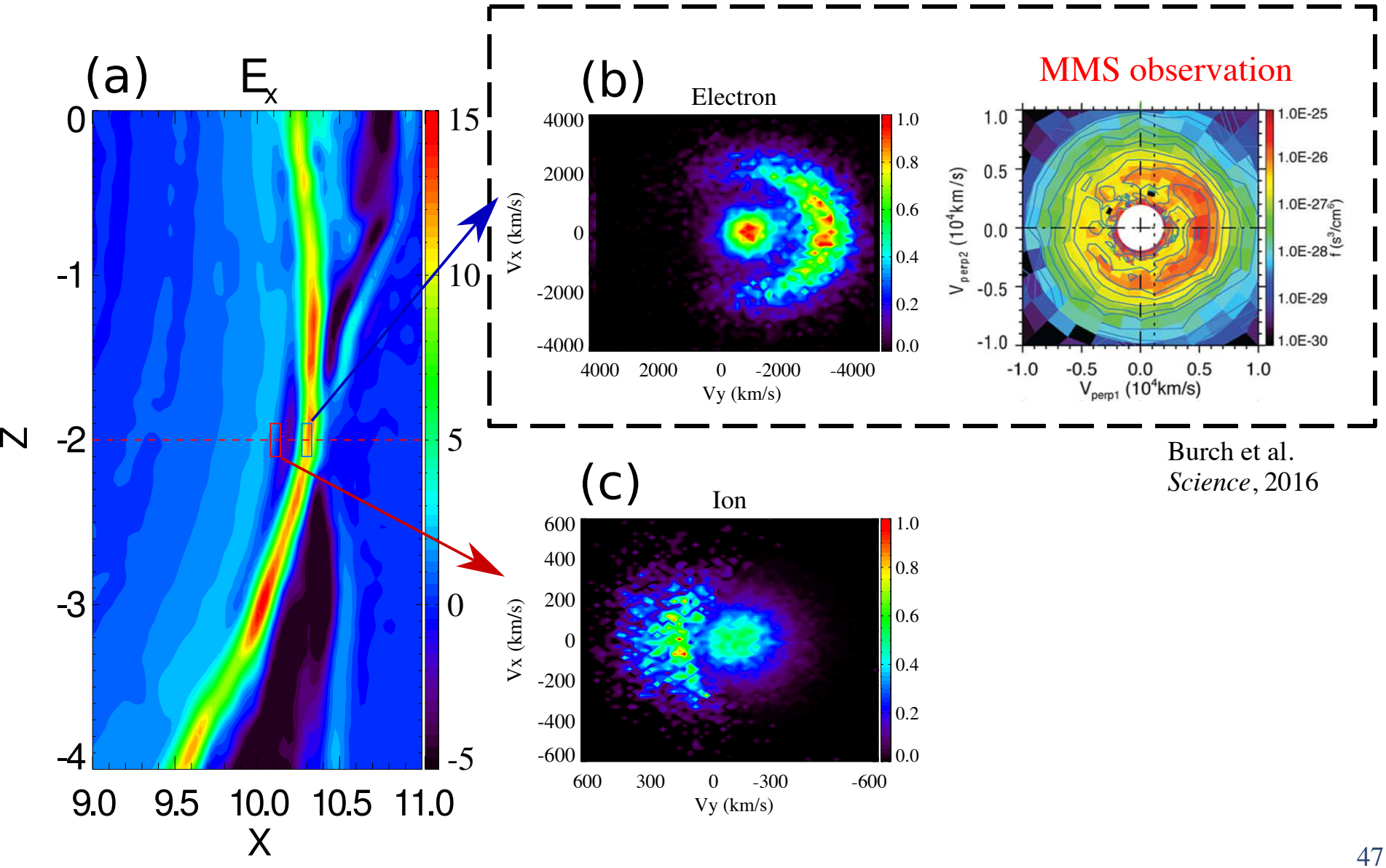
Evolution of FTEs (2)





- The FTE is surrounded by two X lines
- The core field gradually increases to a significant value

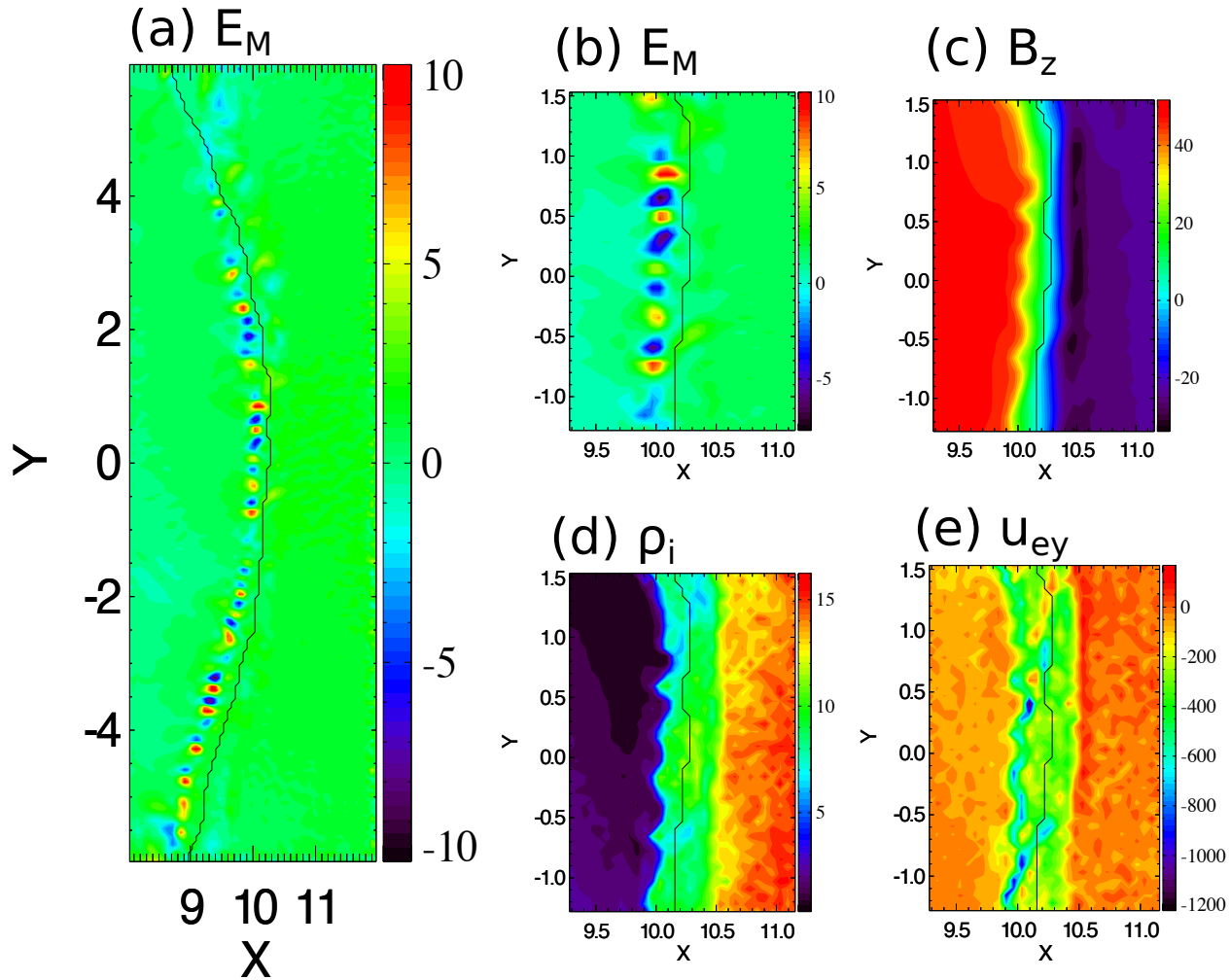
Crescent Distributions



Burch et al.
Science, 2016

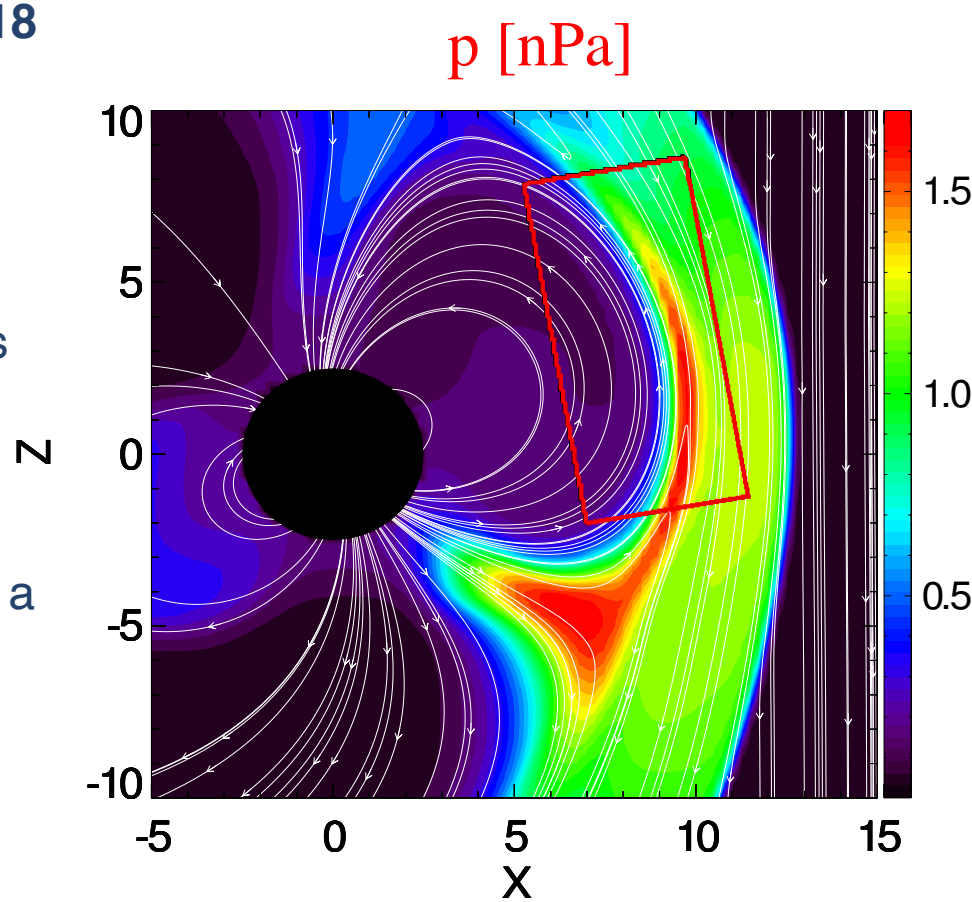
Low Hybrid Drift Instability (LHDI)

- **Simulation agrees with MMS observation**
  - $E_M \sim 8$ mV/m
  - $kr_e \sim 0.4$, $\lambda \sim 16\ r_e$



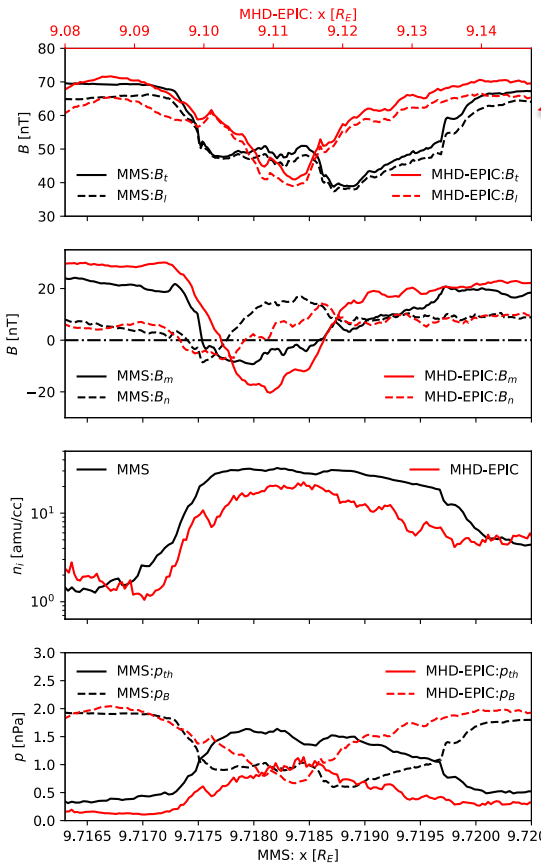
GEM Dayside Kinetic Challenge Event

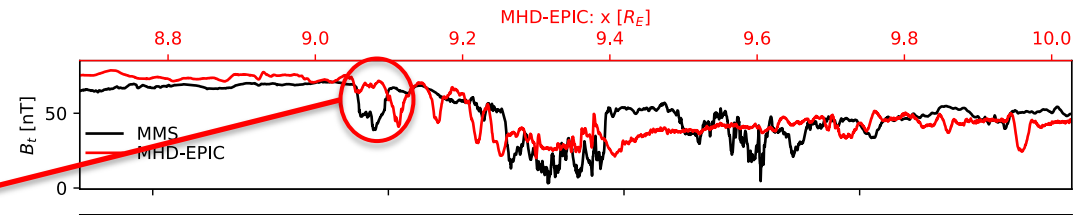
- **The southward IMF event on 2015-11-18 01:50-03:00 UT**
  - Solar wind conditions: ρ= 9.5 amu/cm^3, U_X = -360km/s, $T_i = T_e$ = 9eV, B = [0,0,-6] nT
  - The dipole is 27° tilted from the Z-axis towards the midnight: rotated PIC region
- **Numerical parameters**
  - Artificially increase ion kinetic scale by a factor of 16, so $d_i \sim 1/6\ R_E$ in magnetosheath
  - $m_i/m_e = 100$
  - $\Delta x = 1/25\ R_E$: 4 cells per d_i

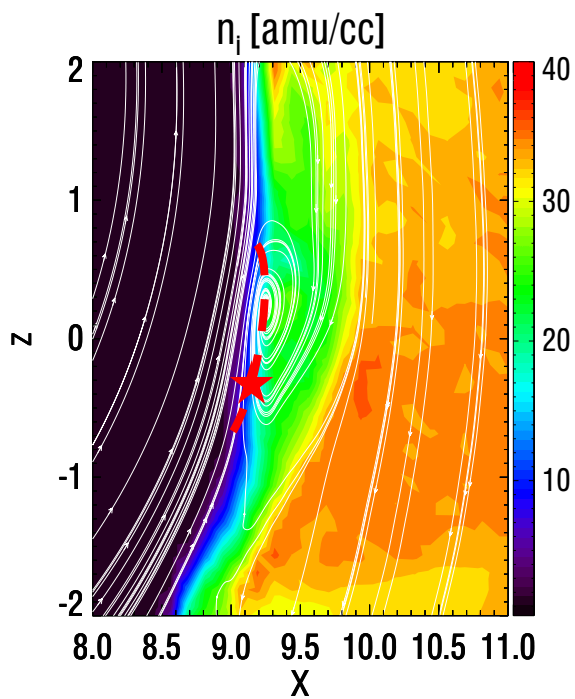


Chen et al., 2020, ESS

MHD-EPIC vs. MMS: FTE-Like Structure



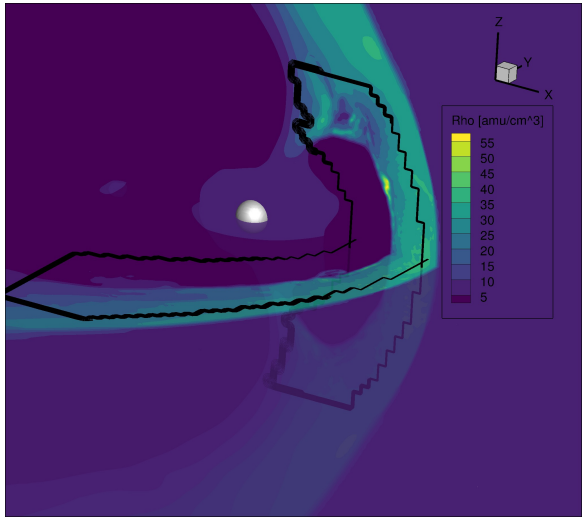




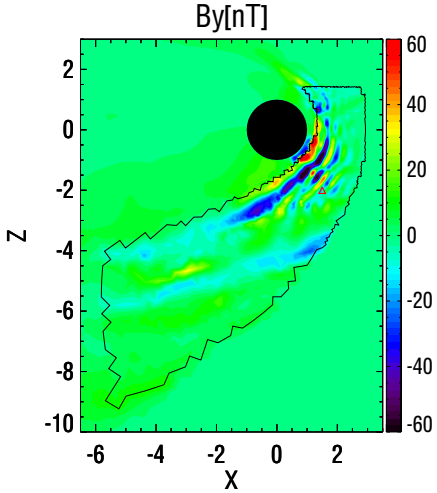
- **Flux rope**
  - Bulge of a flux rope propagates through the virtual satellite/MMS
  - Increase of density/plasma pressure, decrease of magnetic field
  - B_n changes sign

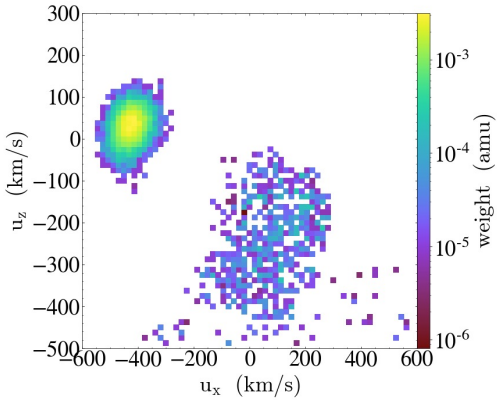
Simulations with FLEKS

Earth: cusp?

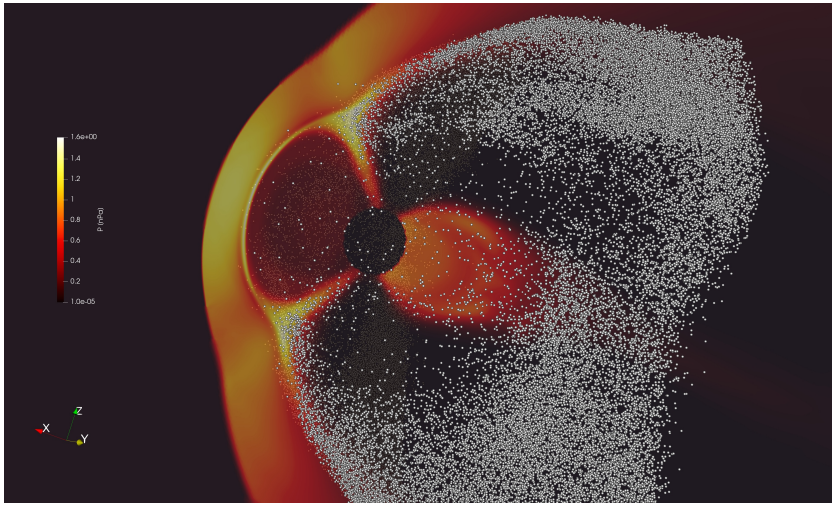


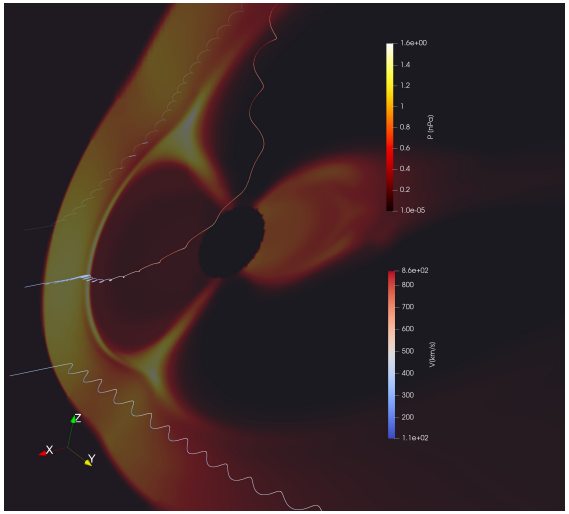
Mercury: foreshock?





FLEKS: newly developed test particle module





Summary

- **MHD-EPIC couples global MHD model with local PIC**
- **Improvement of the PIC component**
  - Gauss's Law satisfying Energy Conserving Semi-Implicit Method (GL-ECSIM)
    - Adjusts particle positions to satisfy Gauss's law
    - Improves robustness and accuracy
  - FLexible Exascale Kinetic Simulator (FLEKS)
    - Adaptive PIC region
    - Particle resampling algorithms
- **Applications**
  - Mercury's magnetotail
    - Dawn-dusk asymmetry
  - Earth's dayside magnetopause
    - Asymmetric reconnection
    - Flux transfer events (FTEs)
    - MMS data comparison