

Highly-Coupled Hall-MHD Algorithm for Hybrid PIC code Chicago*

C. Thoma, R.E. Clark, D. R. Welch, and D. V. Rose

Voss Scientific, LLC

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Introduction

Rudiments of PIC-based single-fluid (2 temperature) MHD algorithm outlined in C. Thoma, et al, Phys. of Plasmas **20**, 082128 (2013)

Extension of algorithm to allow for multiple ion species described in C. Thoma, et al., Phys. of Plasmas **24**, 062707 (2017), based on formulation given by A. Glocer et al., J. Geophys. Res **114**, A12203 (2009).

A highly-coupled version of the algorithm which allows timesteps large compared to the timescales σ and ν_e^{-1} , has recently been added to the hybrid-PIC code Chicago.

In the standard MHD formulation [e.g., N. Krall and A. Trivelpiece, *Principles of Plasma Physics* (McGraw-Hill, New York, 1973)] the Hall term in the generalized Ohm's law can be dropped when the Hall parameter, $\omega_{ce}/\nu_e \ll 1$. But this term must be retained in regimes where the Hall parameter is non-negligible. In this poster we discuss the implementation of highly-coupled Hall-MHD algorithm into Chicago. The algorithm has been developed for multiple ion species, but in this poster we restrict consideration to the case of a single MHD ion species.

Displacement current may either be retained or neglected in the algorithm, but there are some more stringent timestep constraints when displacement current is included.

Numerical dispersion analysis is performed and compared with analytic dispersion relations to demonstrate the feasibility of the approach and to assess regimes of stability.

Results from Chicago simulations of 1D and 2D test problem of plasma diffusion in a magnetic field are then discussed.

Hall-MHD Governing Equations + Analytic Dispersion

Hall-MHD equations for plasma $\beta \ll 1$.

For simplicity, assume 1 MHD species only and cold plasma ($\beta \ll 1$) so all pressure, thermoelectric terms vanish, etc. Also assume $\bar{Z} = 1$.

Eulerian Hall-MHD equations:

$$m_i n \left(\frac{\partial \bar{v}}{\partial t} + (\bar{v} \cdot \nabla) \bar{v} \right) = \frac{\bar{J} \times \bar{B}}{c}$$

$$\frac{1}{c} \frac{\partial \bar{B}}{\partial t} = -\nabla \times \bar{E},$$

$$\frac{1}{c} \frac{\partial \bar{E}}{\partial t} = -\frac{4\pi}{c} \bar{J} + \nabla \times \bar{B},$$

Displacement Current

$$\frac{\bar{J}}{\sigma} + \frac{\bar{J} \times \bar{B}}{nec} = \bar{E} + \frac{\bar{v} \times \bar{B}}{c}$$

Hall Term

where

$$\sigma = n / v_e.$$

These equations assume quasi-neutrality and neglect electron inertia.

The Hall term can be neglected if

$$H \equiv \frac{\omega_{ce}}{v_e} \ll 1$$

Guide field \bar{B}_0 , assume $\bar{k} \parallel \bar{B}_0$ and $\bar{k} \perp \bar{B}_0$

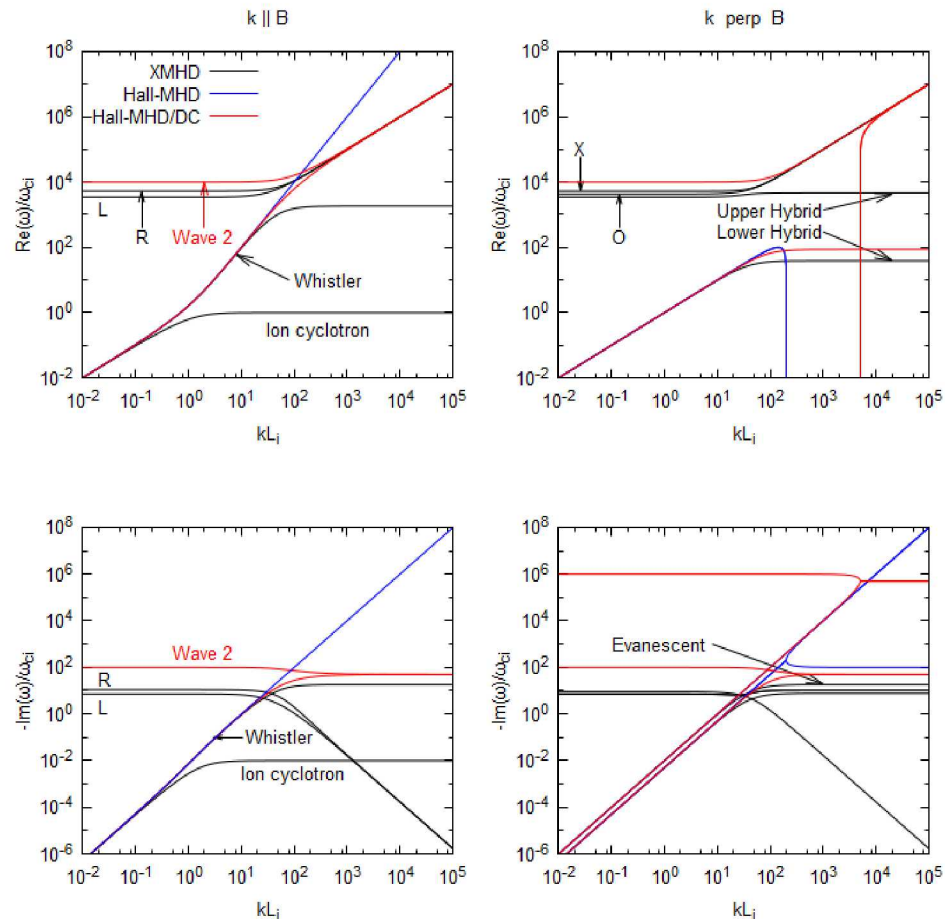
Linearize equations to obtain dispersion relation.

[Srinivasan] B. Srinivasan and U. Shumlak, Phys. Of Plasmas **18**, 092113 (2011).

[Huba] J. D. Huba, "Hall Magnetohydrodynamics", J Buechner, C. T. Dum, M. Scholer (Eds.): LNP 615, pp. 1660192, 2003. © Springer-Verlag Berlin Heidelberg 2003./

Three propagating dispersion branches when Hall term and displacement current are retained [Srinivasan].

$$H = 100, \beta_A = \omega_{ci} / \omega_{pi} = v_A / c = 0.1$$



Consider 2 variants:

Hall-MHD/DC:

Retain DC.

whistler branch: $\omega \sim k$ at large kL_i

Quasi-EM modes present ($\omega \sim kc$ at large kL_i)

Hall-MHD (Blue curves)

Drop displacement current.

Whistler branch: $\omega \sim k^2$ at large kL_i . Problematic for explicit Hall-MHD codes.

Quasi-EM modes vanish.

Recall from Srinivasan (Fig. 1)

In two fluid treatment whistler mode asymptotes to ω_{ce} (electron-cyclotron resonance).

The ion acoustic wave branch is also absent because we assumed a cold plasma.

Single-Ion Highly-Coupled Hall-MHD/DC: Local Velocity update and Electric Field Advance

Update ion velocity on cell nodes

by equations:

$$\frac{d\vec{v}}{dt} = \gamma \bar{\bar{B}}_c \cdot \left(\bar{\bar{v}}_e' \right)^{-1} \cdot \left[\bar{\bar{E}} + \bar{\bar{B}}_c \cdot \vec{v} \right] + \bar{\bar{F}}_V$$

$$\frac{d\bar{\bar{E}}}{dt} = -\bar{\bar{\sigma}}' \cdot \left[\bar{\bar{E}} + \bar{\bar{B}}_c \cdot \vec{v} \right] + \bar{\bar{F}}_E$$

where

$$\bar{\bar{F}}_V = \left(\frac{\Delta \vec{v}}{\Delta t} \right) - \gamma \bar{\bar{B}}_c \cdot \left(\bar{\bar{v}}_e' \right)^{-1} \cdot \left(\frac{\Delta \vec{v}_e}{\Delta t} \right)$$

$$\bar{\bar{F}}_E = \bar{\bar{\sigma}}' \cdot \left(\frac{\Delta \vec{v}_e}{\Delta t} \right) + \nabla \times \bar{\bar{B}}$$

$$\bar{\bar{v}}_e' = v_e \bar{\bar{1}} + \bar{\bar{B}}_c$$

$$\bar{\bar{B}}_c = \begin{bmatrix} 0 & B_z & -B_y \\ -B_z & 0 & B_x \\ B_y & -B_x & 0 \end{bmatrix} \text{Assume B is in +z direction}$$

$$\bar{\bar{\sigma}}' = n_e \left(\bar{\bar{v}}_e' \right)^{-1}$$

$$\left(\frac{\Delta \vec{v}}{\Delta t} \right) = \text{Ion fluid forces due to gradients.}$$

$$\left(\frac{\Delta \vec{v}_e}{\Delta t} \right) = \text{Electron fluid forces due to gradients.}$$

All gradient terms assumed constant during push, as is B field. Allows velocity and electric field to be pushed locally.

Solve by matrix methods (i.e., diagonalization):

$$\vec{v}(t) = \bar{\bar{M}}_{VV} \cdot \vec{v}(0) + \bar{\bar{M}}_{VE} \cdot \bar{\bar{E}}(0) + \bar{\bar{M}}_{V FY} \cdot \bar{\bar{F}}_Y + \bar{\bar{M}}_{V FV} \cdot \bar{\bar{F}}_V t$$

where

$$\bar{\bar{F}}_Y = \bar{\bar{F}}_E + \bar{\bar{B}}_c \cdot \bar{\bar{F}}_V$$

Update field equations at standard

Yee cell positions.

Hall-MHD field equations (assume no non-MHD species)

$$\frac{d\bar{\bar{B}}}{dt} = -\nabla \times \bar{\bar{E}},$$

$$\frac{d\bar{\bar{E}}}{dt} = -\bar{\bar{\sigma}}' \cdot \bar{\bar{E}} + \bar{\bar{G}}_E,$$

where

$$\bar{\bar{G}}_E = -\bar{\bar{\sigma}}' \cdot \bar{\bar{B}}_c \cdot \vec{v} + \bar{\bar{\sigma}}' \cdot \left(\frac{\Delta \vec{v}_e}{\Delta t} \right) + \nabla \times \bar{\bar{B}}$$

Advance electric fields by usual linear algebra methods:

assuming $\bar{\bar{\sigma}}'$, and $\bar{\bar{G}}_E$ are constant.

$$\bar{\bar{E}}(t) = \bar{\bar{M}}_{EE} \cdot \bar{\bar{E}}(0) + t \bar{\bar{M}}_{EG} \cdot \bar{\bar{G}}_E$$

or

$$\bar{\bar{M}}_{EG}^{-1} \cdot \bar{\bar{E}}(t) = \bar{\bar{M}}_{EG}^{-1} \cdot \bar{\bar{M}}_{EE} \cdot \bar{\bar{E}}(0) + t \bar{\bar{G}}_E$$

Hall-MHD: Drop DC

Velocity advance:

$$\frac{d\vec{v}}{dt} = \gamma \bar{\bar{B}}_c \cdot \left(\bar{\bar{v}}_e' \right)^{-1} \cdot \left(\bar{\bar{\sigma}}' \right)^{-1} \cdot \bar{\bar{F}}_E + \bar{\bar{F}}_V$$

Field advance:

$$\left(\bar{\bar{\sigma}}' \right)^{-1} \cdot \left(\alpha_\sigma \bar{\bar{E}}(t) + (1 - \alpha_\sigma) \bar{\bar{E}}(0) \right) = \bar{\bar{G}}_E,$$

where $\alpha_\sigma = [0, 1]$ is a time-biasing coefficient, default 1/2.

Both velocity and field advance can be written in previous form:

$$\vec{v}(t) = \bar{\bar{M}}_{VV} \cdot \vec{v}(0) + \bar{\bar{M}}_{VE} \cdot \bar{\bar{E}}(0) + \bar{\bar{M}}_{V FY} \cdot \bar{\bar{F}}_Y + \bar{\bar{M}}_{V FV} \cdot \bar{\bar{F}}_V t$$

$$\bar{\bar{M}}_{EG}^{-1} \cdot \bar{\bar{E}}(t) = \bar{\bar{M}}_{EG}^{-1} \cdot \bar{\bar{M}}_{EE} \cdot \bar{\bar{E}}(0) + t \bar{\bar{G}}_E$$

by redefining matrices.

Solving equations in a “highly-coupled” fashion, i.e., using matrix diagonalization to solve the underlying ODEs, allows for use of timesteps larger than timescales such as v_e^{-1} and σ^{-1} .

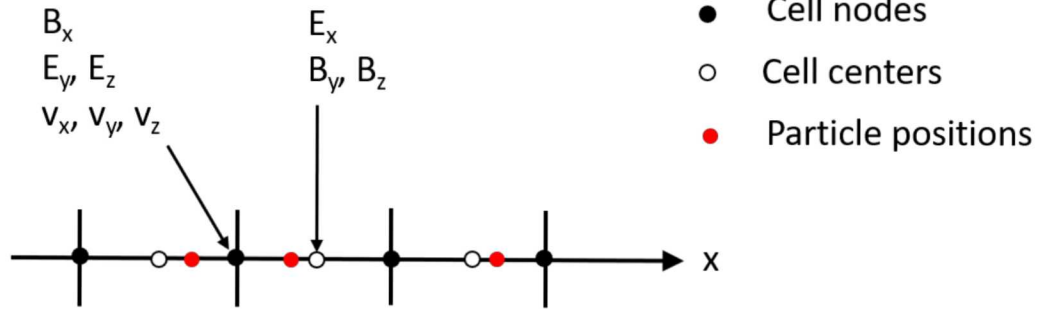
Highly-Coupled Leap-Frog Hall-MHD Solver

Electric and Magnetic fields at usual Yee positions.

Ion velocity and Temperature advanced at cell nodes.

Lagrangian particles may be remapped to cell centers once per timestep (Eulerian remap).

1D Cartesian Example:



Field Advance

Electric and magnetic fields advanced at full timesteps.

Time discretized version of field solution:

$$\vec{B}^{n+1} - \vec{B}^n = -\Delta t (\nabla \times \vec{E})^{n+1/2} \approx -\Delta t \left[\alpha_E (\nabla \times \vec{E})^{n+1} + (1 - \alpha_E) (\nabla \times \vec{E})^n \right]$$

$$\vec{M}_{EG}^{-1} \cdot \vec{E}^{n+1} = \vec{M}_{EG}^{-1} \cdot \vec{M}_{EE} \cdot \vec{E}^n + \Delta t \vec{G}_E^{n+1/2},$$

$$\vec{G}_E^{n+1/2} = \vec{\sigma}' \cdot [-\vec{v} \times \vec{B}^{n+1/2}] + \Delta t \left[\alpha_B (\nabla \times \vec{B})^{n+1} + (1 - \alpha_B) (\nabla \times \vec{B})^n \right]$$

Ion velocities are known at time level $n + 1/2$.

In $\vec{v} \times \vec{B}$ term, use explicit advance of \vec{B} for a 1/2 timestep:

$$\vec{B}^{n+1/2} \approx \vec{B}^n - \frac{\Delta t}{2} (\nabla \times \vec{E})^n.$$

Use same magnetic field to calculate $\vec{\sigma}'$, \vec{N}^{-1} , and \vec{M}_{ee} matrices.

Time-bias coefficients, α_E, α_B , set to values between 0 and 1 (1/2 default).

Particle Advance

We calculate new node velocities (\vec{v}') from old ion velocities (\vec{v}) at half-integer time-values.

$$\begin{aligned} \vec{v}_i^{n+1/2} = & \vec{M}_{EE} \cdot \vec{v}_i^{n-1/2} + \vec{M}_{VE} \cdot \left(\frac{\vec{E}_i^n + \vec{E}_i^{n-1}}{2} \right) \\ & + \vec{M}_{VFY} \cdot \left[\vec{\sigma}' \cdot \left(\frac{\Delta \vec{v}_e}{\Delta t} \right) + (\nabla \times \vec{B})_i^n + \vec{B}_c \cdot \left(\left(\frac{\Delta \vec{v}}{\Delta t} \right) - \gamma \vec{B}_c \cdot (\vec{v}_e')^{-1} \cdot \left(\frac{\Delta \vec{v}_e}{\Delta t} \right) \right) \right] \\ & + t \vec{M}_{VfV} \cdot \left(\left(\frac{\Delta \vec{v}}{\Delta t} \right) - \gamma \vec{B}_c \cdot (\vec{v}_e')^{-1} \cdot \left(\frac{\Delta \vec{v}_e}{\Delta t} \right) \right) \end{aligned}$$

Calculate $\Delta \vec{v}$ on the grid:

$$\Delta \vec{v}_i^{n+1/2} = \vec{v}_i^{n+1/2} - \vec{v}_i^{n-1/2}$$

Particle velocities (\vec{V}) are updated by gathering \vec{v}' , $\Delta \vec{v}$ from cell nodes to particle locations.

E.g., for a particle at the cell center ($i + 1/2$)

$$\begin{aligned} \vec{V}^{n+1/2} = & \left(\vec{v}^{n+1/2} + \frac{\Delta \vec{v}_i^{n+1/2} + \Delta \vec{v}_{i+1}^{n+1/2}}{2} \right) (1 - \alpha_S) \\ & + \left(\frac{\vec{v}'_i^{n+1/2} + \vec{v}'_{i+1}^{n+1/2}}{2} \right) \alpha_S \end{aligned}$$

where, α_S , is the streaming factor between 0 and 1 (default 0).

Following particle position advance

grid velocities are scattered back at cell nodes

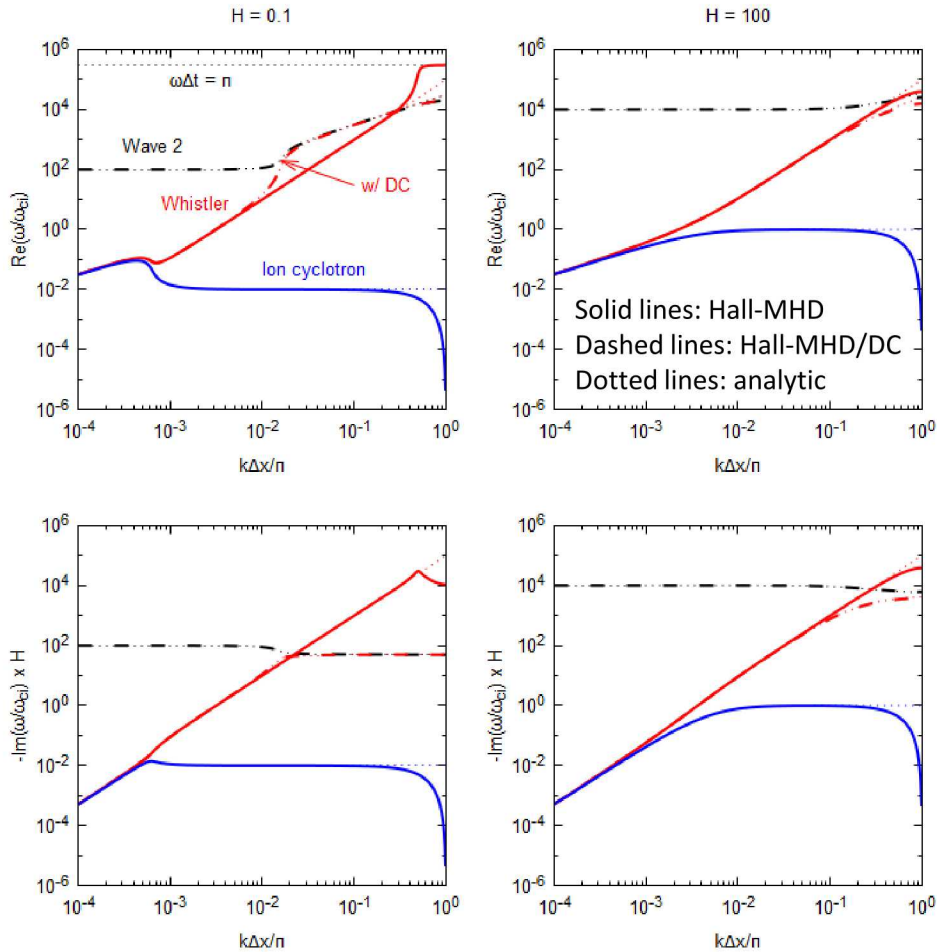
Particles may be remapped to cell centers.

Numerical Dispersion Analysis: $E \perp k \perp B_0$

$$\beta_A = 10^{-2}, \omega_A \Delta t = 0.1, s = c\Delta t / \Delta x = 0.1$$

$$(\alpha_E = \alpha_B = \alpha_\sigma = 1/2, \alpha_S = 0)$$

Vary $k\Delta x$ from 0 to π



Relevant frequencies

$$\omega_A = \frac{\omega_{pi}^2}{\omega_{ci}} = \frac{\omega_{ci}}{\beta_A^2} = \frac{\sigma}{H}$$

$$\sigma_\perp = \frac{\sigma}{1+H^2}$$

$$\sigma_\wedge = \frac{H\sigma}{1+H^2}$$

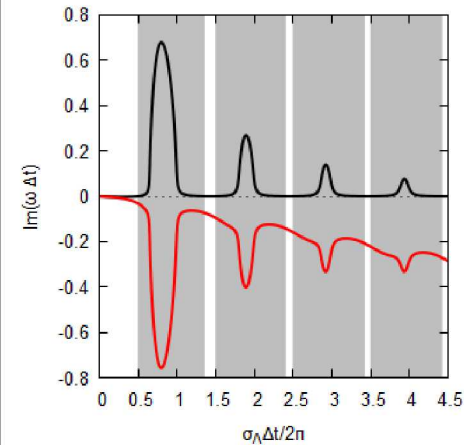
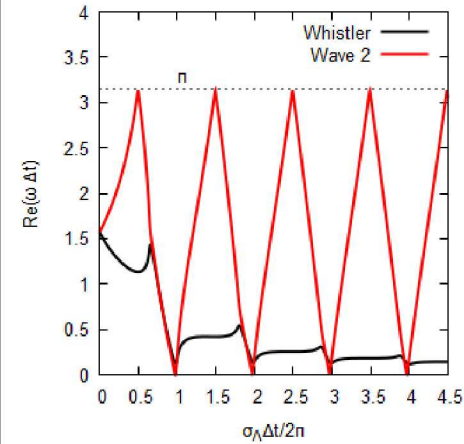
For $H \gg 1$ and $\beta_A \ll 1$,

$$\omega_{2c} \approx \omega_A \approx \sigma_\wedge$$

Hall-MHD/DC

$$H = 100, s = 1, k\Delta z = \pi$$

$$(\alpha_E = \alpha_B = 1/2)$$



Unstable bands around integer multiples of $\sigma_\wedge \Delta t / 2\pi$.

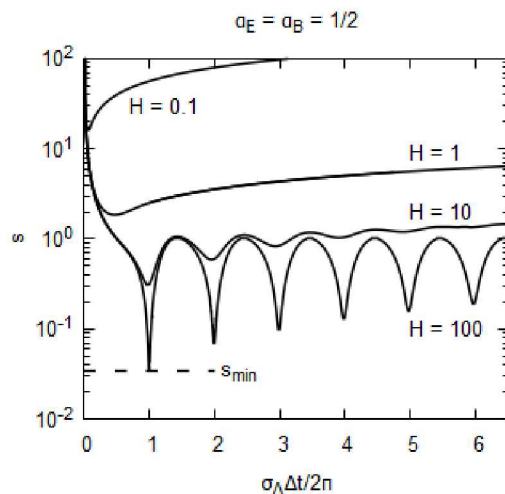
Due to numerical resonance between whistler branch and (aliased) wave 2.

At $k\Delta x = \pi$ ion cyclotron mode drops out due to spatial averaging of particles
If you drop DC no noticeable difference in IC dispersion, and Wave 2 goes away.

With DC, wave 2 is absent and instability mechanism vanishes.

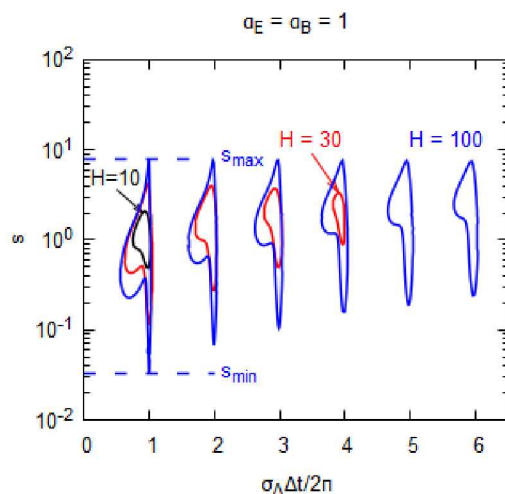
Hall-MHD/DC Instable regions

$k \parallel B_0$ at $k\Delta x = \pi$ Map out regions of stability where $\text{Im}(\omega\Delta t) > 0$



Time-centered case

Regions below black curves are stable, above unstable.



Fully time-biased case

Only regions inside closed curves are unstable.

Note that with full time-biasing can get stable again at large enough values of s . You're under-resolving EM waves but damping is so strong you can get away with it.

For fixed $s_{\min} < s < s_{\max}$ and large but finite H stability returns for large $\sigma_{\wedge} \Delta t / 2\pi$

This is because at large enough Δt collisional damping suppresses numerical resonance due to aliasing of quasi-EM mode..

Hall-MHD/DC Analytic dispersion for $\vec{E} \parallel \vec{k} \perp \vec{B}_0$ at $k\Delta x = \pi$

Hall-MHD/DC algorithm
 Numerical Dispersion analysis
 for $\vec{E} \parallel \vec{k} \perp \vec{B}_0$ at $k\Delta x = \pi$.

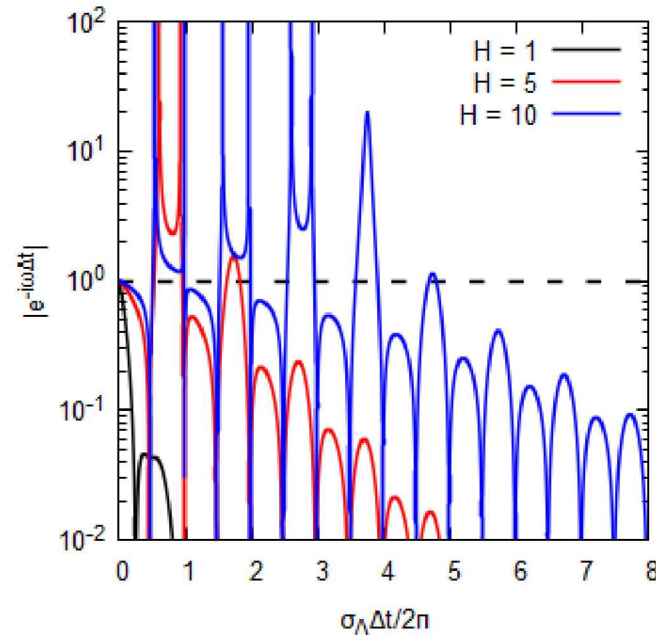
k is in +x direction
 Guide field in +z direction.
 Dispersion relation:

$$e^{-i\omega\Delta t} = \frac{(\bar{\bar{M}}_{EG}^{-1} \cdot \bar{\bar{M}}_{EE})_{11}}{(\bar{\bar{M}}_{EE}^{-1})_{11}}$$

So the mode is stable if

$$\left| \frac{(\bar{\bar{M}}_{EG}^{-1} \cdot \bar{\bar{M}}_{EE})_{11}}{(\bar{\bar{M}}_{EE}^{-1})_{11}} \right| \leq 1$$

Note for $\vec{E} \parallel \vec{k} \parallel \vec{B}_0$ at $k\Delta x = \pi$
 is uniformly stable.



Approximate stability regime for $H \gg 1$

$$\sigma_{\perp} \Delta t \leq \pi$$

$$\sigma_{\perp} \Delta t \geq \ln(H)$$

At large enough $\sigma_{\perp} \Delta t$ collisional damping
 suppresses numerical resonance.

Note: the stability behavior at Nyquist
 for this mode is independent of s .

**The instability is again due to a
 numerical resonance between an
 aliased quasi-EM mode and low
 frequency mode.**

When DC is dropped:

$$|e^{-i\omega\Delta t}| = |1 - \alpha_{\sigma}|$$

Stable for α_{σ} between 0 and 1.

1D Test of Hall-MHD/DC : Diffusion in Fully-ionized Magnetized Plasma

Hall-MHD/DC

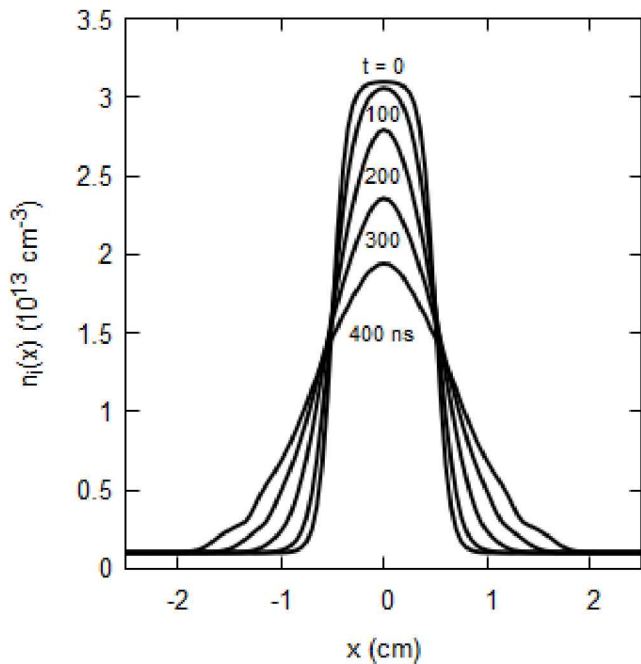
First unmagnetized case:

$$B_z = 0 \text{ G}$$

$$\alpha_E = \alpha_B = \alpha_S = 1$$

$$\Delta x = 0.05 \text{ cm}$$

$$c\Delta t = 50 \text{ cm}$$



$$T_e = T_i = 1 \text{ eV}$$

Varying values of Magnetic field: $B_z = 0, 100, 300 \text{ G}$

Hall-MHD/DC

$$\alpha_E = \alpha_B = \alpha_S = 1$$

$$\Delta x = 0.05 \text{ cm}$$

$$c\Delta t = 50 \text{ cm}$$

Hall-MHD

$$\alpha_E = \alpha_B = \alpha_\sigma = \alpha_S = 1$$

$$\Delta x = 0.05 \text{ cm}$$

$$c\Delta t = 50 \text{ cm}$$

Note density floor of 10^{12} cm^{-3} :

Keeps H finite.

Peak density = $3 \times 10^{13} \text{ cm}^{-3}$

v_{ei} at 1 eV and peak density = $6 \times 10^8 \text{ Hz}$ ($H \sim 3$ at 100 G)

Density Floor = $1 \times 10^{12} \text{ cm}^{-3}$

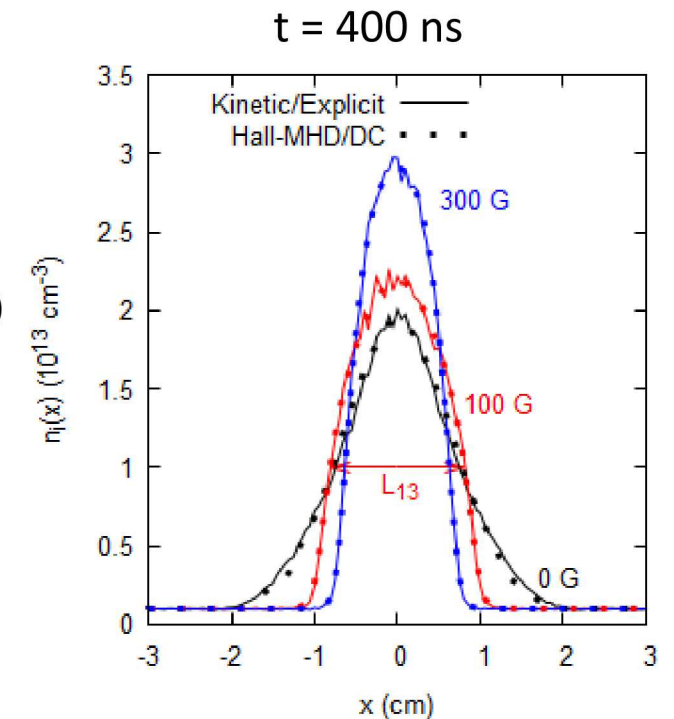
v_{ei} at 1 eV and floor density = $2.5 \times 10^7 \text{ Hz}$ ($H \sim 70$ at 100 G)

Kinetic explicit PIC

$$\Delta x = 0.05 \text{ cm}$$

$$c\Delta t = 0.02 \text{ cm}$$

Excellent agreement with fully kinetic explicit PIC, despite timestep x 2500. Hall-MHD and Hall-MHD/DC virtually indistinguishable.



Effect of streaming factor, α_S ($B_z = 100$ G, No DC)

Classical Diffusion theory (neglects Hall term)

Diffusion coefficient

$$D = \frac{2m_e T v_{ei}}{e^2 B^2}$$

Velocity

$$v_D = D / L_D$$

$$L_D = \frac{n}{\left| \frac{dn}{dx} \right|}$$

Diffusion time

$$\tau_D = L_W / v_D$$

L_W = initial column width

For 100 G field initial plasma conditions:

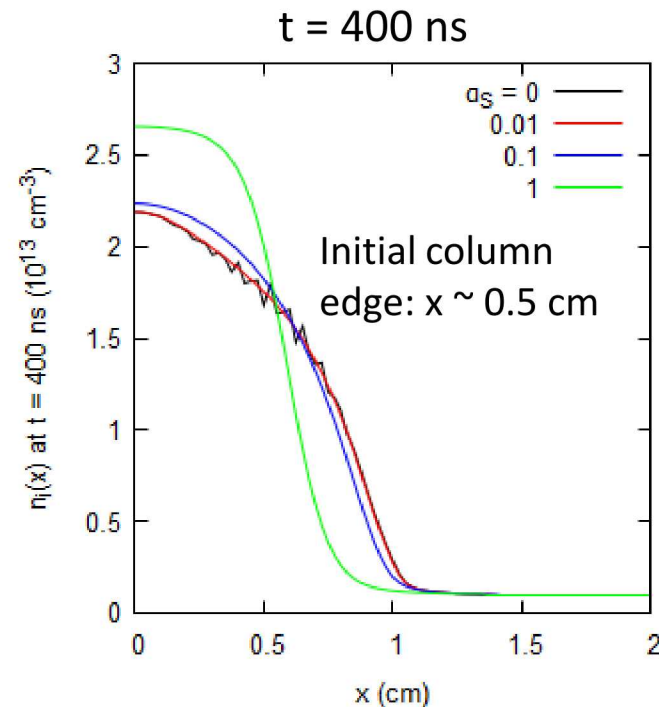
$$D \approx 6.8 \times 10^5 \text{ cm}^2 / \text{s}$$

$$L_n \approx 0.27 \text{ cm}, L_W \approx 1 \text{ cm}$$

$$v_D \approx 2.6 \times 10^6 \text{ cm} / \text{s}$$

$$\tau_D \approx 200 \text{ ns}$$

Even though classical diffusion neglects Hall term, use theory to estimate timescales.



Hall-MHD (no DC)

$$\alpha_E = \alpha_B = \alpha_\sigma = 1$$

$$\Delta x = 0.025 \text{ cm}, c\Delta t = 1 \text{ cm}$$

$$s_D \equiv 2D \Delta t / \Delta x^2 \sim 0.07$$

Note: $s_D \leq 1$ is stability criterion for explicit FDTD diffusion equation solver.

With a zero streaming factor can get high frequency stuff at steep gradients

Small amount of α_S helps suppress this.

But too much and you modify the shape too much.

We have noticed:

$$\alpha_S \Delta x^2 / \Delta t = \text{Constant}$$

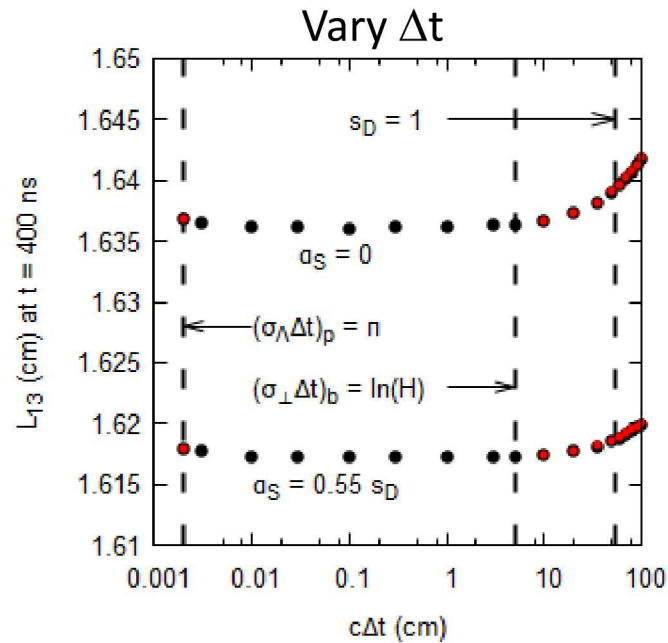
Get “self similar profiles”

And for:

$$\alpha_S \leq s_D$$

negligible distortion of shape

Convergence of L_{13} at $t = 400$ ns for 100 G Sim

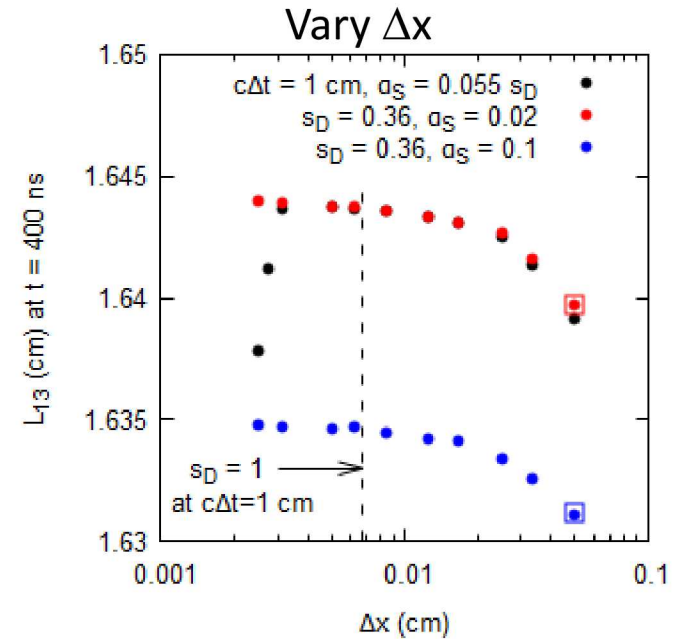


Fixed $\Delta x = 0.05$ cm
 $\alpha_E = \alpha_B = 1$ for all runs
 $\alpha_\sigma = 1$ for all Hall-MHD runs

Black dots Hall-MHD runs
 Red dots stable Hall-MHD/DC runs

p = Calculated at peak density ($H = 3$)
 b = Calculate at background density ($H = 70$)

Stable regions for Hall-MHD/DC predicted well with estimates from numerical Dispersion analysis.



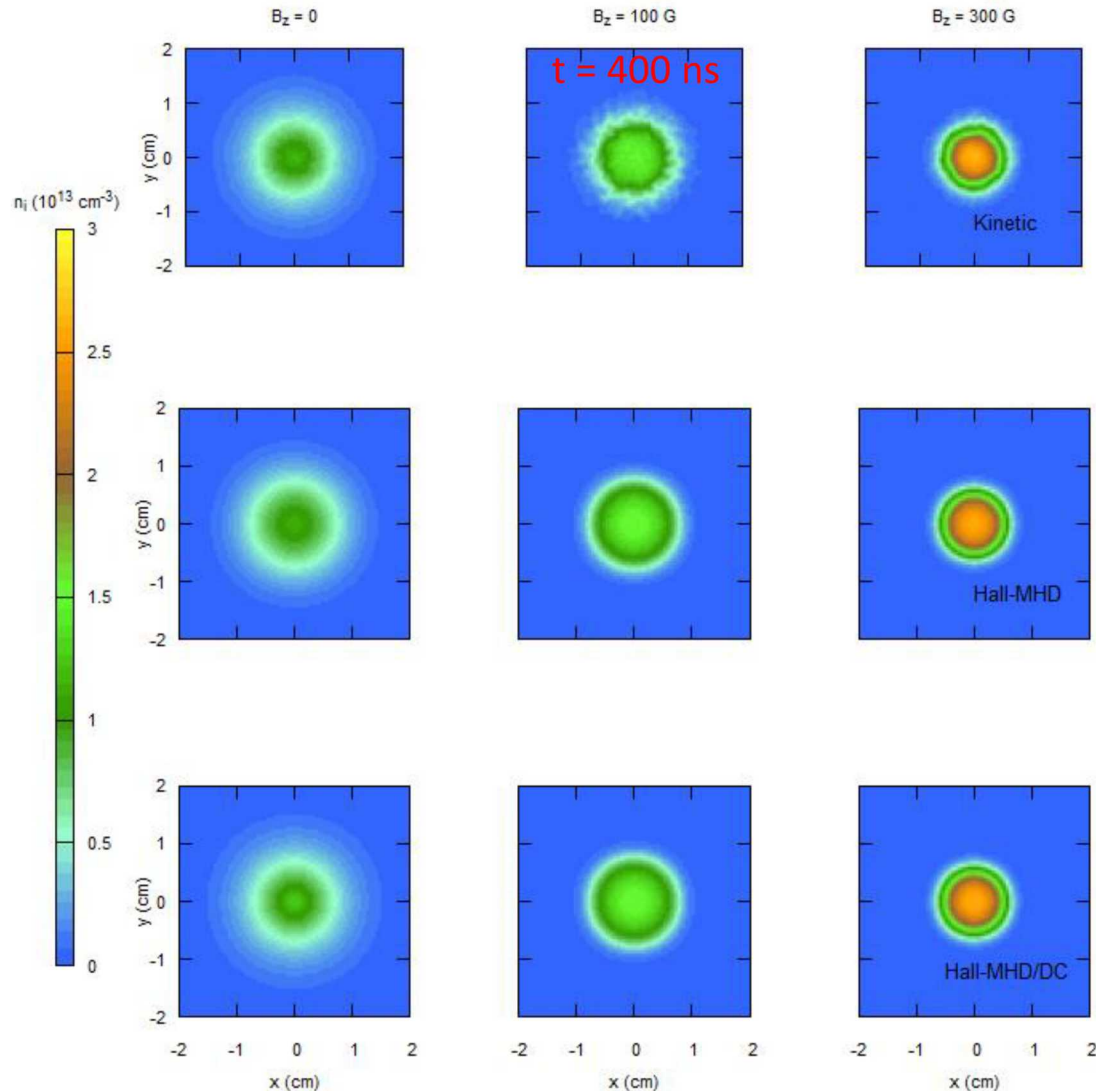
For $c\Delta t = 1$ cm, $s_D = 1$ at
 $\Delta x = 0.0067443$ cm

Black curve turns over when $s_D \gg 1$

Good convergence over wide range of Δt and Δx .

2D Cartesian Magnetic Diffusion Test

Repeat diffusion problem with axisymmetric initial density profile



Hall-MHD/DC

$$\alpha_E = \alpha_B = \alpha_S = 1$$

$$\Delta x = 0.05 \text{ cm}$$

$$c\Delta t = 50 \text{ cm}$$

Hall-MHD

$$\alpha_S = 1$$

Kinetic explicit PIC

$$\Delta x = 0.05 \text{ cm}$$

$$c\Delta t = 0.02 \text{ cm}$$

Good general agreement of Hall-MHD and Hall-MHD/DC with kinetic PIC results for plasma column expansion.

But kinetic PIC results show evidence of flute-like drift instability, which is purely kinetic in 2D [see e.g. D.V. Rose et al, Phys. of Plasmas **13**, 092507 (2006)]

The Hall-MHD and Hall-MHD/DC lack both charge-separation and kinetic effects so it cannot pick up this behavior.

Status and Future Work

- We have here described a single ion version of a highly-coupled Hall-MHD algorithm implemented into the code Chicago.
- Multi-ion implementation has been added to the code as well, but still needs to be made more robust (some numerical troubles with matrix diagonalization in certain parameter regimes).
- Hall-MHD formulation which retains displacement current requires $\omega_A \Delta t < \pi$ for numerically stable operation at high hall parameters. This restriction is lifted when displacement current is neglected.
- Highly-coupled version of Hall-MHD has no problems with the quadratic dispersion of whistler mode, which plagues explicit Hall-MHD codes.
- Braginskii [S. I. Braginskii, in *Reviews of Plasma Physics* (Plenum, New York, 1965)] has shown that corrections to the transport coefficients for a simple plasma (one ion and one electron species) due to magnetic field effects must also be included at non-negligible values of the Hall parameter. This effect has been included in Chicago only for thermal conductivity in the fluid energy equations. This effect needs to be added for all transport coefficients.
- The extension of Braginskii's transport theory to account for multiple ion-species has been done by Simakov and Molvig [A. N. Simakov and K. Molvig, *Phys. of Plasmas* 21, 024503 (2014)], but only in the absence of magnetic fields
- Our ultimate goal is to update the Braginskii transport coefficients to account for **both** multiple ion species and magnetic field corrections, and to implement these generalizations into a general multi-species Hall-MHD capability in Chicago.