Analysis of Numerical Algorithms for Two-Fluid Multiscale Computation

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Outline

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  - Comparison of semi-implicit two-fluid algorithms
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- NIMROD implementation
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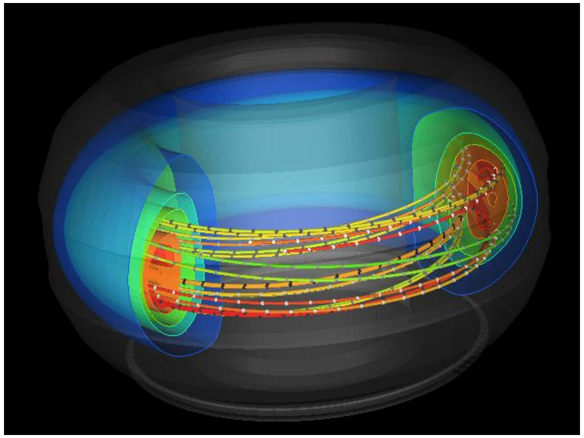
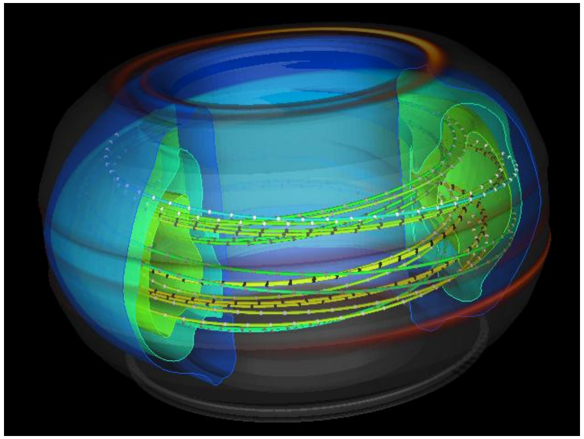
Introduction

- Modeling the evolution of MHD-like instabilities poses many challenges.
  - The modes extend over the device scale and are therefore sensitive to geometry.
  - Nonlinear effects are required to understand how magnetic topology and confinement are affected.
  - There are extreme anisotropies with respect to the direction of the evolving magnetic field.
  - The time-scales for wave propagation and nonlinear evolution are separated by many orders of magnitude.





NIMROD simulation of high-β disruption in DIII-D. [Courtesy of Scott Kruger, Tech-X]

Introduction (continued)

- Two-fluid contributions, such as the Hall electric field and gyroviscosity, are known to be important for macroscopic dynamics.
  - Drift effects lead to rotation and change stability thresholds.
  - Magnetic reconnection changes qualitatively with two-fluid effects.
- Two-fluid nonlinear macroscopic simulation requires numerical algorithms that can deal with greater ranges of temporal and spatial scales.
  - For resistive MHD, the NIMROD code uses a semi-implicit method with flow velocity staggered in time from magnetic field and pressure [JCP **195**, 355 (2004)].
  - Here, we investigate and analyze possible algorithms for incorporating two-fluid effects.
  - The analyses and test results have led us to a leap-frog scheme with implicit steps.

Non-Ideal Hall MHD Model

• Like other algorithms for MHD and extended-MHD, we cast the evolution equations in a single-fluid *form*.

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \left(\eta \mathbf{J} - \mathbf{V} \times \mathbf{B} + \frac{1}{ne} \mathbf{J} \times \mathbf{B} - \frac{1}{ne} \nabla p_e \right)$$ Faraday's / Ohm's law

$$\mu_0 \mathbf{J} = \nabla \times \mathbf{B}$$ low-ω Ampere's law

$$\nabla \cdot \mathbf{B} = 0$$ divergence constraint

$$\rho \left(\frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} \right) = \mathbf{J} \times \mathbf{B} - \nabla p - \nabla \cdot \Pi$$ flow evolution

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{V}) = \nabla \cdot D \nabla n$$ particle continuity

$$\frac{n}{\gamma - 1} \left(\frac{\partial T_\alpha}{\partial t} + \mathbf{V}_\alpha \cdot \nabla T_\alpha \right) = -p_\alpha \nabla \cdot \mathbf{V}_\alpha - \nabla \cdot \mathbf{q}_\alpha + Q_\alpha$$ temperature evolution

• The relations used for $\mathbf{E}$, Π, and $\mathbf{q}_\alpha$ determine which theoretical model is solved. [resistive MHD, two-fluid, kinetic effects, etc.]

Numerical Analyses

- A semi-implicit Hall-MHD algorithm based on [Harned and Mikic, JCP **83**, 1 (1989)] had been implemented in NIMROD.
  - Tests of waves in homogeneous equilibria demonstrated numerical stability for EMHD but not HMHD.
  - In general, numerical dispersion relations contain truncation errors, are not Hermitian, and are more complicated than corresponding analytic dispersion relations.
  - We were able to apply von Neumann stability analysis to the EMHD system by hand but found the numerical HMHD analysis to be too cumbersome.
- We therefore developed the 'DISPERSION' code for rapid construction and analysis of general linear algebraic systems.

DISPERSION scans a wavenumber parameter and evaluates the spectra of analytical and numerical linear systems.

- LAPACK routines for general linear systems are used to allow non-Hermitian matrices and 'defective' matrices (matrices where the set of eigenvectors do not form a complete basis). [Golub and van Loan, *Matrix Computations*]
  - Step 1: ZGEBAL separates triangular parts

$$\mathbf{A} \Rightarrow \begin{pmatrix} \mathbf{T}_1 & \mathbf{X} & \mathbf{X} \\ \mathbf{0} & \mathbf{X} & \mathbf{X} \\ \mathbf{0} & \mathbf{0} & \mathbf{T}_2 \end{pmatrix}$$

– Step 2: ZGEHRD forms the upper Hessenberg **H**, $\mathbf{A} = \mathbf{Q}^H \mathbf{H}\mathbf{Q}$

$$\mathbf{H} \sim \begin{pmatrix} x & x & x & x \\ x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \end{pmatrix}$$

The unitary **Q** is the product of Givens rotations,

$$\mathbf{Q} = \mathbf{H}(1)\mathbf{H}(2)\ldots\ ,$$

$$\mathbf{H}(i) = \mathbf{I} - \tau_i \mathbf{v}_i \mathbf{v}_i^H$$

– Step 3: ZHEQR performs QR-factorization from the upper Hessenberg matrix.

$$\mathbf{HZ} = \mathbf{ZT}$$

$$\mathbf{A}(\mathbf{QZ}) = (\mathbf{QZ})\mathbf{T}$$

- **T** is the Schur matrix, and eigenvalues appear on the diagonal.
- Nonzeros above the diagonal only appear for repeated eigenvalues with geometric multiplicity < algebraic multiplicity.

– Step 4: ZTREVC determine eigenvectors if desired.

The normalizations and post-processing conventions used in DISPERSION are:

- Time is normalized with the ion cyclotron frequency (Ω_i).
- Wavenumbers are normalized with the ion skin-depth (c/ω_i).
- In these units, $$v_A = \frac{c\Omega_i}{\omega_i} \Rightarrow 1, \quad \omega_{whistler} = kk_{\|}$$
- For numerical analysis, the eigenvalue of the time-step operation is reported as

$$\omega_r = \frac{1}{\Delta t}\tan^{-1}\left(\frac{-\mathrm{Im}(\lambda)}{\mathrm{Re}(\lambda)}\right) \qquad \text{for} \qquad (\mathbf{x})_j^{n+1} \to \lambda_j (\mathbf{x})_j^n$$
$$\omega_i = \frac{1}{2\Delta t}\ln\left(\lambda\lambda^*\right)$$

Aside on DISPERSION: Coding is an F90 version of symbolic manipulation to create the linear time-step matrix.

Example for MHD without flow.

6-vector is $(V_x, V_y, V_z, B_x, B_z, p)$ and $\mathbf{k}$ is in the y-direction.

F90 coding, where si_v, jxb_v, etc. are 6×6 matrices.

```
c
c     invert the semi-implicit operator:
c
      det=d_determ(si_v)
      CALL d_cofactor(si_v,work1)
      work1=TRANSPOSE(work1)/det
c
c     velocity advance:
c
      mat=MATMUL(work1,si_v+jxb_v+grp_v)
c
c     pressure advance:
c
      mat=MATMUL(iden+dvv_p,mat)
c
c     magnetic field advance:
c
      mat=MATMUL(iden+vxb_b,mat)
```

Corresponding numerical time-advance operation.

Find $\left(1+\Delta t^2 L\right)^{-1}$

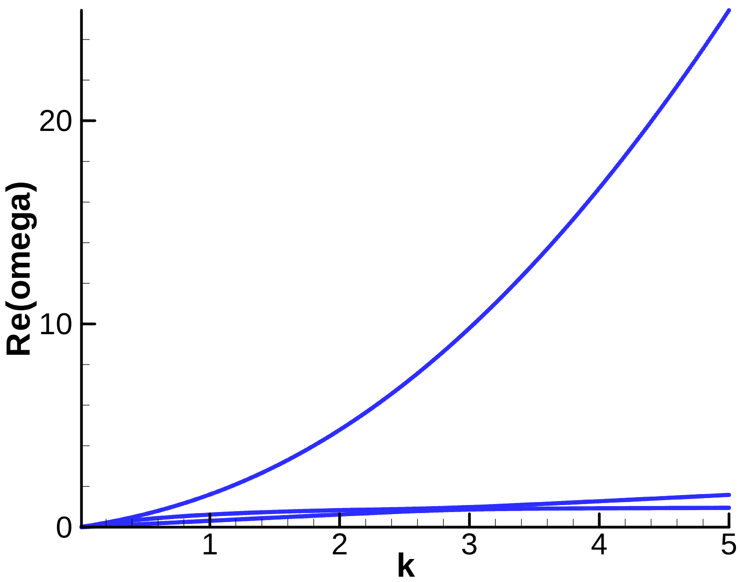
$$\mathbf{V}^{n+1} = \mathbf{V}^n + \left(1+\Delta t^2 L\right)^{-1}\left(\Delta t \mathbf{J}^{n+1/2} \times \mathbf{B}_0 - \Delta t \nabla p^{n+1/2}\right)$$

$$p^{n+3/2} = p^{n+1/2} - \Delta t \gamma\, p_0 \nabla \cdot \mathbf{V}^{n+1}$$

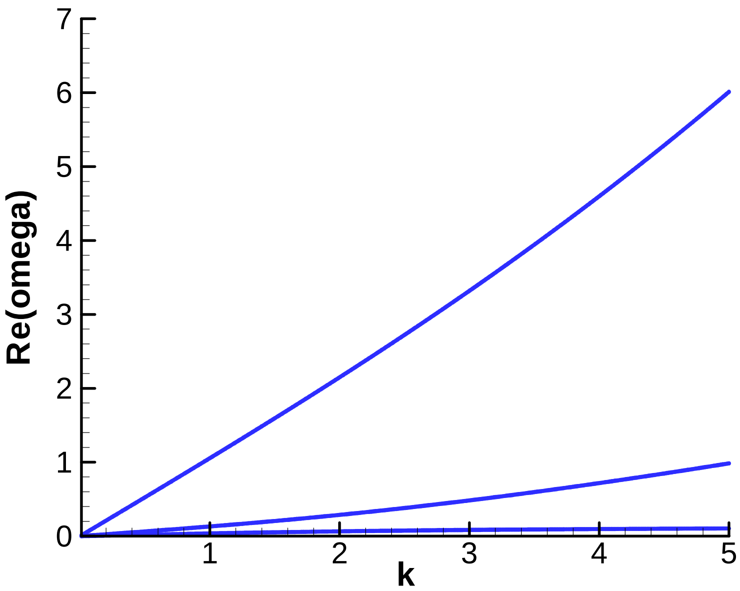
$$\mathbf{B}^{n+3/2} = \mathbf{B}^{n+1/2} + \Delta t \nabla \times \left(\mathbf{V}^{n+1} \times \mathbf{B}_0\right)$$

- **Matrices for complicated time-advances are also built from individual pieces, making it possible to analyze different algorithms quickly.**

EXAMPLE: Analytical Dispersion Relations for Two-Fluid Waves



$\theta = 0.04\pi$

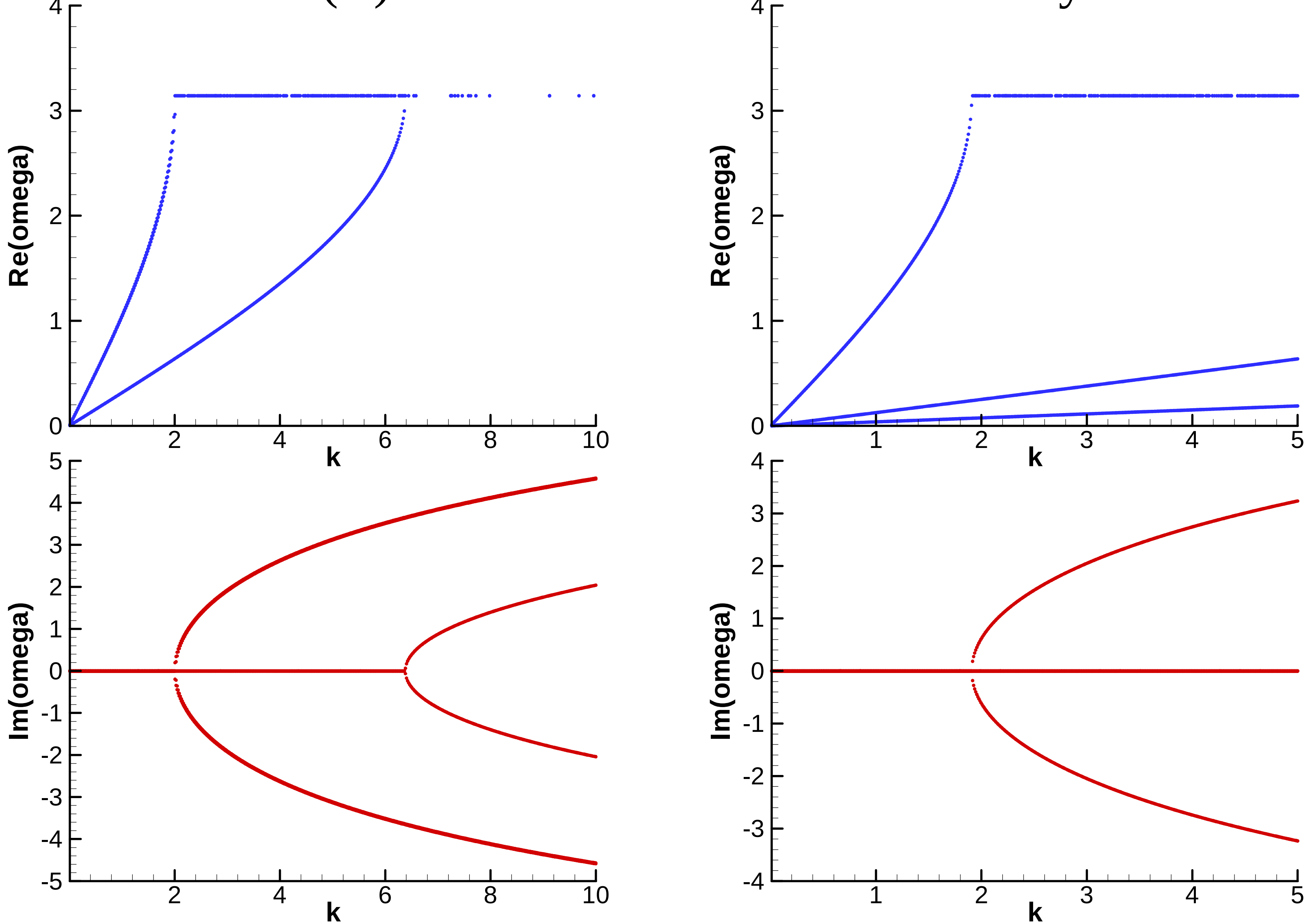


$\theta = 0.46\pi$

θ is the angle between **k** and $\mathbf{B}_0$. Here, $c_s^2/ v_A^2 = 0.1$.

EXAMPLE: Numerical Leapfrog for MHD Only

Im(ω)>0 indicates numerical instability.

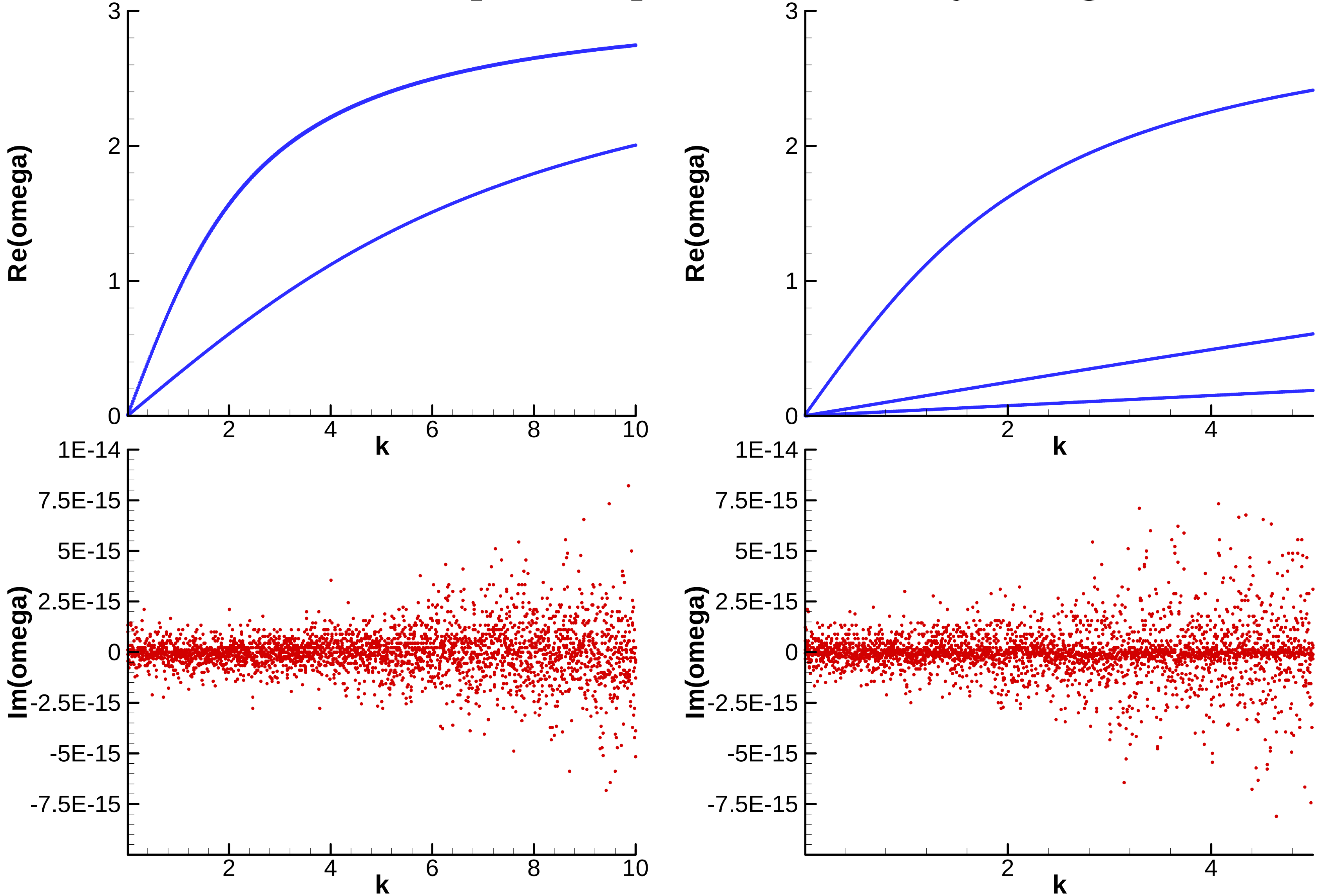


θ=0.04π θ=0.46π

Δt =1, c_s^2 / v_A^2=0.1.

EXAMPLE: Semi-Implicit MHD Leapfrog

Numerical dispersion provides stability at high-*k*.



$\theta = 0.04\pi$ $\theta = 0.46\pi$

$\Delta t = 1,\ c_s^2 / v_A^2 = 0.1.$

Semi-implicit algorithms for the Hall advance are intended to stabilize waves by adding numerical dispersion to the advance of magnetic field.

- A predictor/corrector advance is needed. (**B** drives itself via the Hall term.)
- A self-adjoint fourth-order differential operator is recommended for the semi-implicit operator in [Harned-Mikic, JCP **83**, 1 (1989)]. We initially used it in p&c steps.

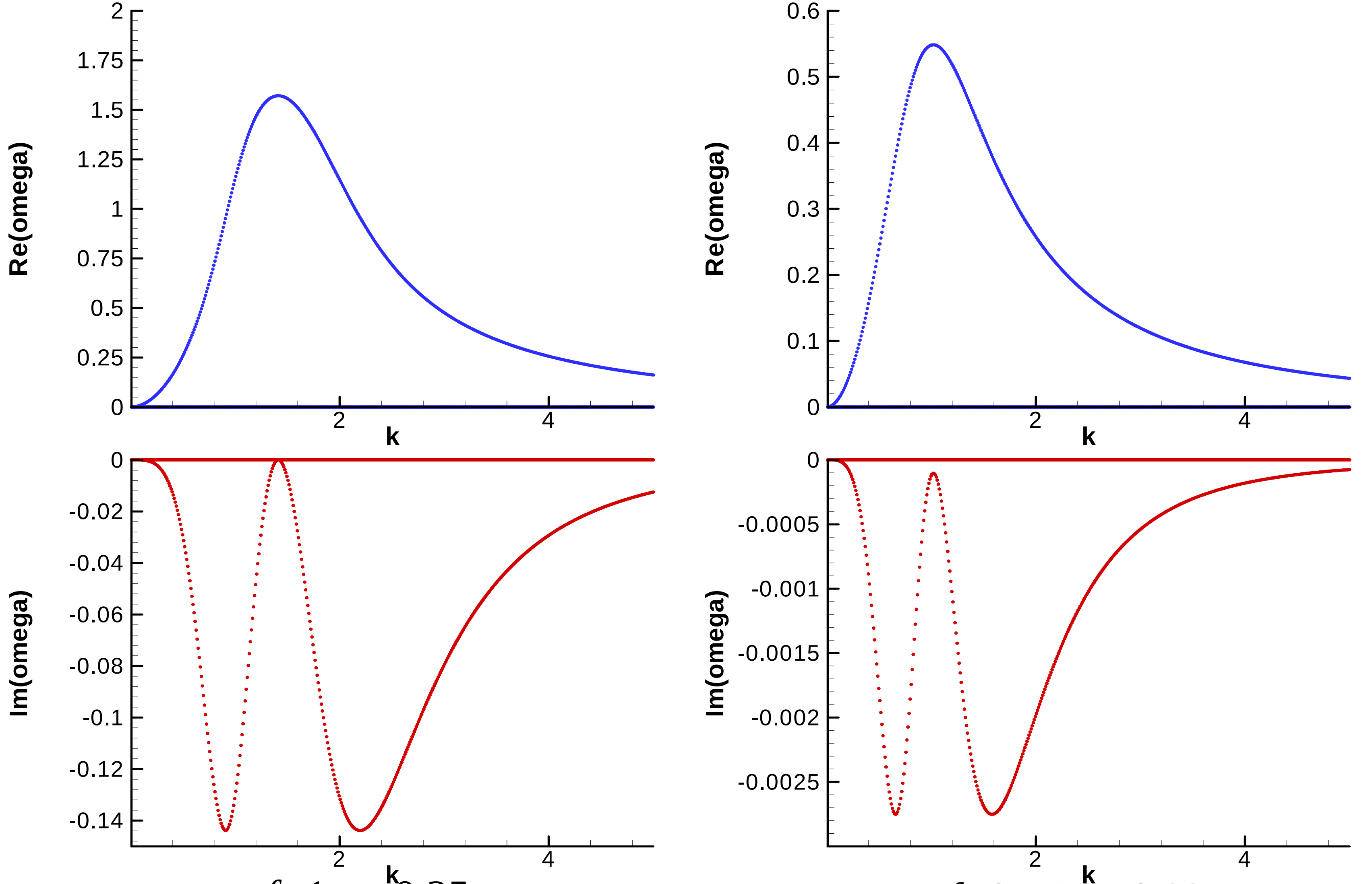
$$\Delta\mathbf{B} - \nabla\times\left(\frac{\Delta t}{\mu_0 ne}\left(\nabla\times\nabla\times\left(\frac{\Delta t}{\mu_0 ne}(\nabla\times\Delta\mathbf{B})\times\mathbf{B}_0\right)\right)\times\mathbf{B}_0\right) = rhs$$

- Our implementation in NIMROD uses an auxiliary field, so that all terms in the weak form are integrable with C^0 elements.

$$\int d\mathbf{x}\,\mathbf{A}\cdot\Delta\mathbf{B} + \int d\mathbf{x}\,\nabla\times\mathbf{f}\cdot\left(\frac{\Delta t}{\mu_0 ne}(\nabla\times\mathbf{A})\times\mathbf{B}_0\right) \quad = rhs$$

$$\int d\mathbf{x}\,\mathbf{g}\cdot\mathbf{f} \quad - \int d\mathbf{x}\,\nabla\times\mathbf{g}\cdot\left(\frac{\Delta t}{\mu_0 ne}(\nabla\times\Delta\mathbf{B})\times\mathbf{B}_0\right) = \mathbf{0}$$

NIMROD tests and numerical analysis show that the semi-implicit Hall advance is stable for EMHD.

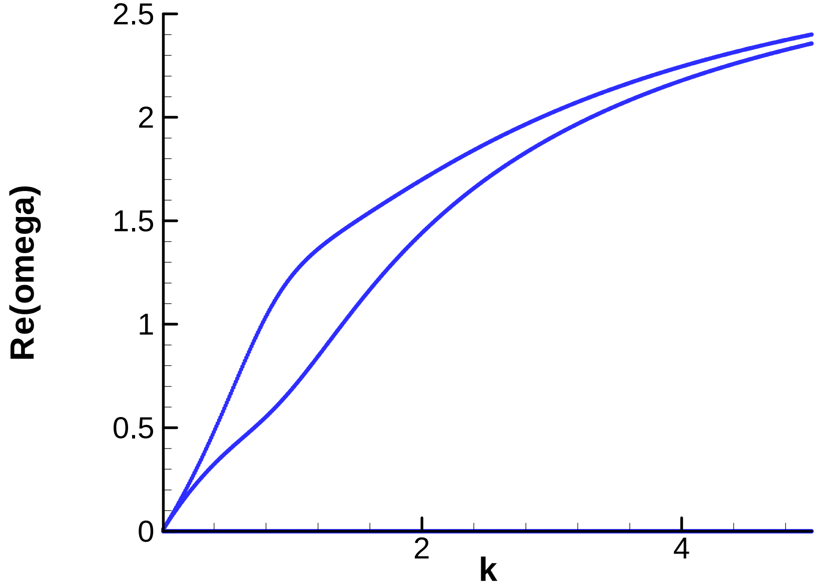


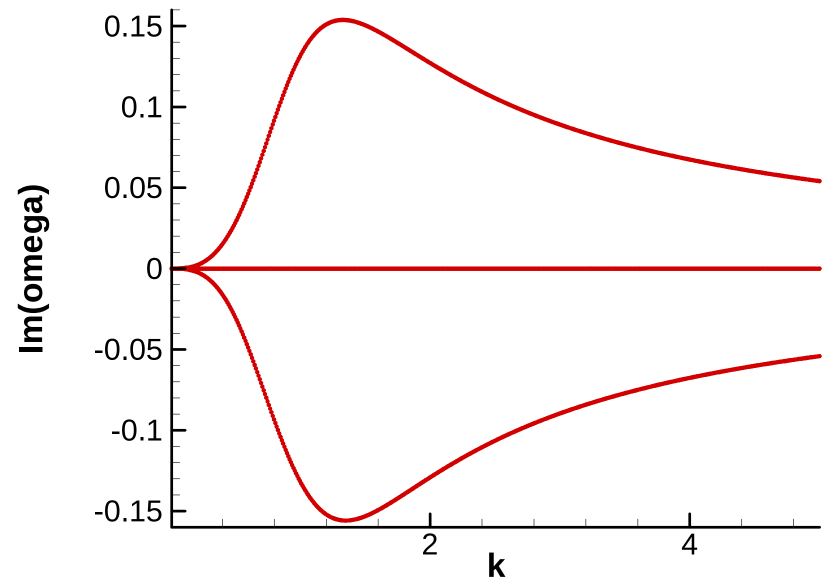
f=1, s=0.25

f=0.54, s=0.92

Δt =1, c_s^2/ v_A^2=0, f is P/C centering, and s is SI coefficient. (θ=0)

Tests indicate numerical instability when the algorithm is applied to HMHD, as confirmed by analysis.



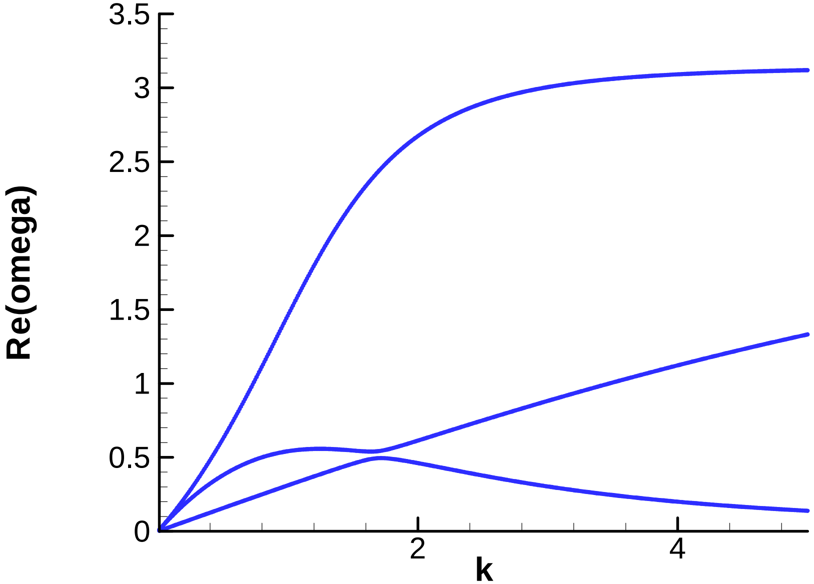


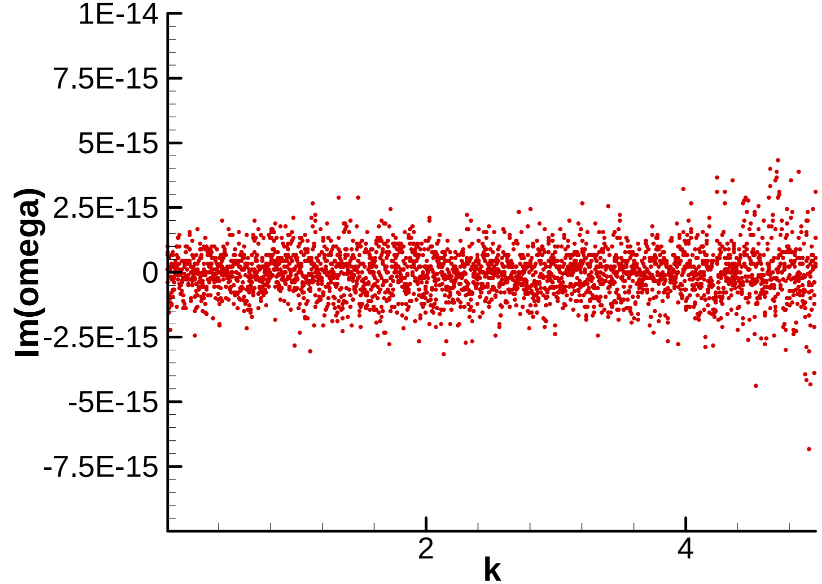
f=0.54, s_{Hall}=0.92

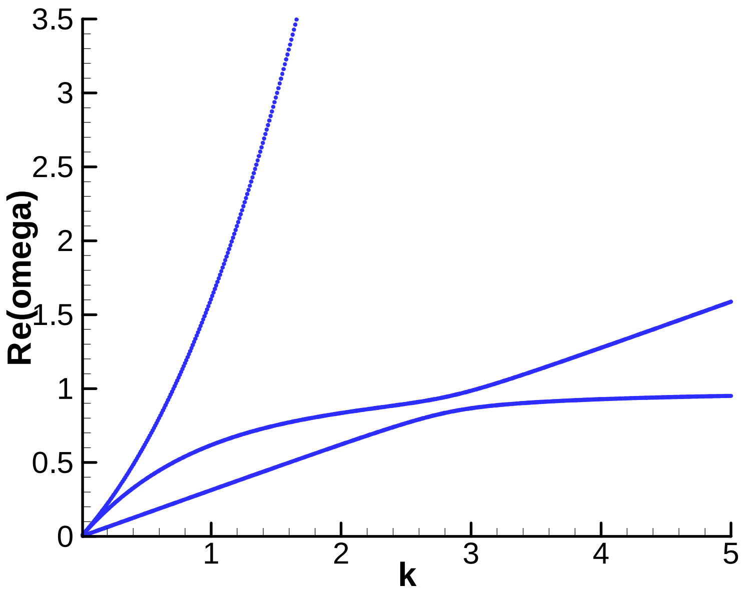
Δt =1, $c_s^2/\ v_A^2$=0 (θ=0)

- The Hall advance of **B** is time-split from the MHD advance of **B**, and the Hall semi-implicit operator is applied to predictor and corrector steps.
- Note that with the same code, SI MHD and SI EMHD are stable.

Applying the 4-th order operator to the corrector step only (with an unsplit **B** advance) initially looked promising.



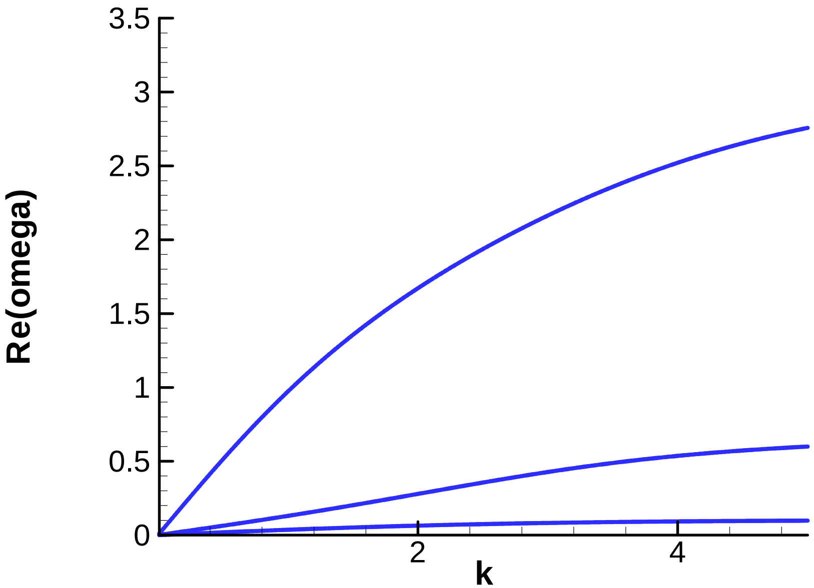


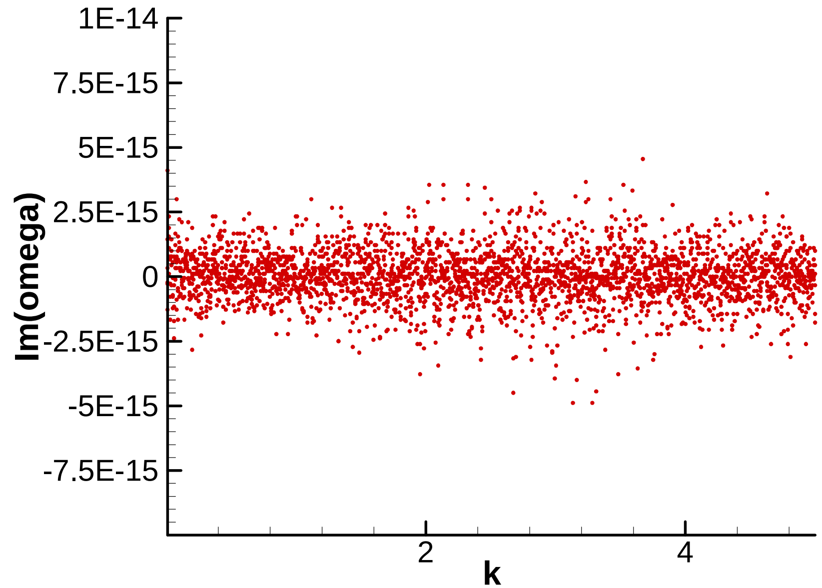


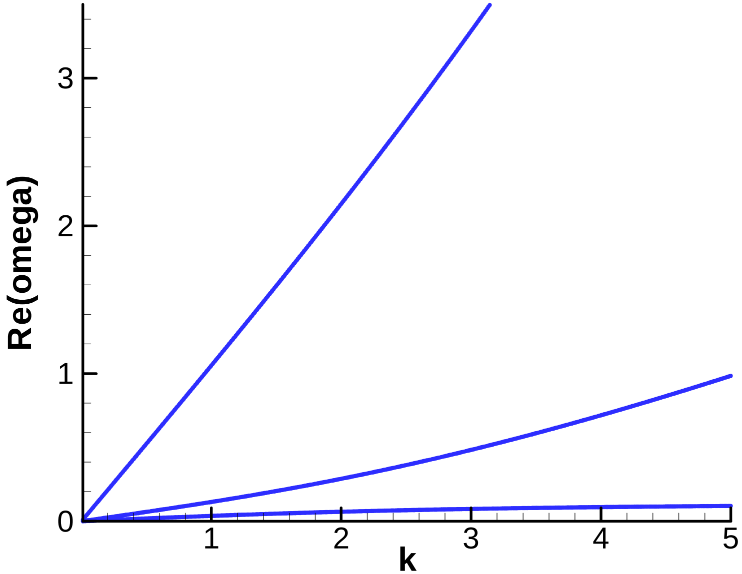
f=0.5, s_{Hall}=0.25, Δt =1, $c_s^{\,2}/\,v_A^{\,2}$=0.1 (θ=0.04π)

- The Hall semi-implicit operator is only applied to the corrector step.
- Bottom plot shows analytical dispersion for comparison.

Numerical Semi-Implicit Hall-MHD (Unsplit **B**)







f=0.5, s_{Hall}=0.25, Δt =1, $c_s^{\,2}/\, v_A^{\,2}$=0.1
(θ=0.46π)

- Bottom plot shows analytical dispersion for comparison.

- **Unfortunately, the NIMROD implementation found another numerical stability problem when applied to inhomogeneous equilibria.**

A new algorithm uses the leap-frog staggered data representation with a time-centered magnetic field update.

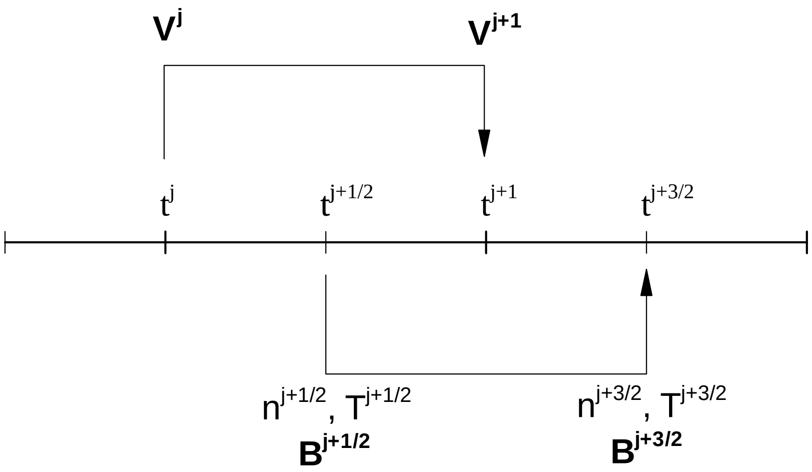
• This approach was motivated by the successful combination of the semi-implicit algorithm and time-centered advection (reported in http://www.cptc.wisc.edu/sovinec_research/meetings/sovinec_aps03poster.pdf)

Neglecting advection, dissipation, and the separate *n* and *T* advances for clarity:

$$\left(\rho + \Delta t^2 L\right)\Delta\mathbf{V} = \left(\Delta t\mathbf{J}^{n+1/2} \times \mathbf{B}^{n+1/2} - \Delta t\nabla p^{n+1/2}\right)$$

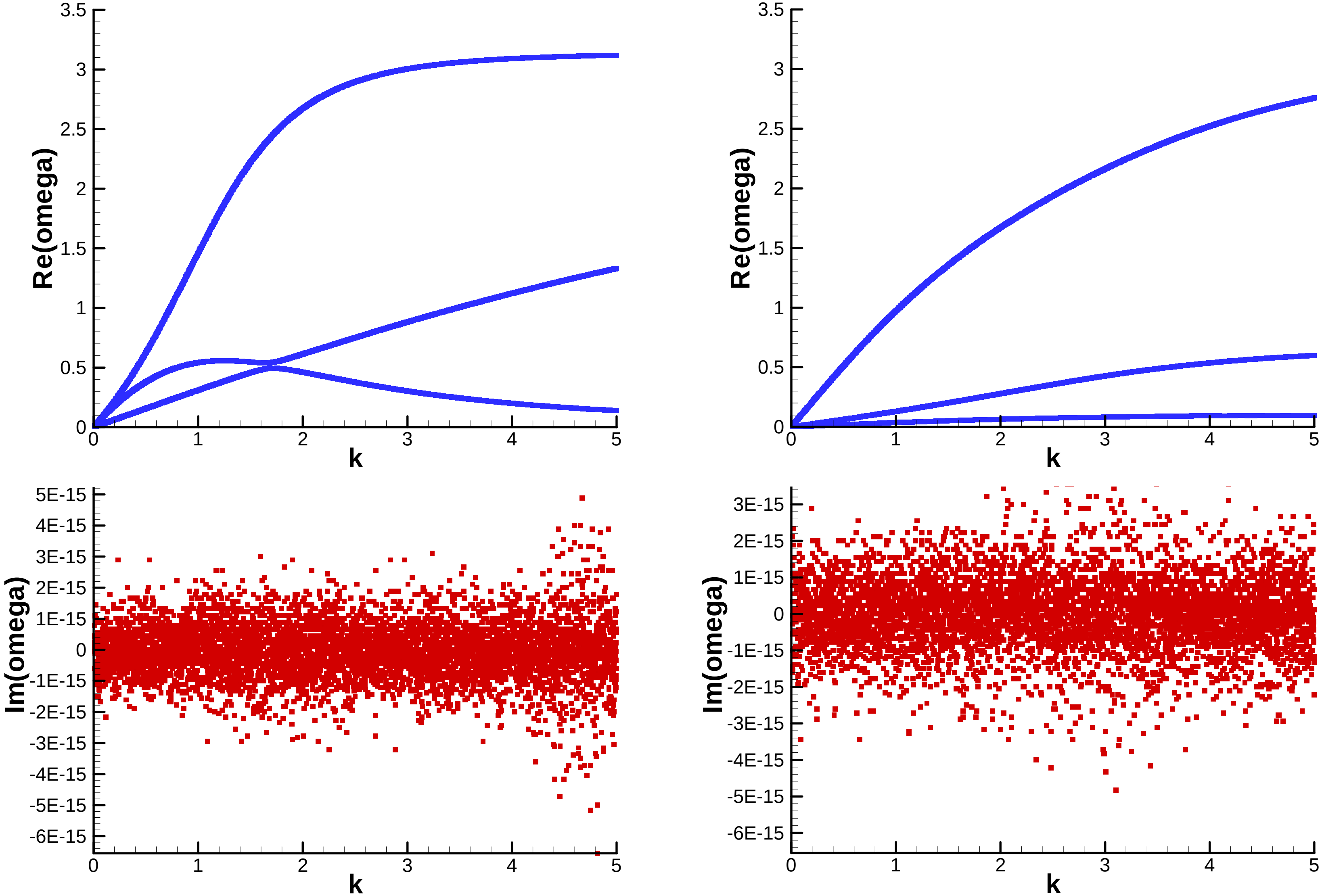
$$\Delta p = -\Delta t\gamma\, p^{n+1/2}\nabla\cdot\mathbf{V}^{n+1}$$

$$\Delta\mathbf{B} + \frac{\Delta t}{2}\nabla\times\frac{1}{ne}\left(\mathbf{J}^{n+1/2}\times\Delta\mathbf{B} + \frac{\nabla\times\Delta\mathbf{B}}{\mu_0}\times\mathbf{B}^{n+1/2}\right) = \Delta t\nabla\times\left(\mathbf{V}^{n+1}\times\mathbf{B}^{n+1/2}\right) - \Delta t\nabla\times\frac{1}{ne}\left(\mathbf{J}^{n+1/2}\times\mathbf{B}^{n+1/2} - \nabla p_e\right)$$



• The implicit Hall terms are linearized from the beginning of a time-step.

The leap-frog with implicit magnetic advance shows favorable numerical properties.

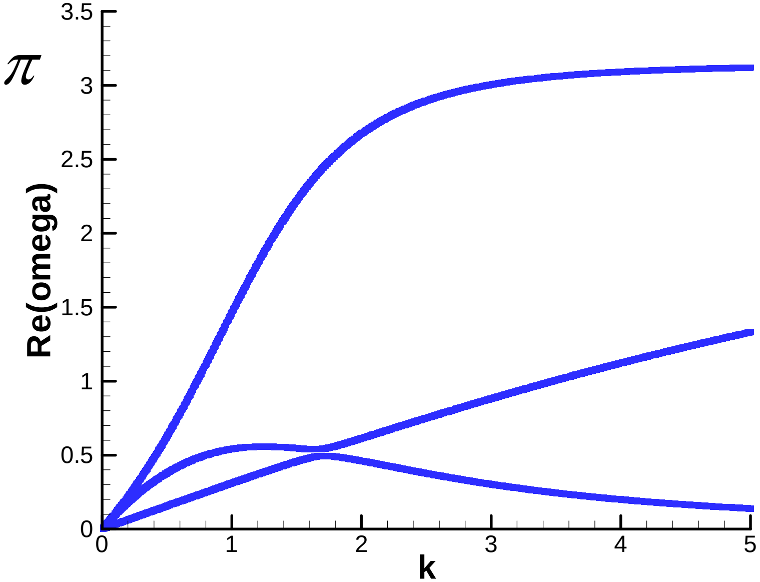


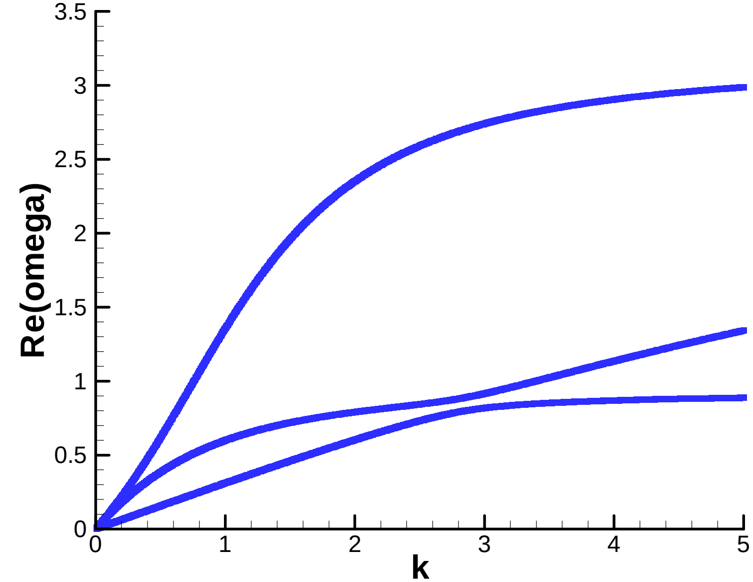
$\theta = 0.04\pi$ $\theta = 0.46\pi$

$\Delta t = 1,\ c_s^2 / v_A^2 = 0.1.$

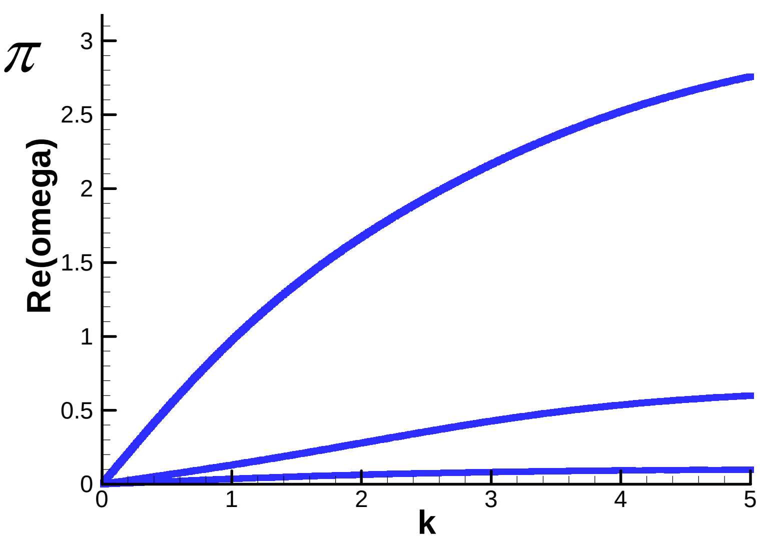
The leap-frog shows somewhat more numerical dispersion in the slow waves (for $\omega\Delta t$ >0.5) than a time-centered advance.

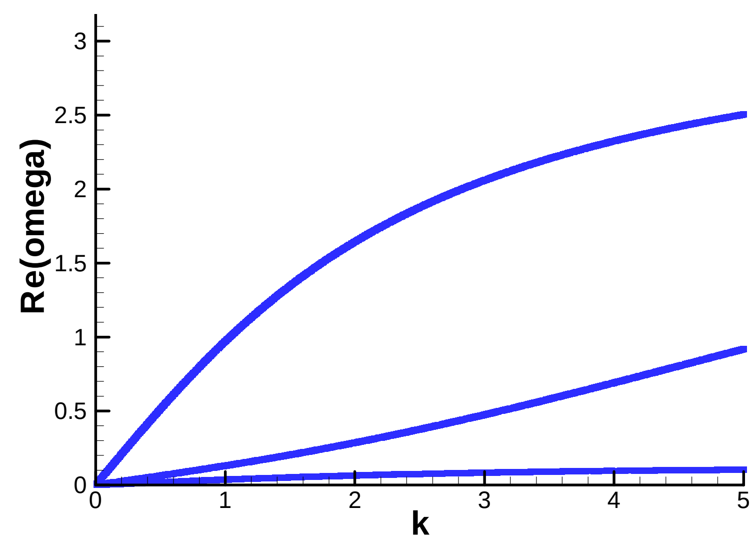
$\theta = 0.04\pi$





$\theta = 0.46\pi$





New Leap-frog

Time-centered

NIMROD Implementation

• The new leap-frog scheme has been partly implemented in NIMROD.

• The two-fluid magnetic advance requires solution of a non-Hermitian matrix.

• For 2D problems, we are able to solve non-Hermitian matrices using to the SuperLU software library.

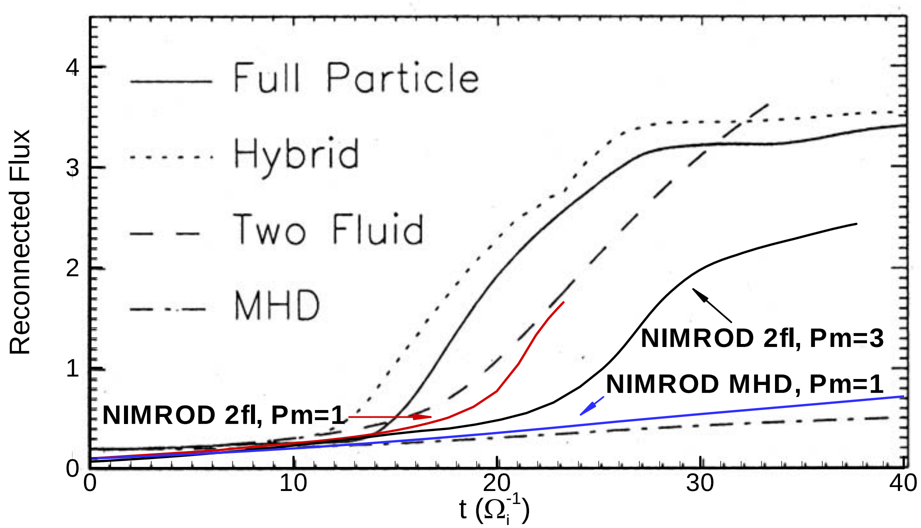
• For nonlinear 3D problems, we will need a matrix-free iterative approach; generating 3D matrix elements with the Fourier representation of the toroidal angle is not practical.

• Parallel software for performing matrix-free system solves is available (PETSc, for example) and will be implemented.

Results on the GEM Challenge Problem

• This comparison shows recent NIMROD Hall-MHD and resistive MHD results together with results published in Birn, Drake *et al.*, JGR (2001).

• This problem has no guide field, and reconnection generates sonic flows well into the nonlinear phase of the 2-fluid computations.



Reconnected magnetic flux as a function of time.

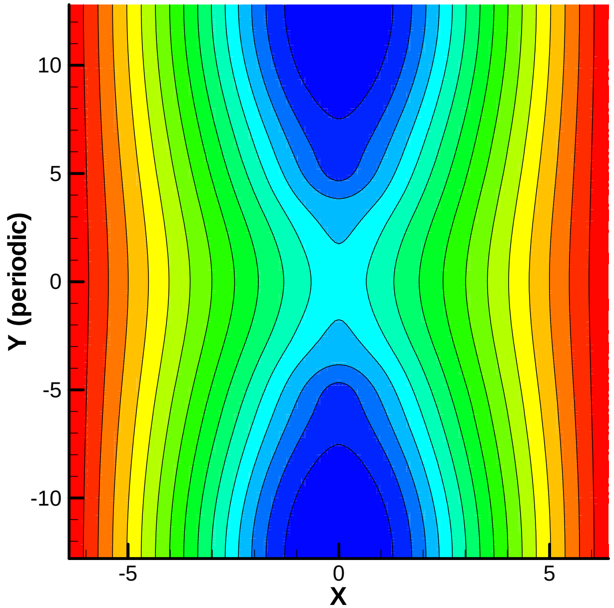
• Resistivity $\eta = 0.005$

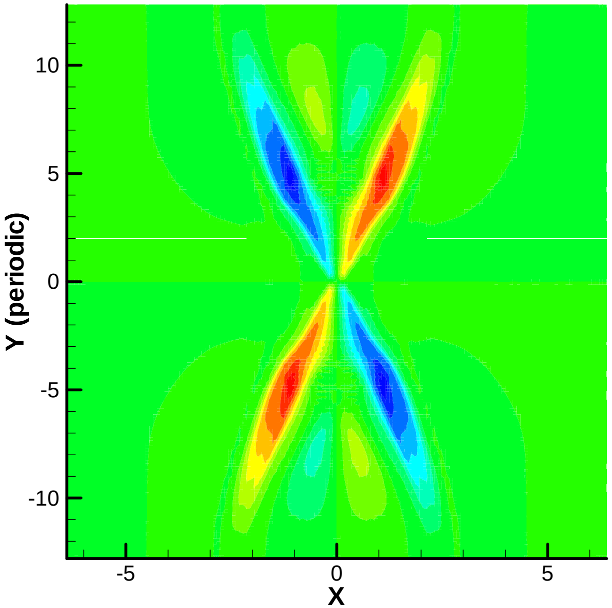
• NIMROD simulations have

- $\chi_{iso} = 0.005$
- $D = 0.005$
- $0.005 \leq \nu \leq 0.015$

• Since NIMROD does not have shock-capturing capabilities, dissipation is used to maintain some degree of smoothness. With a 72×96 mesh of biquadratic elements, Pm=3 is required to achieve saturation.

The NIMROD Hall-MHD computation with Pm=1 shows important characteristics of two-fluid reconnection.

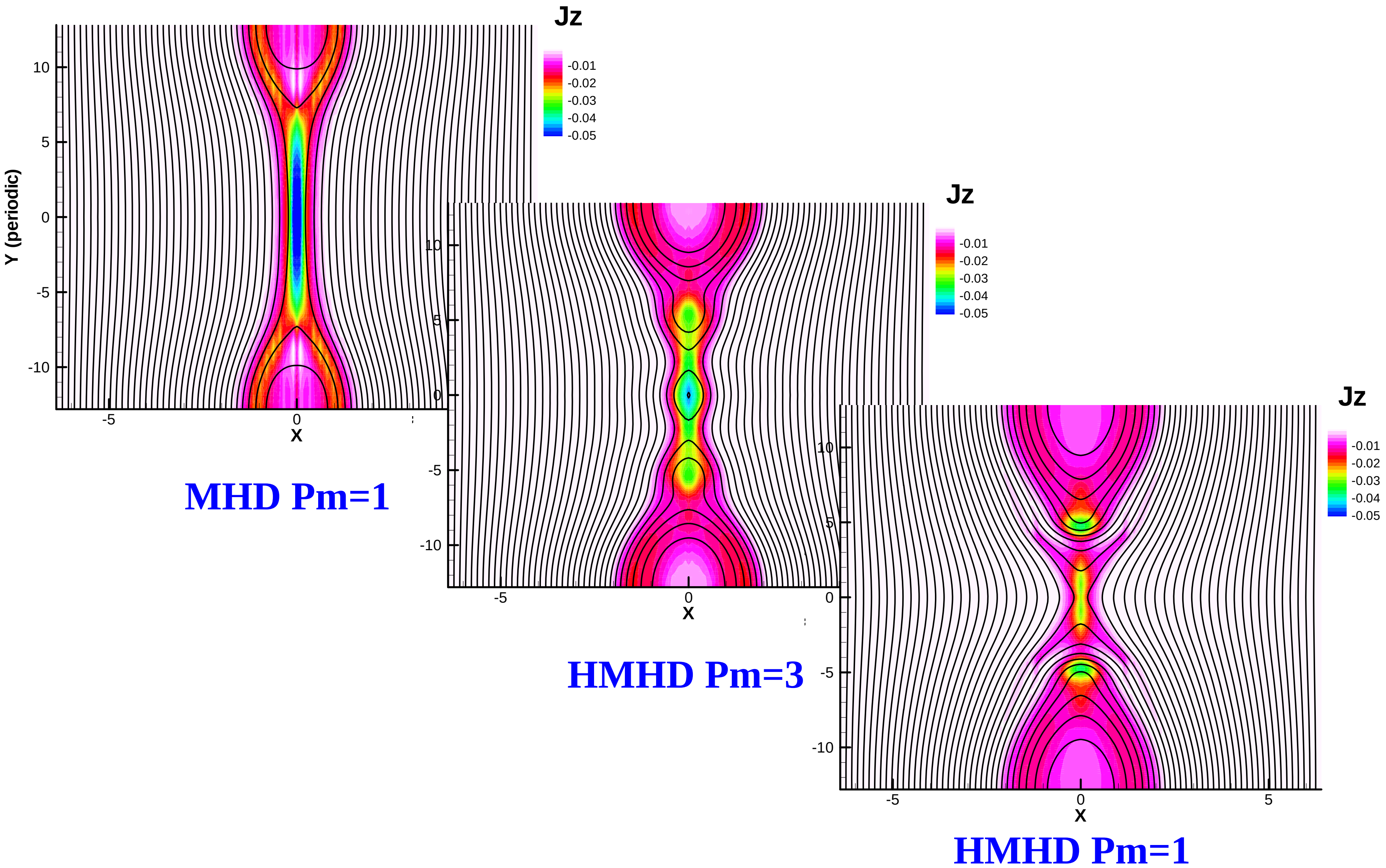




The characteristic results from t=23 Ω_i^{-1} are the open geometry of the reconnecting magnetic flux (left) and the quadrupole out-of-plane magnetic field (right).

• See the next poster (Tian) for results on low-beta equilibria with a large guide field.

Out-of-plane current density and poloidal flux at t=23-24 Ω_i^{-1} show sensitivity to viscosity.



Conclusions

• Algorithms with a semi-implicit operator for stabilizing two-fluid waves (including whistler waves) are numerically unstable in the full HMHD system; though, they are stable for EMHD alone. This finding may be at odds with what is published in [Harned and Mikic], however.

• A numerical tool for analyzing the spectra of general matrices has been constructed using LAPACK routines. Time-steps are built-up in a symbolic way, which facilitates tests of different algorithms.

• A new leap-frog based scheme with an implicit magnetic field advance has been proposed, analyzed, and implemented in NIMROD. It is numerically stable for waves and has been exercised on the GEM Challenge problem. Accuracy appears to be close to a fully centered advance, and the algebraic systems should be easier to solve.

• This presentation will be posted on nimrodteam.org and www.cptc.wisc.edu/sovinec_research.