Semi-Implicit Extended MHD Simulation

C. R. Sovinec, H. Tian, University of Wisconsin-Madison D. D. Schnack, A. Y. Pankin, Science Applications International Corporation D. C. Barnes University of Colorado at Boulder

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Introduction

- Modeling the evolution of MHD-like instabilities poses many challenges.
 - 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.
 - Nonlinear Hall contributions can produce dynamo effects.
- The ranges of temporal and spatial scales in two-fluid computations are yet more extreme than with resistive MHD.
 - 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)].
 - Analyses and test results for the two-fluid system have led us to a leapfrog scheme with implicit steps.
 - A suite of test cases is required to benchmark the algorithm and understand its properties.

Evolution Equations

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

$$\begin{aligned} \frac{\partial \mathbf{B}}{\partial t} &= -\nabla \times \left(\eta \mathbf{J} - \mathbf{V} \times \mathbf{B} + \frac{1}{ne} \mathbf{J} \times \mathbf{B} - \frac{1}{ne} \nabla p_e \right) & \text{Faraday's / Ohm's law} \\ \mu_0 \mathbf{J} &= \nabla \times \mathbf{B} & \text{low-} \omega \text{ Ampere's law} \\ \nabla \cdot \mathbf{B} &= 0 & \text{divergence constraint} \\ \rho \left(\frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} \right) &= \mathbf{J} \times \mathbf{B} - \nabla p - \nabla \cdot \Pi_i (\mathbf{V}) & \text{flow evolution} \\ \frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{V}) &= \nabla \cdot D \nabla n & \text{particle continuity} \\ \frac{n}{\gamma - 1} \left(\frac{\partial T_\alpha}{\partial t} + \mathbf{V}_\alpha \cdot \nabla T_\alpha \right) &= -p_\alpha \nabla \cdot \mathbf{V}_\alpha - \nabla \cdot \mathbf{q}_\alpha + Q_\alpha & \text{temperature evolution} \end{aligned}$$

The relations used for **E**, Π , and \mathbf{q}_{α} determine which theoretical model is solved. [resistive MHD, two-fluid, kinetic effects, etc.] • Collisional closure relations have limited applicability, but they provide dissipation that is <u>necessary</u> for nonlinear simulations if the algorithm is not

inherently dissipative.

$$\Pi_{gv} = \frac{m_{i}p_{i}}{4eB} \left[\hat{\mathbf{b}} \times \mathbf{W} \cdot \left(\mathbf{I} + 3\hat{\mathbf{b}}\hat{\mathbf{b}} \right) - \left(\mathbf{I} + 3\hat{\mathbf{b}}\hat{\mathbf{b}} \right) \cdot \mathbf{W} \times \hat{\mathbf{b}} \right], \qquad \left(\mathbf{W} \equiv \nabla \mathbf{V} + \nabla \mathbf{V}^{T} - \frac{2}{3}\mathbf{I}\nabla \cdot \mathbf{V} \right)$$
$$\Pi_{\parallel} = \frac{p_{i}\tau_{i}}{2} \left(\hat{\mathbf{b}} \cdot \mathbf{W} \cdot \hat{\mathbf{b}} \right) \left(\mathbf{I} - 3\hat{\mathbf{b}}\hat{\mathbf{b}} \right)$$
$$\Pi_{\perp} \sim -\frac{3p_{i}m_{i}^{2}}{10e^{2}B^{2}\tau_{i}} \mathbf{W}$$
$$\mathbf{q}_{i} = -n \left[\chi_{\parallel_{i}}\hat{\mathbf{b}}\hat{\mathbf{b}} + \chi_{\perp_{i}} \left(\mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}} \right) \right] \cdot \nabla T_{i} + 2.5 p_{i}(eB)^{-1}\hat{\mathbf{b}} \times \nabla T_{i}$$
$$\mathbf{q}_{e} = -n \left[\chi_{\parallel_{e}}\hat{\mathbf{b}}\hat{\mathbf{b}} + \chi_{\perp_{e}} \left(\mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}} \right) \right] \cdot \nabla T_{e} - 2.5 p_{e}(eB)^{-1}\hat{\mathbf{b}} \times \nabla T_{e}$$

• Closure terms with local gradients may be treated implicitly and can be used in semi-implicit advances with nonlocal closures. [Held, PoP **11**, 2419 (2004)]

• They may also prove useful for moment-implicit simulation-particle closures.

Numerical Algorithm

The NIMROD code has had two-fluid terms available in its Ohm's law, but the advance did not allow time-steps significantly larger than an explicit algorithm.

- Nonlinear computations of global extended-MHD activity in high-temperature plasmas are not possible if Δt is so restricted.
- We have considered / are considering different possible algorithms for the two-fluid system:
 - A **semi-implicit** advance of the magnetic field using a selfadjoint 4th-order spatial differential operator
 - A new **implicit leapfrog** algorithm
 - Implicit time-centering of the entire system of equations

A self-adjoint fourth-order differential operator has been recommended for the **semi-implicit** algorithm. [Harned and Mikic, JCP **83**, 1 (1989)]

• The time-advance is similar to the semi-implicit MHD algorithm, but a second semi-implicit operator is added for the Hall terms.

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



• As with advection, predictor/corrector steps are applied in the magnetic advance to provide forward centering of \mathbf{B}^* and \mathbf{J}^* in the Hall term.

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

The **implicit leapfrog** algorithm also has temporally staggered data, but linear terms are centered in the magnetic-field step.

• 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)

Again neglecting advection, dissipation, and
the separate n and T advances for clarity:
 $(\rho + \Delta t^2 L)\Delta \mathbf{V} = (\Delta t \mathbf{J}^{n+1/2} \times \mathbf{B}^{n+1/2} - \Delta t \nabla p^{n+1/2})$ $\mathbf{V}^{\mathbf{i}}$ $\mathbf{V}^{\mathbf{i}+1}$ $\Delta p = -\Delta t \gamma p^{n+1/2} \nabla \cdot \mathbf{V}^{n+1}$ $\mathbf{V}^{\mathbf{i}}$ $\mathbf{V}^{\mathbf{i}+1}$ $\mathbf{V}^{\mathbf{i}+1}$ $\Delta \mathbf{B} + \frac{\Delta t}{2} \nabla \times \frac{1}{ne} \left(\mathbf{J}^{n+1/2} \times \Delta \mathbf{B} + \frac{\nabla \times \Delta \mathbf{B}}{\mu_0} \times \mathbf{B}^{n+1/2} \right) =$ $\mathbf{N}^{\mathbf{i}+1/2}$ $\mathbf{N}^{\mathbf{i}+1/2}$ $\Delta t \nabla \times (\mathbf{V}^{n+1} \times \mathbf{B}^{n+1/2}) - \Delta t \nabla \times \frac{1}{ne} \left(\mathbf{J}^{n+1/2} \times \mathbf{B}^{n+1/2} - \nabla p_e \right)$ $\mathbf{N}^{\mathbf{i}+1/2}$ $\mathbf{N}^{\mathbf{i}+1/2}$

- The implicit Hall terms are linearized from the beginning of a time-step, resulting in second-order differential operators that are not self-adjoint.
- The advantage over full implicit time-centering is that the resulting algebraic systems are smaller.
- Full implicit time-centering has the best numerical properties, however.

Numerical Analysis

The normalizations and post-processing conventions 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,
$$v_A = \frac{c\Omega_i}{\omega_i} \Longrightarrow 1$$
, $\omega_{whistler} = kk_{\parallel}$

• For numerical analysis, the eigenvalue of the time-step operation is reported as

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

• θ is the angle between **k** and **B**₀.





NIMROD tests and numerical analysis show that the semiimplicit Hall advance is stable for EMHD.



 $\Delta t = 1, c_s^2 / v_A^2 = 0, f \text{ is P/C centering, and } s \text{ is SI coefficient.} (\theta = 0)$

Tests indicate numerical instability when the algorithm is applied to HMHD, however. Analysis also finds instability.



• The Hall advance of **B** is time-split from the MHD advance of **B**, and the Hall semi-implicit operator is applied to both predictor and corrector steps.

• Note that with the same parameters, 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.



 $f=0.5, s_{Hall}=0.25, \Delta t=1, c_s^2/v_A^2=0.1 \ (\theta=0.04\pi)$

- Here, the Hall semi-implicit operator is only applied to the corrector step.
- Unfortunately, the NIMROD implementation found another numerical stability problem when applied to inhomogeneous equilibria.

The leapfrog with implicit magnetic advance is stable for basic HMHD waves.



Gyroviscosity, V_0 , and J_0 have been added to the analyses.



• Here, analytical dispersion relations are shown with $c_s^2 / v_A^2 = 0.1$ and $V_0 = v_A / 3$. • J_0 is added as a separate drift flow at $v_A / 2$, retaining homogeneous **B**₀.



Predictor-corrector advection is unstable with \mathbf{J}_0 and is conditionally stable with $\mathbf{J}_0=\mathbf{0}$.



Returning to HMHD without G.V. and flow, we find somewhat more numerical dispersion in slow waves (for $\omega \Delta t > 0.5$) for leapfrog than implicit time-centering.



NIMROD Implementation

- The new leapfrog scheme is being implemented in NIMROD.
 - Linear terms for Hall, gyroviscosity, and thermal drifts for $T_i \neq T_e$ have been added.
- All of these terms require solution of non-Hermitian matrices.
- For 2D problems, we are able to solve non-Hermitian matrices using to the SuperLU software library.

• For nonlinear 3D problems, we will use 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.

Modeling: Time-advance algorithms (continued)

• A full implicit leapfrog separates pressure evolution into number density and temperature equations.

$$\begin{split} m_{\mathbf{i}} n^{j+1/2} & \left(\frac{\Delta \mathbf{V}}{\Delta t} + \frac{1}{2} \mathbf{V}^{j} \cdot \nabla \Delta \mathbf{V} + \frac{1}{2} \Delta \mathbf{V} \cdot \nabla \mathbf{V}^{j} \right) - \Delta t L^{j+1/2} (\Delta \mathbf{V}) + \nabla \cdot \Pi_{\mathbf{i}} (\Delta \mathbf{V}) = \mathbf{J}^{j+1/2} \times \mathbf{B}^{j+1/2} \\ & - m_{\mathbf{i}} n^{j+1/2} \mathbf{V}^{j} \cdot \nabla \mathbf{V}^{j} - \nabla p^{j+1/2} - \nabla \cdot \Pi_{\mathbf{i}} (\mathbf{V}^{j}) \\ & \frac{\Delta n}{\Delta t} + \frac{1}{2} \mathbf{V}^{j+1} \cdot \nabla \Delta n = -\nabla \cdot \left(\mathbf{V}^{j+1} \cdot n^{j+1/2} \right) \end{split}$$

$$\frac{3n}{2} \left(\frac{\Delta T_{\alpha}}{\Delta t} + \frac{1}{2} \mathbf{V}_{\alpha}^{j+1} \cdot \nabla \Delta T_{\alpha} \right) + \frac{1}{2} \nabla \cdot \mathbf{q}_{\alpha} (\Delta T_{\alpha}) = -\frac{3n}{2} \mathbf{V}_{\alpha}^{j+1} \cdot \nabla T_{\alpha}^{j+1/2} - n T_{\alpha}^{j+1/2} \nabla \cdot \mathbf{V}_{\alpha}^{j+1} - \nabla \cdot \mathbf{q}_{\alpha} (T_{\alpha}^{j+1/2}) + Q_{\alpha}^{j+1/2}$$

$$\frac{\Delta \mathbf{B}}{\Delta t} + \frac{1}{2} \mathbf{V}^{j+1} \cdot \nabla \Delta \mathbf{B} + \frac{1}{2} \nabla \times \frac{1}{ne} \left(\mathbf{J}^{j+1/2} \times \Delta \mathbf{B} + \Delta \mathbf{J} \times \mathbf{B}^{j+1/2} \right) + \frac{1}{2} \nabla \times \eta \Delta \mathbf{J}$$
$$= -\nabla \times \left[\frac{1}{ne} \left(\mathbf{J}^{j+1/2} \times \mathbf{B}^{j+1/2} - \nabla p_{\mathbf{e}} \right) - \mathbf{V}^{j+1} \times \mathbf{B}^{j+1/2} + \eta \mathbf{J}^{j+1/2} \right]$$

• The *T* and **B** advances can be predicted and corrected to center all coefficients in time.

Test Results

• Using HMHD to solve a 0-beta tearing mode benchmark for resistive MHD leads to no rotation (good) and a slightly increased growth rate at a Hall parameter of 0.2.





• The three lowest– Δt results indicate a convergence rate of 2.0. Dissipation coefficients are time-centered.

• Two-fluid tearing calculations in slab geometry are shown in poster LP1.00113 by H. Tian. A finite-beta version of the cylindrical tearing test shows rotation and a reduced growth rate.

• Mode parity changes when the equilibrium has finite pressure.





• Rotation is apparent from the eigenfunction's flow velocity field.

• At S=10⁵, we find: $\gamma \tau_A = 1.2 \times 10^{-2}$ for MHD $\gamma \tau_A = 8.6 \times 10^{-3}$ and $\Omega \tau_A = 2.3 \times 10^{-2}$ HMHD $\gamma \tau_A = 4.3 \times 10^{-3}$ and $\Omega \tau_A = 2.6 \times 10^{-2}$ HMHD+GV

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.

• 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 $t=23 \ \Omega_i^{-1}$ are the open geometry of the reconnecting magnetic flux (left) and the quadrupole out-of-plane magnetic field (right).

• See the poster LP1.00113 (Tian) for nonlinear results on equilibria with a large guide field.

Out-of-plane current density and poloidal flux at $t=23-24 \Omega_i^{-1}$ 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 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.

• We welcome recommendations for two-fluid benchmark computations that have analytical solutions.

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