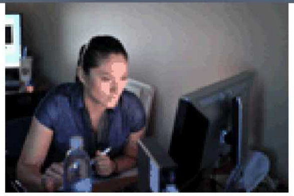
SAND2019-12542C

Implicit-Explicit Time Integration for a Mixed CG-DG Multi-Fluid Plasma Formulation



PRESENTED BY

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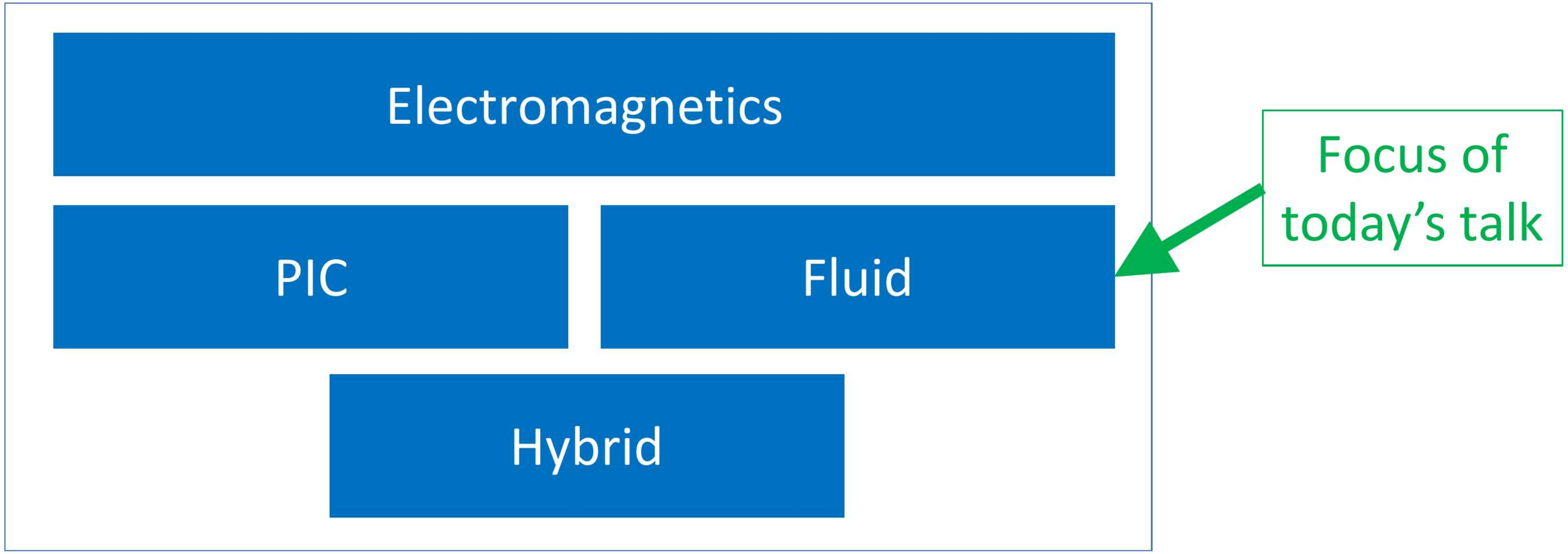
EMPIRE: A hierarchy of capabilities



- <u>EMPIRE’s goal</u>: Accurately simulate plasmas across regimes on next-generation exascale computing platforms
- Expand the range of electromagnetic plasma simulation and Z-power flow applications that we can simulate with high confidence and fidelity

Multiple time scales (yikes!)

Plasma models are replete with multi-scale phenomena:

- Strongly dependent on species mass, density, and temperature
- Speed of light, plasma and cyclotron frequency are often stiff!
- Can be broken into frequency, velocity, and diffusion (not used here) scales:

Plasma frequency

$$\omega_{p\alpha} = \sqrt{\frac{q_\alpha^2 n_\alpha}{m_\alpha \epsilon_0}}$$

Cyclotron frequency

$$\omega_{c\alpha} = \frac{q_\alpha B}{m_\alpha}$$

Collision frequency

$$\nu_{\alpha\beta} \sim \frac{n_\beta}{\sqrt{m_\alpha} T_\alpha^{\frac{3}{2}}} \frac{1 + \frac{m_\alpha}{m_\beta}}{\left(1 + \frac{m_\alpha}{m_\beta}\frac{T_\beta}{T_\alpha}\right)^{\frac{3}{2}}}$$

Flow velocity

$$u_\alpha$$

Speed of sound

$$v_{s\alpha} = \sqrt{\frac{\gamma P_\alpha}{\rho_\alpha}}$$

Speed of light

$$c \gg u_\alpha, v_{s\alpha}$$

Momentum diffusivity

$$\upsilon_\alpha = \frac{\mu_\alpha}{\rho_\alpha}$$

Thermal diffusivity

$$\kappa_\alpha \sim \frac{k_\alpha}{\rho_\alpha}$$

Take home: These plasmas are hard to simulate!

Multi-Fluid Plasma Formulation

- Multi-species Euler coupled to Maxwell
- Strong collisions terms
- Maxwell involutions must be enforced

5-Moment Fluid

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) = \sum_{\text{srcs}} m_\alpha \Gamma^{\text{src}} - \sum_{\text{sinks}} m_\alpha \Gamma^{\text{sink}}$$

$$\frac{\partial (\rho_\alpha \mathbf{u}_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha + p_\alpha \boldsymbol{I} + \Pi_\alpha) = \frac{q_\alpha}{m_\alpha} \rho_\alpha (\mathbf{E} + \mathbf{u}_\alpha \times \mathbf{B}) + \sum_{\text{srcs}} m_\alpha \mathbf{u}_{\text{src}} \Gamma^{\text{src}} - \sum_{\text{sinks}} m_\alpha \mathbf{u}_\alpha \Gamma^{\text{sink}} + \sum_{\beta \neq \alpha} \mathbf{R}^{\alpha,\beta}$$

$$\frac{\partial \mathcal{E}_\alpha}{\partial t} + \nabla \cdot ((\mathcal{E}_\alpha + p_\alpha)\mathbf{u}_\alpha + \mathbf{u}_\alpha \cdot \Pi_\alpha + \mathbf{h}_\alpha) = \frac{q_\alpha}{m_\alpha} \rho_\alpha \mathbf{E} \cdot \mathbf{u}_\alpha + \sum_{\beta \neq \alpha} \left(\mathbf{u}_\alpha \mathbf{R}^{\alpha,\beta} + Q^{\alpha,\beta} \right) + \frac{1}{2} \sum_{\text{srcs}} m_\alpha u_{\text{src}}^2 \Gamma^{\text{src}} - \frac{1}{2} \sum_{\text{sinks}} m_\alpha u_\alpha^2 \Gamma^{\text{sink}}$$

Maxwell Equations

$$\frac{\partial \mathbf{E}}{\partial t} - c^2 \nabla \times \mathbf{B} = -\frac{1}{\epsilon_0} \sum_\alpha \frac{q_\alpha}{m_\alpha} \rho_\alpha \mathbf{u}_\alpha \qquad \nabla \cdot \mathbf{E} = \frac{1}{\epsilon_0} \sum_\alpha \frac{q_\alpha}{m_\alpha} \rho_\alpha$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0 \qquad \nabla \cdot \mathbf{B} = 0$$

Important to satisfy involutions numerically

Discretization Tools

We have (at least) two major challenges:

1. Involutions from Maxwell's equations
2. Multiple time scales

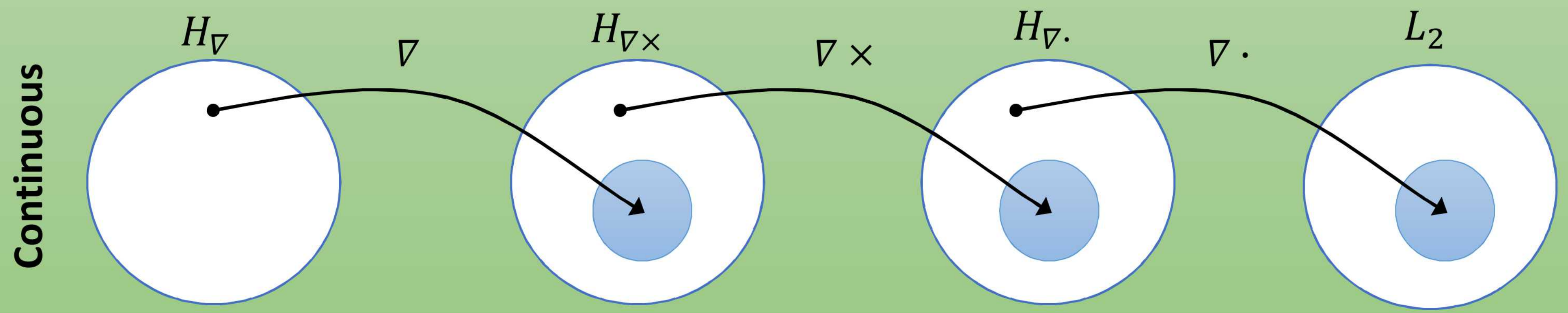
We will attack each of these in turn with two discretization tools

1. "Exact-Sequence" discretizations to structurally enforce involutions
2. Implicit-Explicit (IMEX) time integration to handle multiple time scales

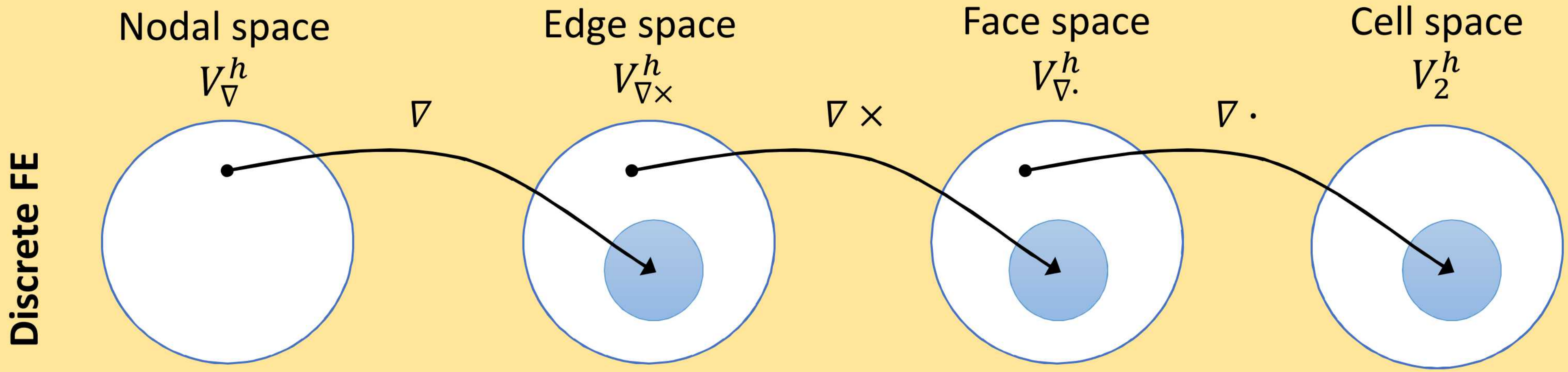
The interesting part is how these interact! (Not to mention boundary conditions! Which I won't talk about)

Exact-Sequence Discretizations

Function spaces posses an exact sequence property where the derivative maps into the next space, e.g.:



Exact sequence finite elements have been constructed[1] (note $V_*^h \subset H_*$):

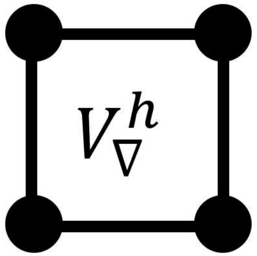


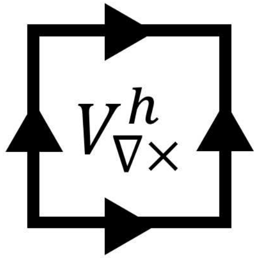
[1]Bochev, P., Edwards, H. C., Kirby, R. C., Peterson, K., & Ridzal, D. (2012). Solving PDEs with intrepid. *Scientific Programming*, *20*(2), 151-180.

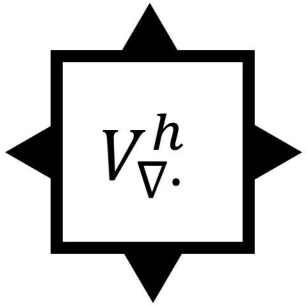
Exact-Sequence and Multi-Fluids

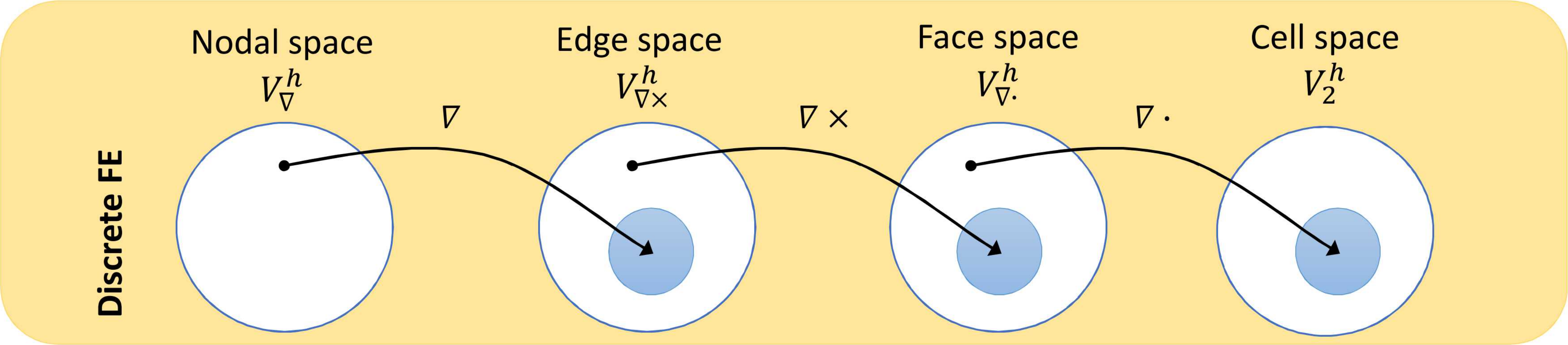
Discretization:

Fields continuous by construction (CG)

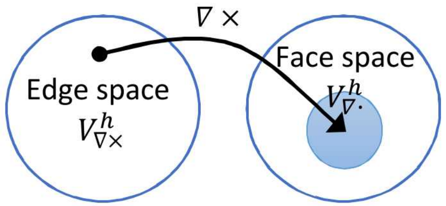
$\begin{bmatrix} \rho_\alpha \\ \rho_\alpha u_\alpha \\ \mathcal{E}_\alpha \end{bmatrix} \in$ 

$E \in$ 

$B \in$ 



No magnetic monopoles example: Let $\mathbf{B}^h \in V_{\nabla\cdot}^h$ and $\mathbf{E}^h \in V_{\nabla\times}^h$, then the argument is straightforward and follows the continuous case:



$$\nabla \cdot \left(\frac{\partial \mathbf{B}^h}{\partial t} + \nabla \times \mathbf{E}^h \right) = 0 \Rightarrow \nabla \cdot \partial_t \mathbf{B}^h = 0$$

$$\Rightarrow \nabla \cdot \mathbf{B}^h = 0 \text{ (assuming satisfied at } t = 0)$$

Enforcing Gauss Law

Discrete Weak Form	Continuous Strong Form
Assume: Let $\mathbf{E}^h \in V^h_{\nabla\times}$ and $\rho^h_\alpha, \rho_\alpha \mathbf{u}^h_\alpha, \mathcal{E}^h_\alpha \in V^h_\nabla$, then using the weak forms:	
$\int \partial_t \mathbf{E}^h \cdot \psi^h - \mathbf{B}^h \cdot \nabla \times \psi^h = -\frac{1}{\epsilon_0}\sum_\alpha \frac{q_\alpha}{m_\alpha}\int \rho^h_\alpha \mathbf{u}^h_\alpha \cdot \psi^h \ \forall \psi^h \in V^h_{\nabla\times}$	$\partial_t \mathbf{E} - c^2 \nabla \times \mathbf{B} = -\frac{1}{\epsilon_0}\sum_\alpha \frac{q_\alpha}{m_\alpha}\rho_\alpha \mathbf{u}_\alpha$
$\int \partial_t \rho^h_\alpha \phi^h = \int \rho^h_\alpha \mathbf{u}^h_\alpha \cdot \nabla \phi^h \ \forall \phi^h \in V^h_\nabla$	$\partial_t \rho_\alpha + \nabla \cdot (\rho_\alpha u_\alpha) = 0$

Derivation

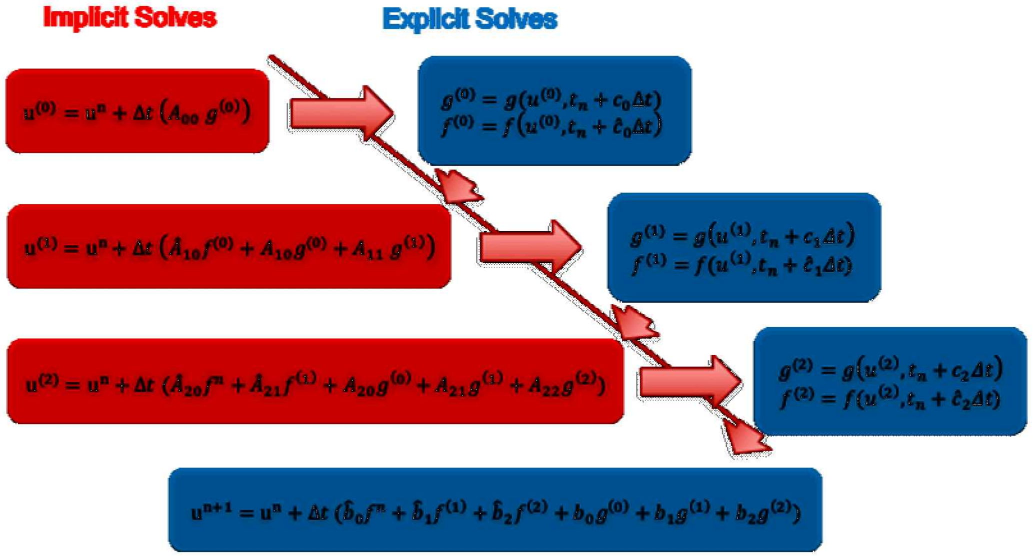
1. $-\int \partial_t \mathbf{E}^h \cdot \nabla \phi^h = \frac{1}{\epsilon_0}\sum_\alpha \frac{q_\alpha}{m_\alpha}\int \rho^h_\alpha \mathbf{u}^h_\alpha \cdot \nabla \phi^h$ — Exact Sequence: $\nabla \phi^h \in V^h_{\nabla\times}$ (take divergence) — $\partial_t \nabla \cdot \mathbf{E} = -\frac{1}{\epsilon_0}\sum_\alpha \frac{q_\alpha}{m_\alpha}\nabla \cdot (\rho_\alpha \mathbf{u}_\alpha)$

2. $= \frac{1}{\epsilon_0}\sum_\alpha \frac{q_\alpha}{m_\alpha}\int \partial_t \rho^h_\alpha \phi^h$ — Apply Continuity — $= \frac{1}{\epsilon_0}\sum_\alpha \frac{q_\alpha}{m_\alpha}\partial_t \rho_\alpha$

3. $-\int \mathbf{E}^h \cdot \nabla \phi^h = \frac{1}{\epsilon_0}\sum_\alpha \frac{q_\alpha}{m_\alpha}\int \rho^h_\alpha \phi^h$ — (weak) Gauss' Law (strong) — $\nabla \cdot \mathbf{E} = \frac{1}{\epsilon_0}\sum_\alpha \frac{q_\alpha}{m_\alpha}\rho_\alpha$

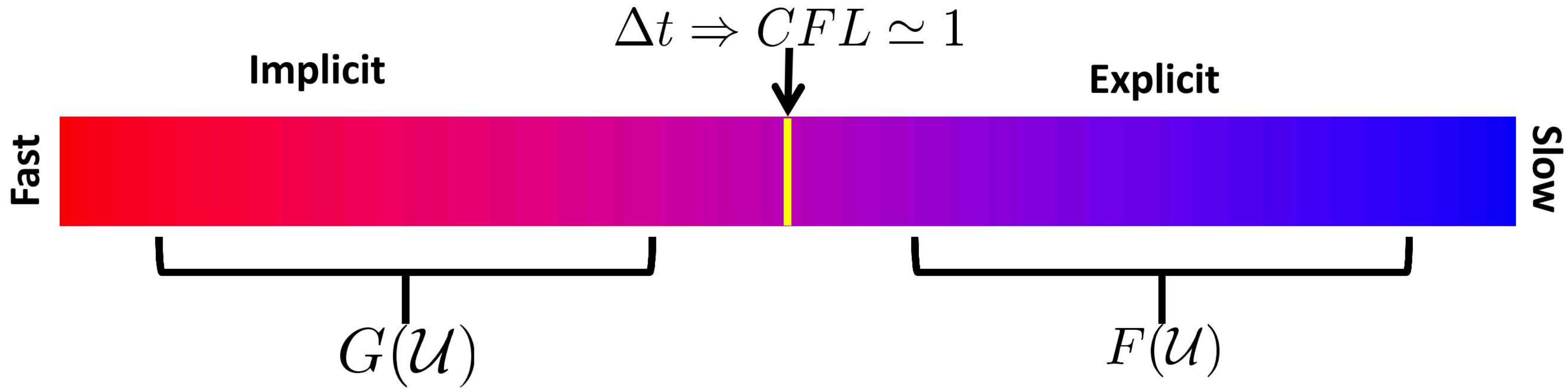
Implicit-Explicit (IMEX) Time Integration

3 Stage IMEX-RK Algorithm



IMEX methods split fast and slow modes

- Implicit terms solve for stiff modes (plasma oscillation, speed of light)
- Explicit terms are accurately resolved
- Combine with block/physics-based preconditioning for implicit solves
- IMEX assumes an additive decomposition: $\dot{\mathcal{U}} + F(\mathcal{U}) + G(\mathcal{U}) = 0$



Fast/Stiff/Implicit modes in plasma model

Stiff Modes:

- Speed of light
- Plasma Oscillation
- Collisions
- Cyclotron frequency

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) = \sum_{\text{srcs}} m_\alpha \Gamma^{\text{src}} - \sum_{\text{sinks}} m_\alpha \Gamma^{\text{sink}}$$

$$\frac{\partial (\rho_\alpha \mathbf{u}_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha + p_\alpha I + \Pi_\alpha) = \frac{q_\alpha}{m_\alpha} \rho_\alpha (\mathbf{E} + \mathbf{u}_\alpha \times \mathbf{B})$$

$$+ \sum_{\text{srcs}} m_\alpha \mathbf{u}_{\text{src}} \Gamma^{\text{src}} - \sum_{\text{sinks}} m_\alpha \mathbf{u}_\alpha \Gamma^{\text{sink}} + \sum_{\beta \neq \alpha} \mathbf{R}^{\alpha,\beta}$$

$$\frac{\partial \mathbf{E}}{\partial t} - c^2 \nabla \times \mathbf{B} = -\frac{1}{\epsilon_0} \sum_\alpha \frac{q_\alpha}{m_\alpha} \rho_\alpha \mathbf{u}_\alpha$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

- Speed of light arises from coupling of electromagnetic field: explicit CFL $\sim c\Delta t/\Delta x$
- Plasma oscillation arises from Ampere's law to momentum conservation: explicit CFL $\sim \Delta t$
- Collisions explicit CFL$\sim \Delta t$
- Cyclotron frequency explicit CFL$\sim |\mathrm{B}| \Delta t$

$\nabla \cdot (\rho_\alpha \mathbf{u}_\alpha)$ If the plasma oscillation is implicit, then the mass flux needs to be implicit to maintain Gauss' law

Two Fluid Plasma Vortex (from Drekar)*

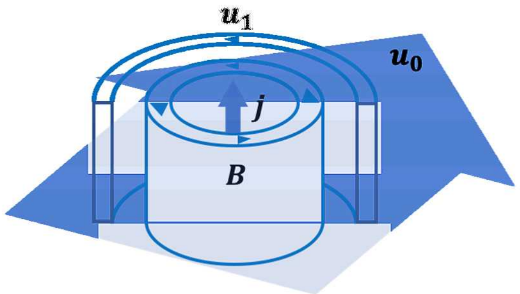
Two fluid plasma vortex in MHD limit

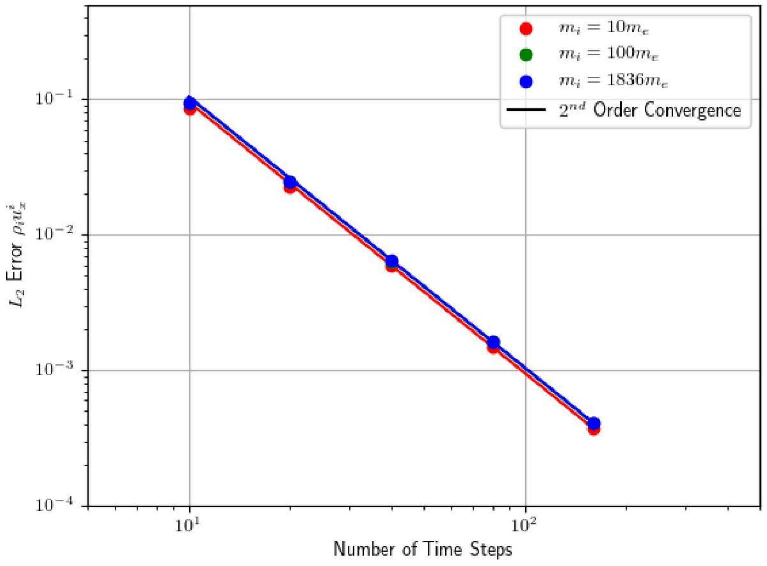
- IMEX time discretization
- Compatible spatial discretization

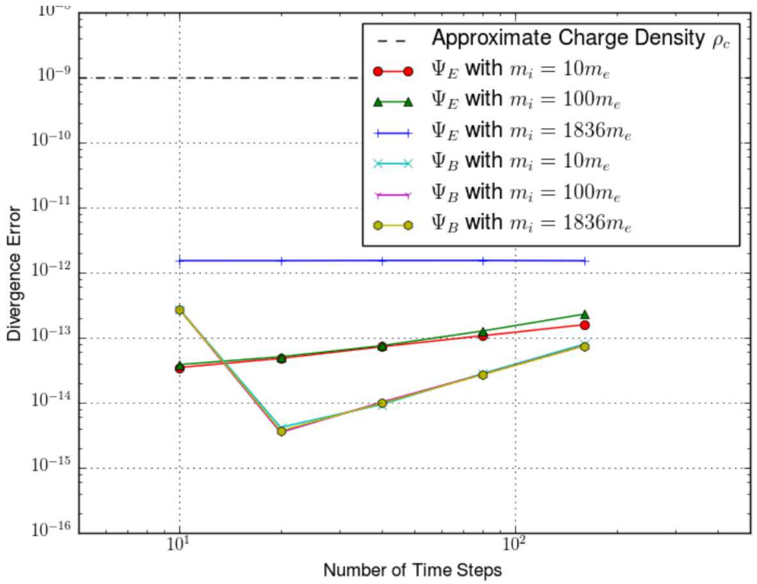
	Electrons	Ions
$\omega_p \Delta t$	**23 - 270**	**0.55 - 6.3**
$\omega_c \Delta t$	**1 - 12**	$\mathbf{5.5 \cdot 10^{-4} - 6.3 \cdot 10^{-3}}$
$v_s \frac{\Delta t}{\Delta x}$	0.25	$5.7 \cdot 10^{-3}$
$c \frac{\Delta t}{\Delta x}$	**6.3**	

Achieves 2nd order conv, satisfies involutions:

- $\nabla \cdot E = \rho$ (weakly enforced)
- $\nabla \cdot B = 0$ (strongly enforced)





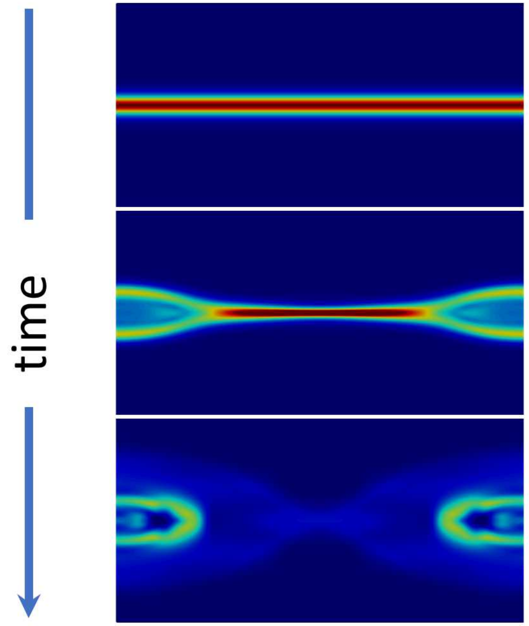


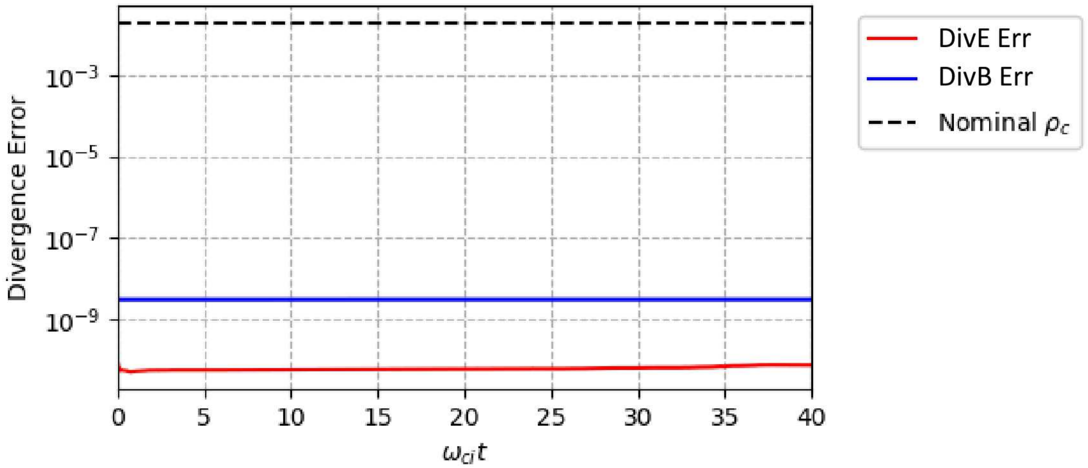
*See Miller, Cyr, Shadid, Kramer, Phillips, Conde, Pawlowski., IMEX and exact sequence discretization of the multi-fluid plasma model, in press JCP, 2019

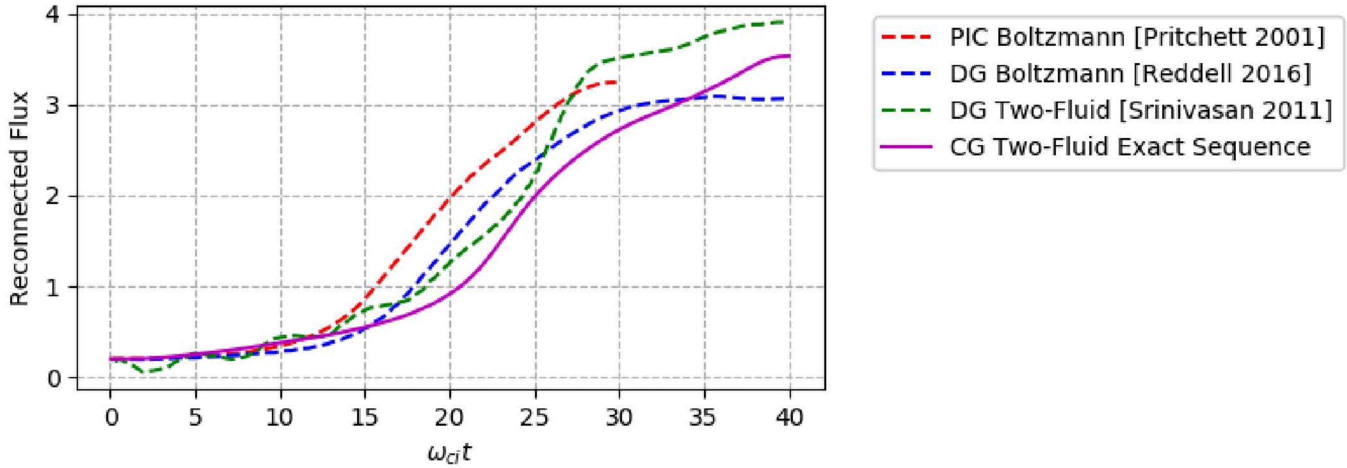
GEM Challenge Problem (from Drekar)*

Using described spatial and temporal discretizations

- Testing magnetic reconnection using multi-fluid
- As run, unstabilized (recent improvements extend this)
- Qualitative agreement with existing reconnection results
- Preserves no magnetic monopoles and charge density involutions







*See Miller, Cyr, Shadid, Kramer, Phillips, Conde, Pawlowski., IMEX and exact sequence discretization of the multi-fluid plasma model, in press JCP, 2019

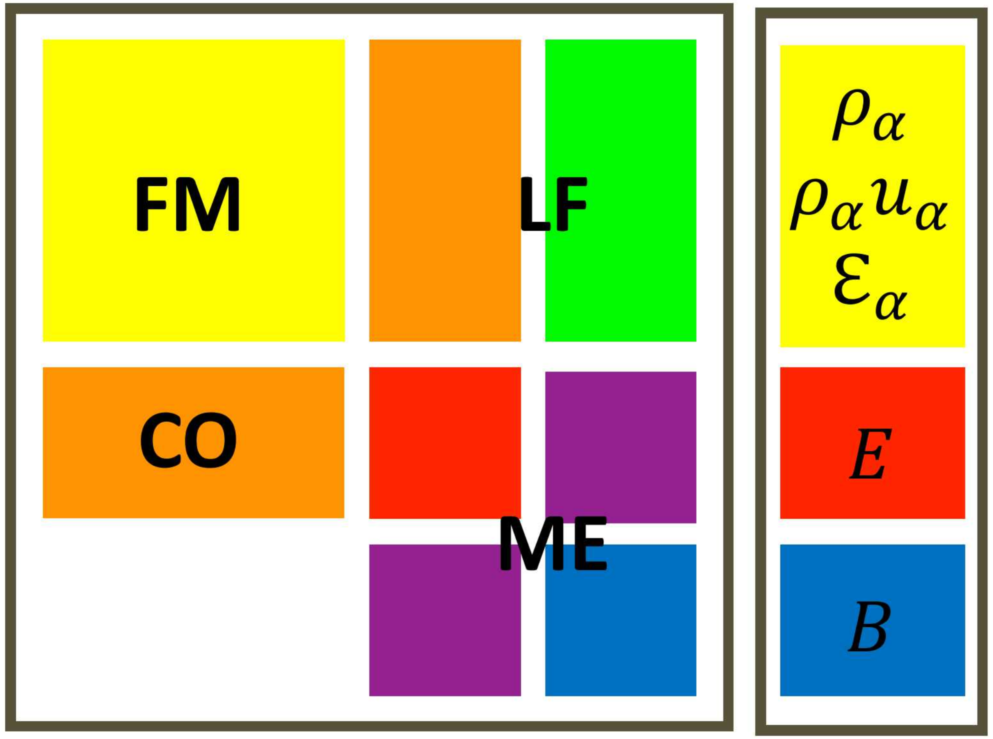
Nonlinear Algorithm

For IMEX we have to solve a nonlinear problem:

- We are using Newton-Krylov
- To get scalability we must precondition*

$$J_k \Delta x_k = -f(x_k)$$
$$x_k = x_k + \Delta x_k$$

$$J_k v =$$



Nonlinear terms

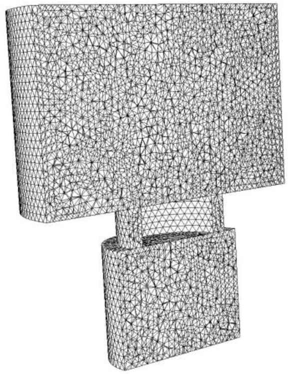
- Fluid matrix (mass like)
- Lorentz Force

Linear terms

- Maxwell equations
- Current Operator

*E. G. Phillips, J. N. Shadid, E. C. Cyr, S. T. Miller, Enabling Scalable Multi-Fluid Plasma Simulations through Block Preconditioning, Accepted to Lecture Notes in Computational Science and Engineering, 2019.

Nonlinear Algorithm: Maxwell Solver

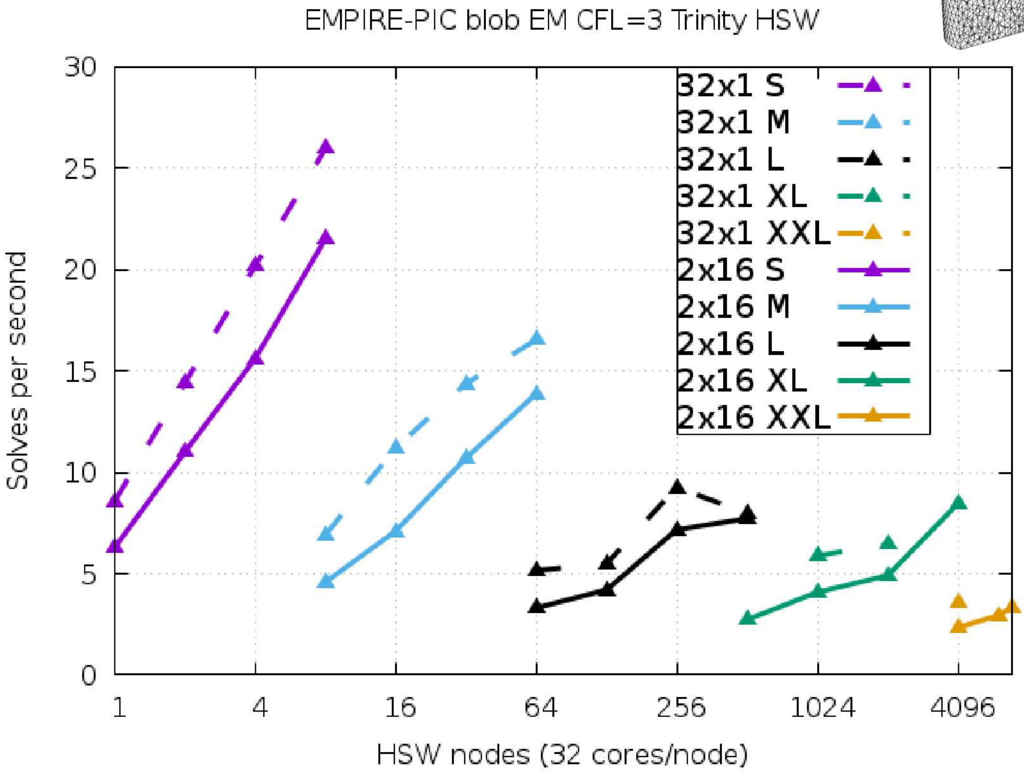


We (Sandia royal*) have made good progress in solving the Maxwell system

- Preconditioner exploits exact-sequence discretization structure

Size	#Elts	#Nodes	#Edges	#Faces
S	337k	60k	406k	683k
M	2.68M	462k	3.18M	5.40M
L	20.7M	3.51M	24.4M	41.6M
XL	166M	27.9M	195M	333M
XXL	1.332B	223M	1.56B	2.67B

Solves per second



- Trinity HSW: scaling study to **entire HSW** partition (9375 nodes, 300,000 cores)
- Trinity KNL: scaling study to **99.2% KNL** partition (9900 nodes, 633,600 cores)

* **Credit (and apologies) to:** Jonathan Hu, Christian Glusa, Paul Lin, Edward Phillips, Matt Bettencourt, James Elliott, Chris Siefert, Siva Rajamanickam

Examining the IMEX Scheme

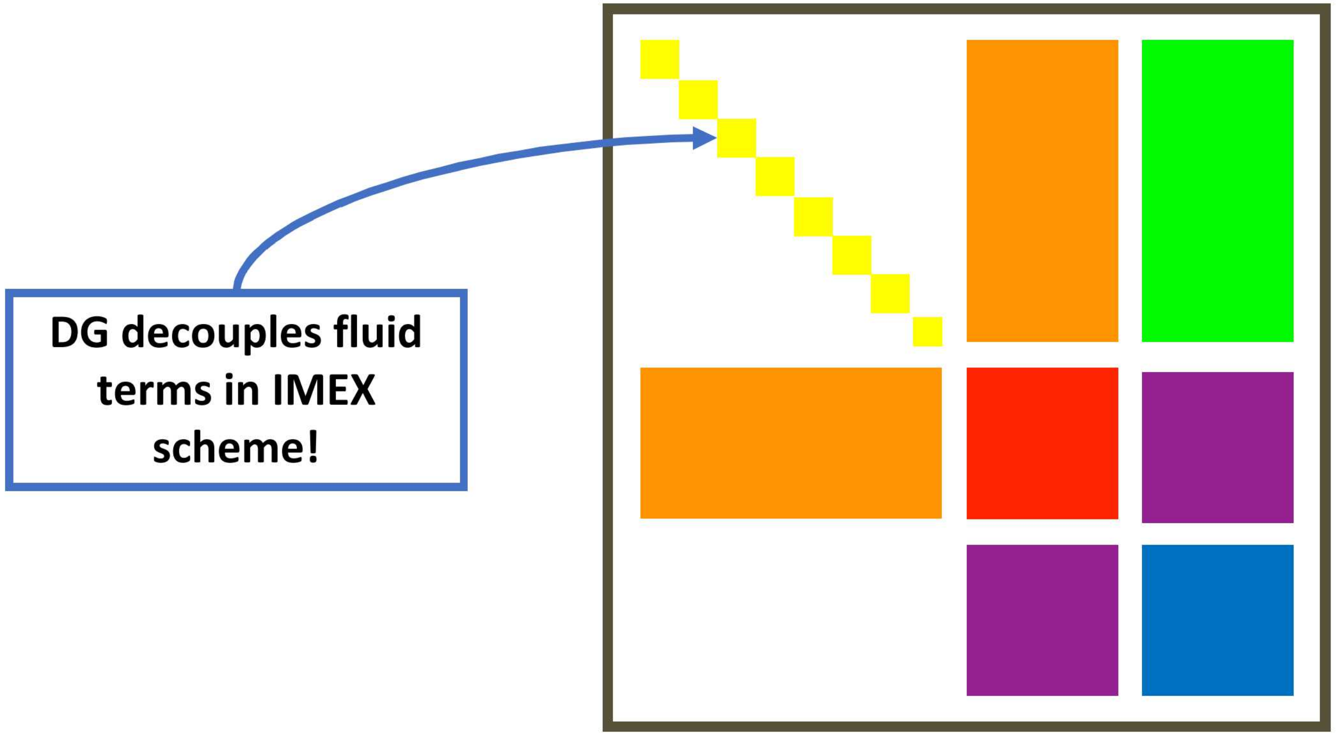
- Fluid matrix is mass matrix (CG fluids gives global coupling)
- Maxwell solver is effective (and should remain unperturbed)
  - Handles speed of light coupling
- Important to get plasma frequency and cyclotron frequency coupling
  - Handled by preconditioning
  - These are local (ODE-like) coupling terms
- Many linear operators that can be computed once and reused

We will try to construct a scheme:

- Take advantage of only local coupling in fluid operators
- Maxwell solver is effective (and should remain unperturbed)
- Handle plasma/cyclotron frequency coupling efficiently
- Reduce the number of recomputations required per nonlinear step

Introduce DG Fluids/CG Maxwell

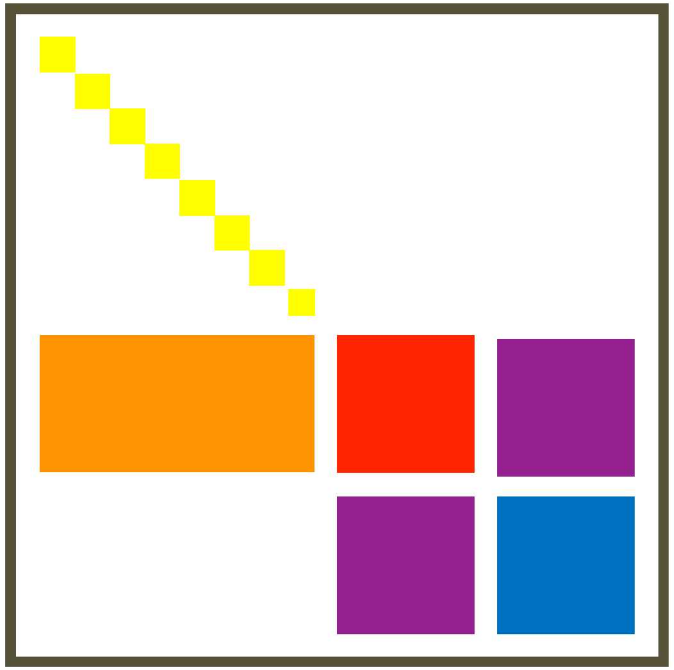
- DG Fluids will make the fluid contribution block diagonal on each element
  - Local nature of DG discretization
  - IMEX splitting choice
- Support for involutions still preserved
  - No Magnetic monopoles is the same
  - Weak enforcement of Gauss' law works (math is more complex)



Quasi-Newton Method

Typically I would do Newton-Krylov, but…

Block lower Gauss-Seidel



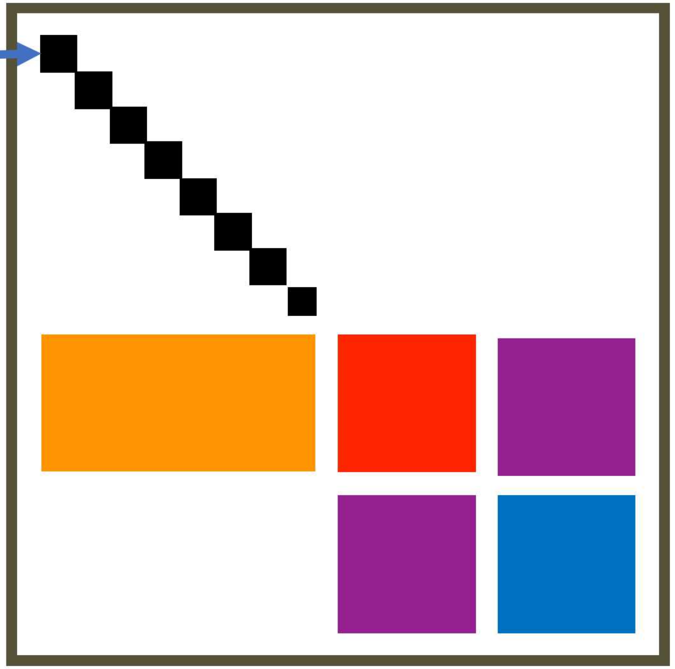
- ✓ Triangular solve
- ✓ Leverages Maxwell solver
- ✓ Block diagonal fluid solve
- ✓ Implicit cyclotron frequency
- ✗ Implicit plasma frequency

Couple in plasma frequency using Schur complement

Both schemes:

- Simplified linear construction
- Only inner Maxwell Krylov solve
- Will require more iterations than Newton
- Maybe cheaper then Newton

Block GS with Schur Complement



- ✓ Triangular solve
- ✓ Leverages Maxwell solver
- ✓ Block diagonal fluid solve
- ✓ Implicit cyclotron frequency
- ✓ Implicit plasma frequency

Plasma Frequency Schur Complement

To step over plasma frequency we must work it into the "black" part of the approximate Jacobian.

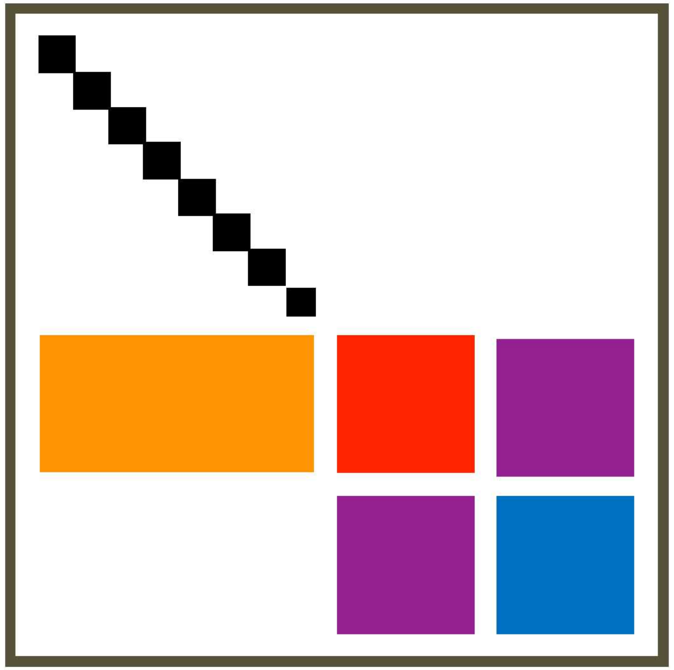
- Mode derived from coupling Ampere's law and momentum equation

$$\left.\begin{aligned} \frac{\partial(\rho_\alpha \mathbf{u}_\alpha)}{\partial t} &= \frac{q_\alpha}{m_\alpha}\rho_\alpha \mathbf{E} \\ \frac{\partial \mathbf{E}}{\partial t} &= -\frac{1}{\epsilon_0}\frac{q_\alpha}{m_\alpha}(\rho_\alpha \mathbf{u}_\alpha) \end{aligned}\right\} \frac{\partial^2(\rho_\alpha \mathbf{u}_\alpha)}{\partial t^2} = -\frac{1}{\epsilon_0}\frac{q_\alpha^2}{m_\alpha^2}\rho_\alpha(\rho_\alpha \mathbf{u}_\alpha)$$

- We apply the local Schur complement to the fluid contribution as a correction

$$\frac{(\rho_\alpha \mathbf{u}_\alpha)}{\Delta t} + \underbrace{\Delta t \frac{1}{\epsilon_0}\frac{q_\alpha}{m_\alpha}\rho_\alpha \sum_\beta \frac{q_\beta}{m_\beta}\rho_\beta \mathbf{u}_\beta}_{\text{Correction}}$$

Block GS with Schur Complement



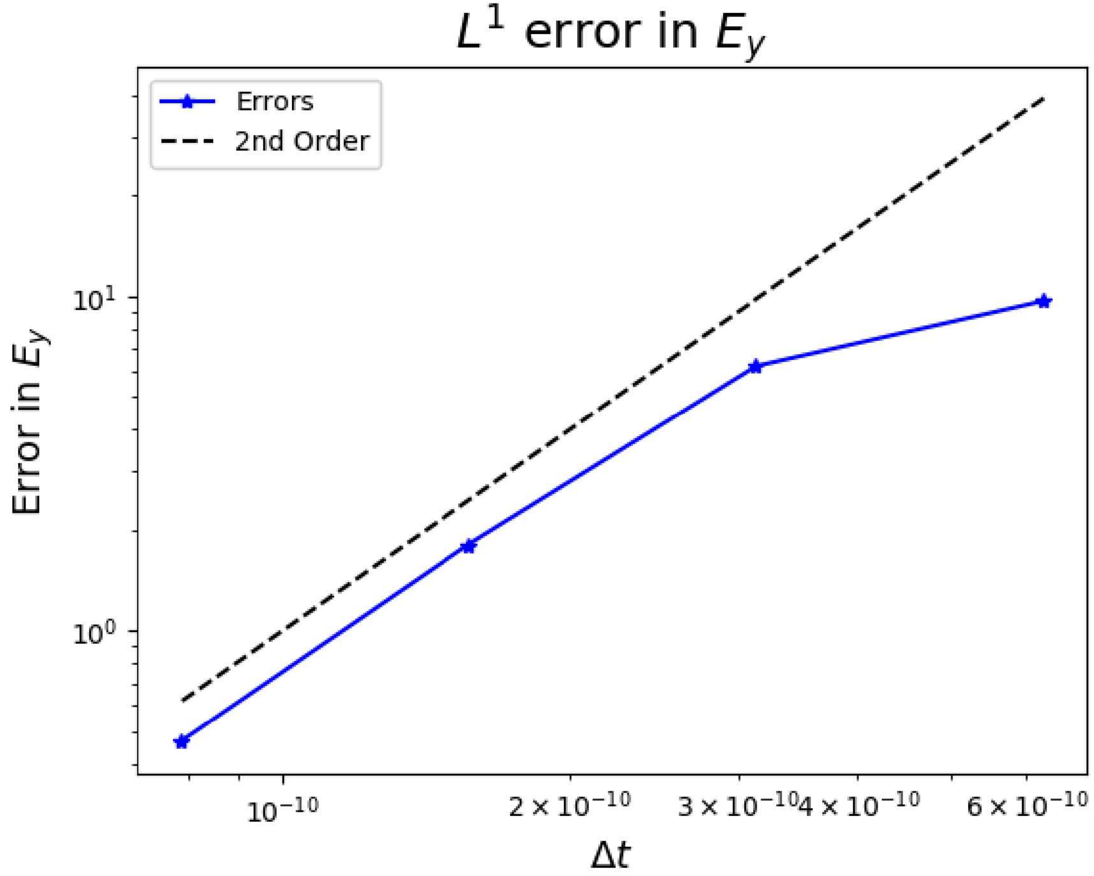
(Unlike the "analysis" above, we use the full current in the Schur complement correction)

O-Wave Convergence Results (EMPIRE-Fluid)

A linear wave verification test*

- Refining in space and time
- Running IMEX SSPRK2

Analytical Solution



* S. Miller, J. Niederhaus, R.M.J. Kramer, and G. Radtke, Robust Verification of the Multi-Fluid Plasma Model in Drekar.. United States: N. p., 2017. Web.

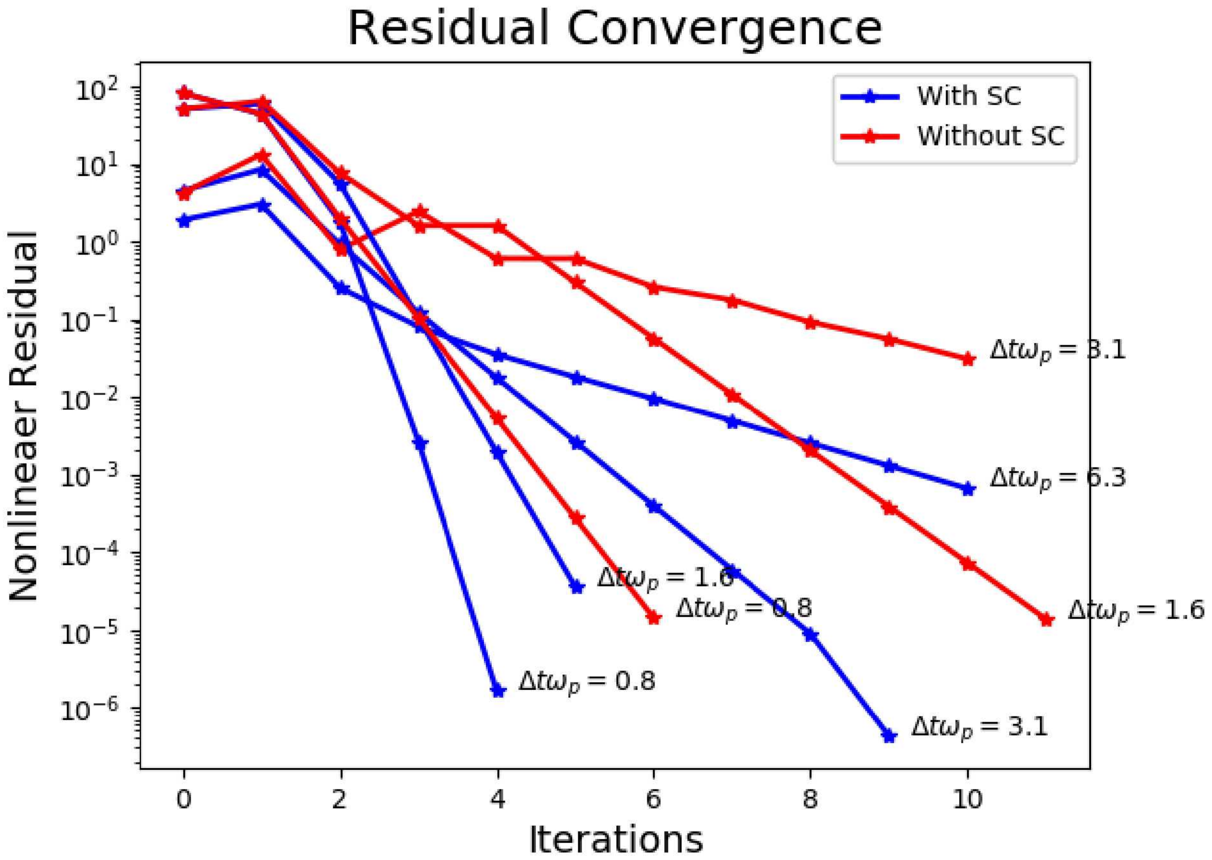
O-Wave Nonlinear Solver (EMPIRE-Fluid)

Adding Schur complement improves nonlinear convergence

- Still has strong growth in iteration count with increasing time steps
- Cost/benefit tradeoff study against Newton-Krylov with similar preconditioner required

Each nonlinear iteration requires:

1. Reconstruction of fluid Jacobian inverse
2. Solve of Maxwell system



One More Trick: Anderson Acceleration

Anderson Acceleration

- Requires same computations as Quasi-Newton
- Fixed point around $x = g(x)$
- Combines multiple nonlinear steps improving convergence
- Typically less complex to implement than full Newton
- Walker and Ni, SINUM 2011: **"Essentially equivalent" to GMRES**

Algorithm AA: Anderson Acceleration

GIVEN x_0 AND $m \geq 1$.
SET $x_1 = g(x_0)$.
FOR $k = 1, 2, \ldots$ (UNTIL CONVERGED) DO:
SET $m_k = min\{m, k\}$.
DETERMINE $\gamma^{(k)} = (\gamma_0^{(k)}, \ldots, \gamma_{m_k-1})^T$ THAT SOLVES
$min_{\gamma^{(k)}=(\gamma_0^{(k)},\ldots,\gamma_{m_k-1})^T} \|f_k - \mathcal{F}_k\|_2$.
SET $x_{k+1} = g(x_k) - \mathcal{G}_k \gamma^{(k)}$.

$f_i = g(x_i) - x_i$
$\mathcal{F}_k = (\Delta f_{k-m_k}, \ldots, \Delta f_{k-1})$ with $\Delta f_i = f(x_{i+1}) - f(x_i)$.
$\mathcal{G}_k = (\Delta g_{k-m_k}, \ldots, \Delta g_{k-1})$ with $\Delta g_i = g(x_{i+1}) - g(x_i)$.

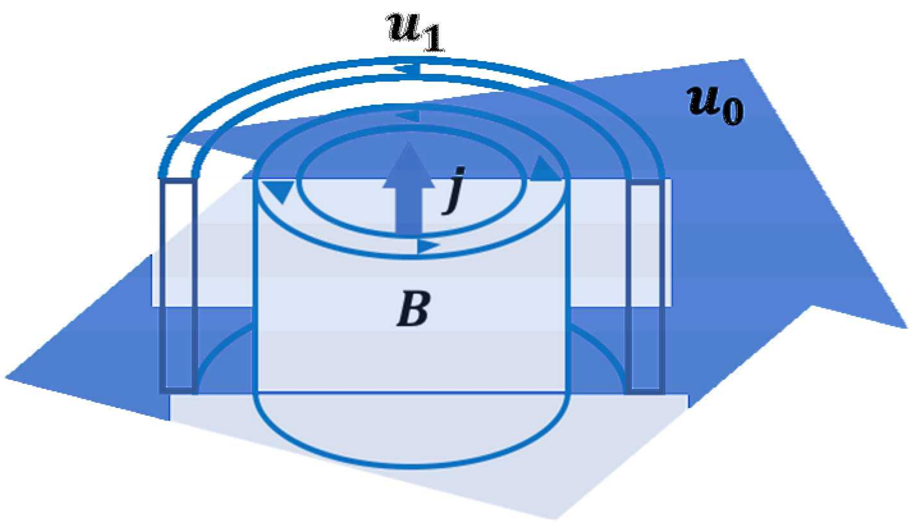
Anderson, ACM 1965

This is what I remember (understand) about Anderson (thanks Homer!). If you want more details about Anderson, talk with Roger Pawlowski and then tell me what you learned!

Two Fluid Plasma Vortex

Two fluid plasma vortex in MHD limit

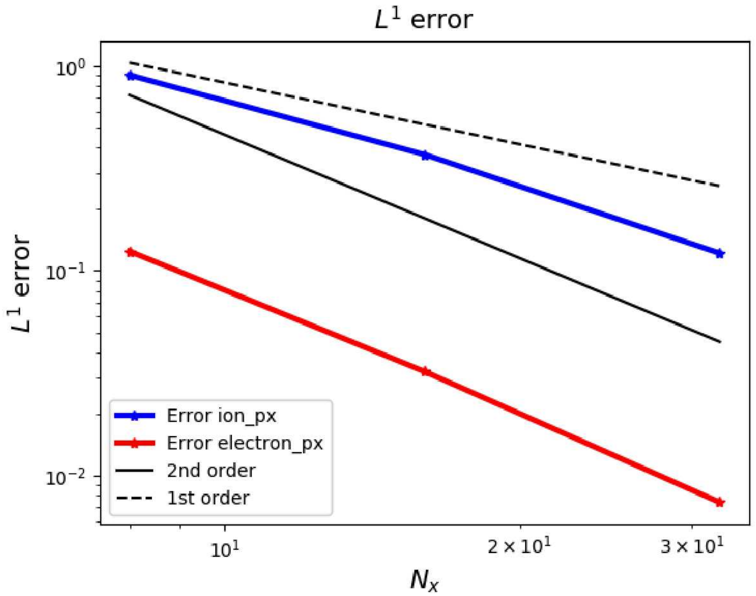
- IMEX time discretization, DG fluid discretization, CG Maxwell discretization
- Using Schur-Complement in all simulations

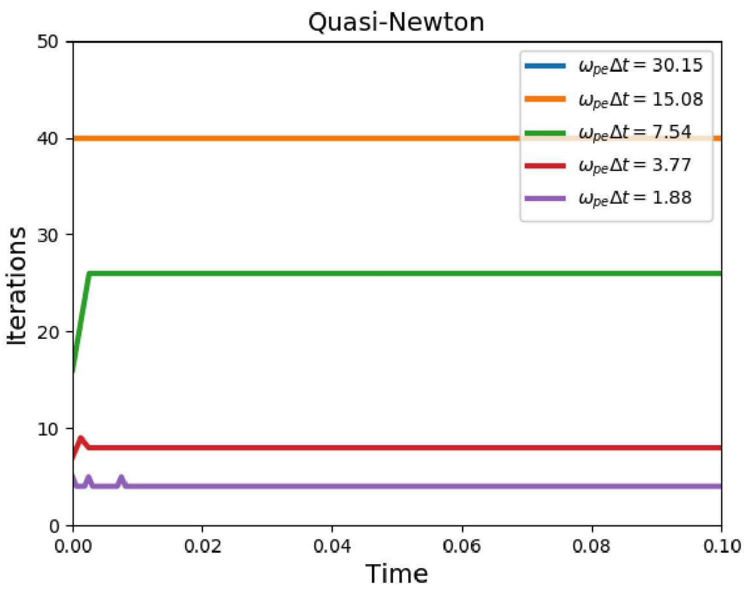


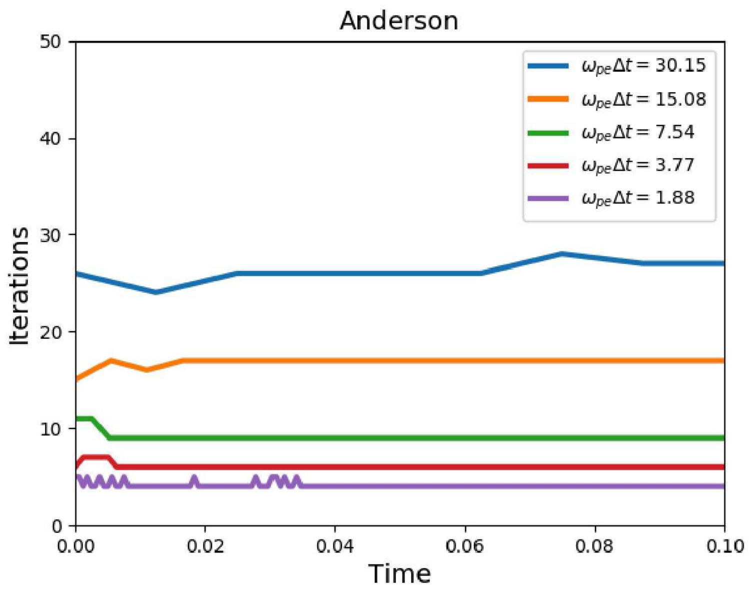
Convergence study:

- N_x x N_x x N_x =[8x8x8, 16x16x16, 32x32x32]
- N_t = [10,20,40]
- Speed of light: C dt/dx = 8

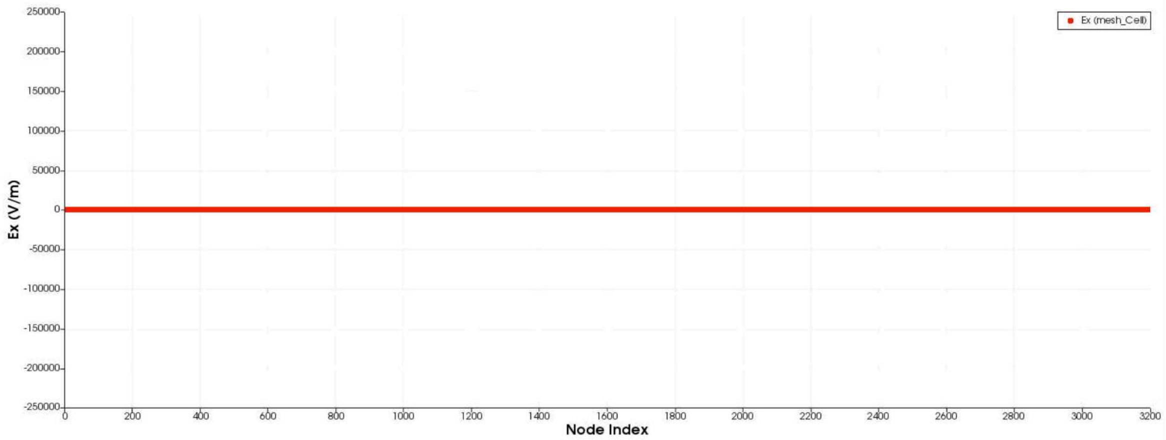
Iteration study: 8x8x8 grid

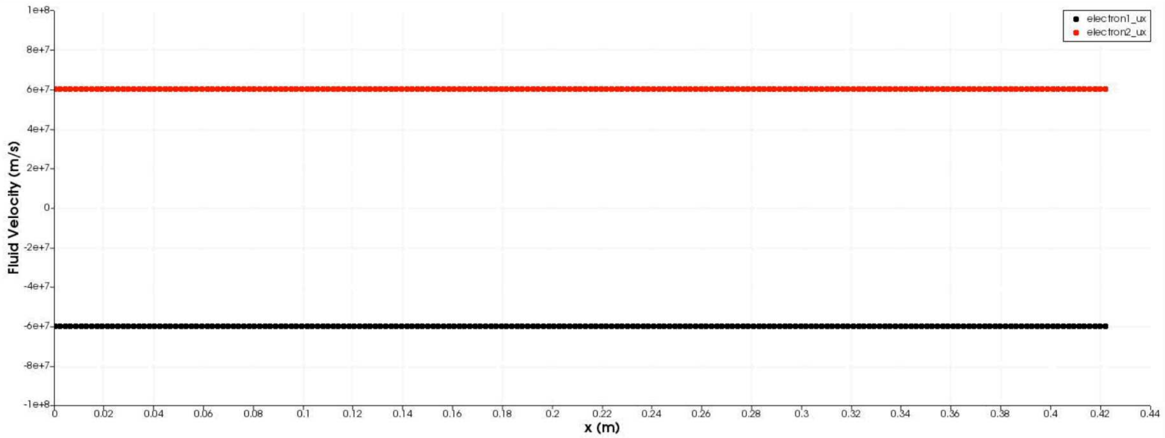


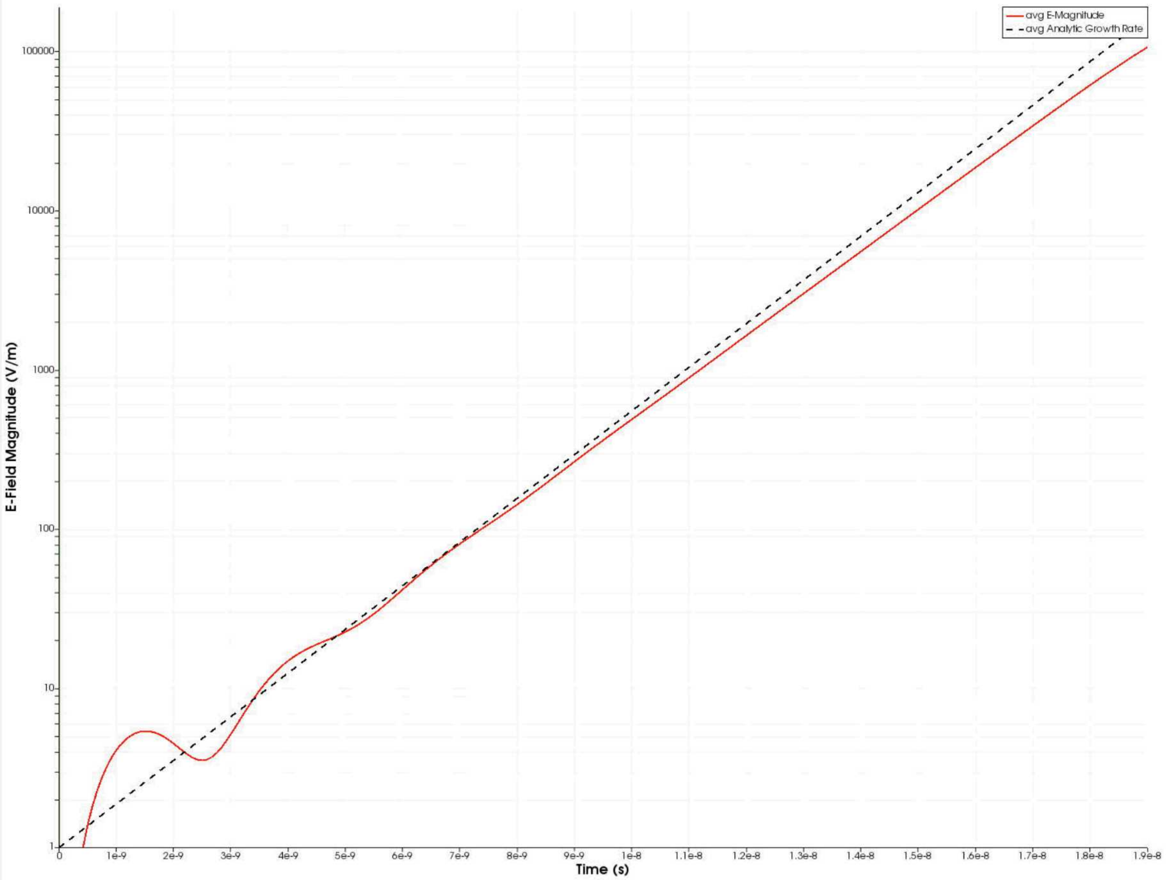




Two Stream Instability*







* We run this only through the linear growth regime

Final Thoughts

In Review:

- Mixture of IMEX temporal and Exact-Sequence discretizations has been shown to enforce involutions
- Extending previous work to DG fluid/CG Maxwell discretization
- Developed quasi-Newton/Anderson nonlinear solver for DG/CG discretization
  - Takes advantage of IMEX, DG structure, and linearity
  - Schur complement correction required for improved performance
- Early results for DG/CG discretizations are encouraging

Open questions:

1. How does quasi-Newton/Anderson compare with Newton-Krylov?
2. How does quasi-Newton/Anderson converge in other scenarios? (e.g. scalability)
3. Numerical study of DG/CG enforcement of the involutions
4. How does stabilization interact with Exact-Sequence/IMEX discretization?