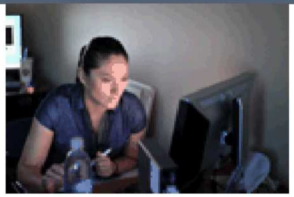
SAND2019-9480C

Multi-Fluid Plasma Simulation with an IMEX CG/DG Discretization



PRESENTED BY

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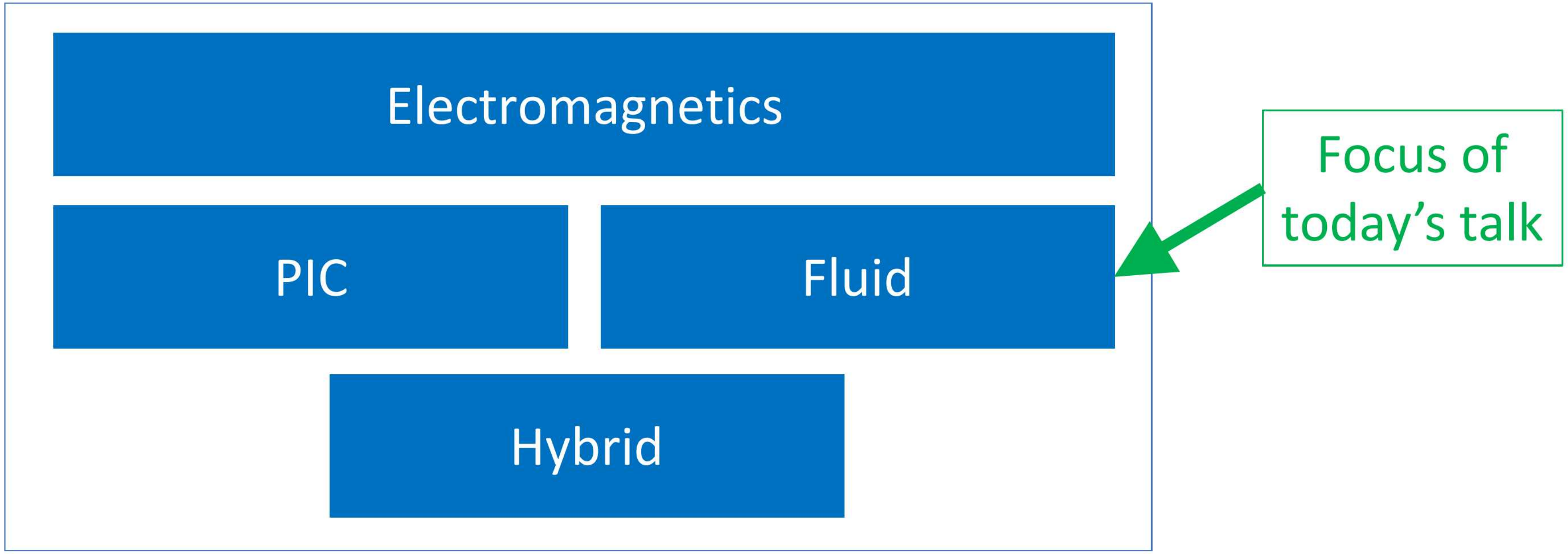
EMPIRE: A hierarchy of capabilities



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

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

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!

Discretization Tools

We have (at least) two major challenges:

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

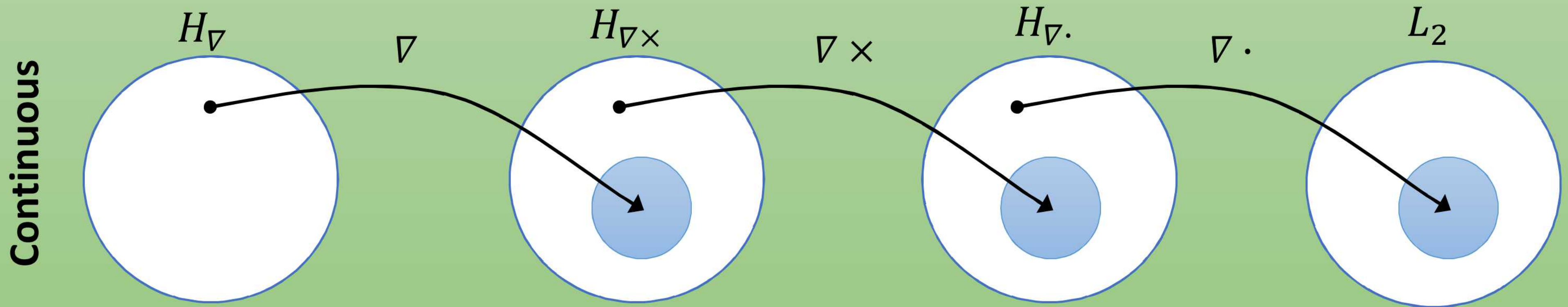
We will attack each of these in turn with two discretization tools

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

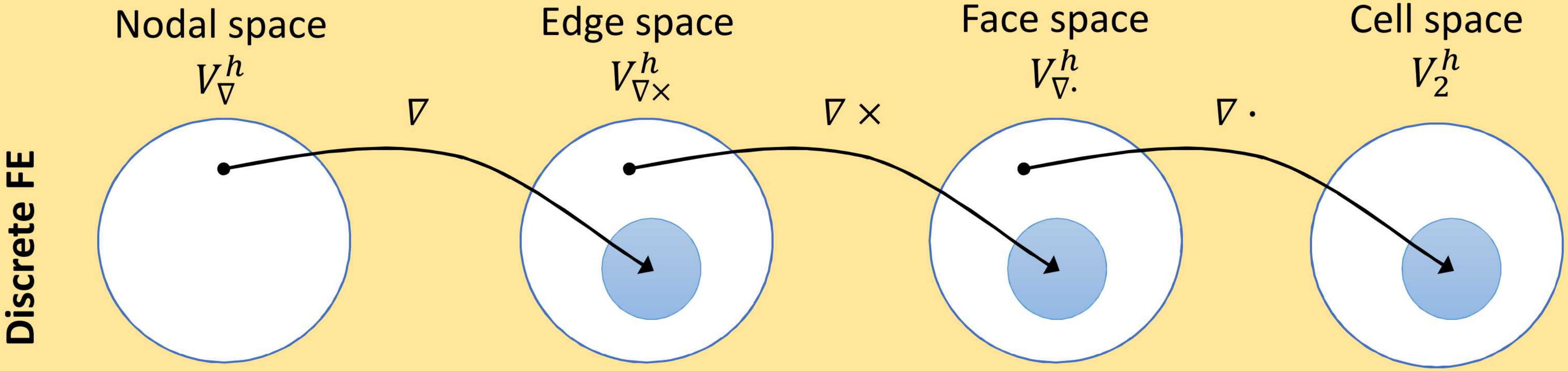
The interesting part is how these interact! (Not to mention boundary conditions! Which I won't talk about)

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 $V_*^h \subset H_*$):

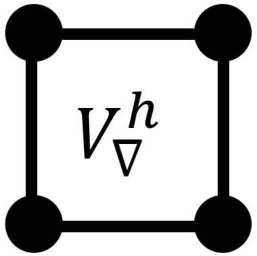


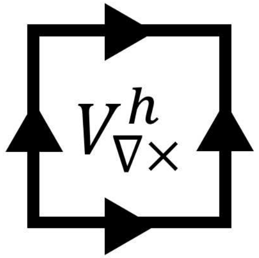
[1]Bochev, P., Edwards, H. C., Kirby, R. C., Peterson, K., & Ridzal, D. (2012). Solving PDEs with intrepid. *Scientific Programming*, *20*(2), 151-180.

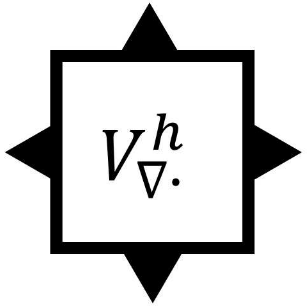
Exact-Sequence and Multi-Fluids

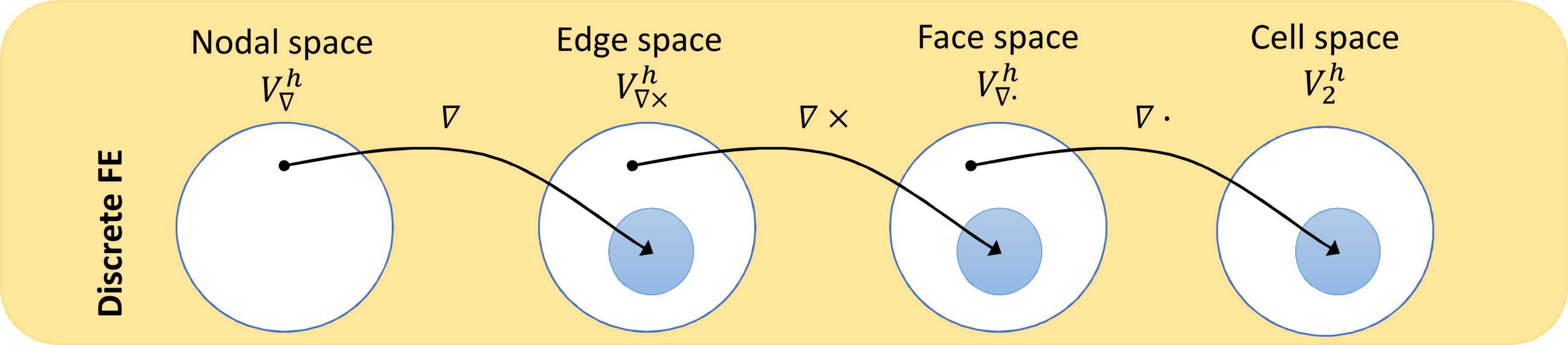
Discretization:

Fields continuous by construction (CG)

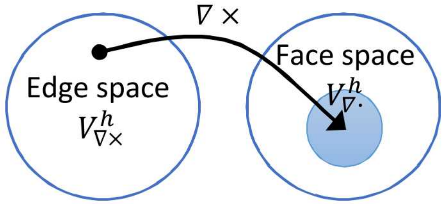
$\begin{bmatrix}\rho_\alpha \\ \rho_\alpha u_\alpha \\ \mathcal{E}_\alpha\end{bmatrix} \in$ 

$E \in$ 

$B \in$ 



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

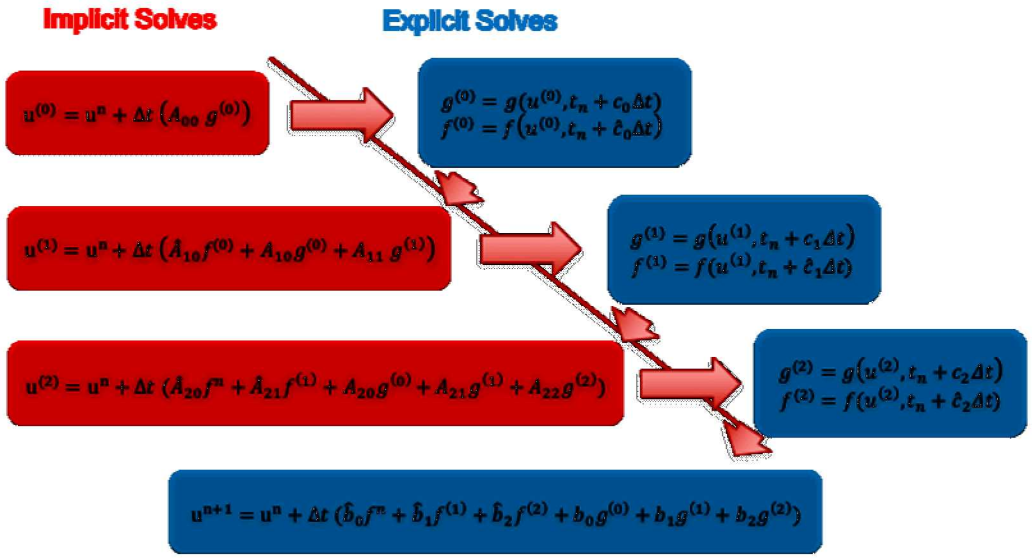


$$\nabla\cdot\left(\frac{\partial \mathbf{B}^h}{\partial t} + \nabla\times\mathbf{E}^h\right) = 0 \Rightarrow \nabla\cdot\partial_t\mathbf{B}^h = 0$$

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

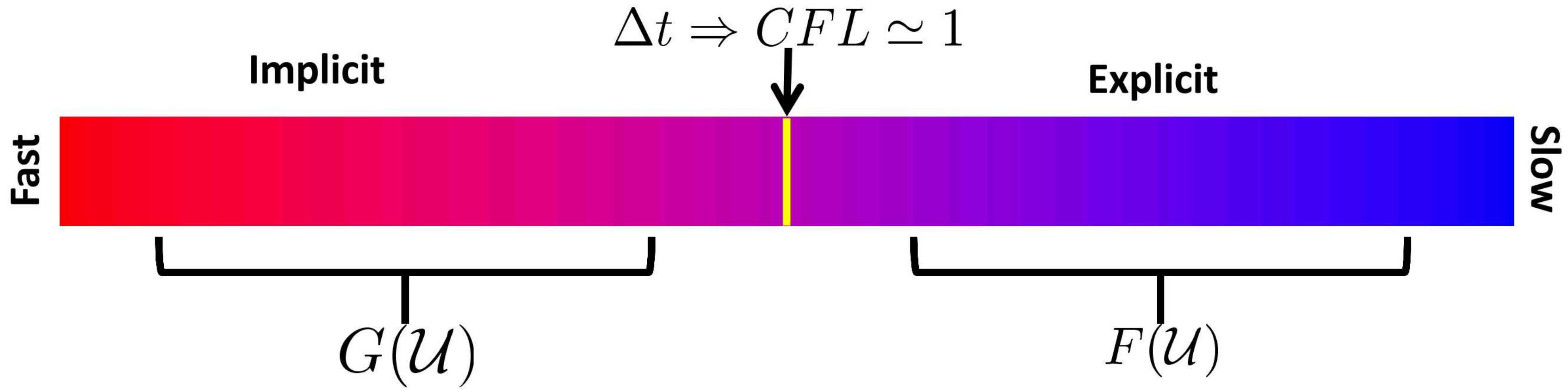
Implicit-Explicit (IMEX) Time Integration

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)*

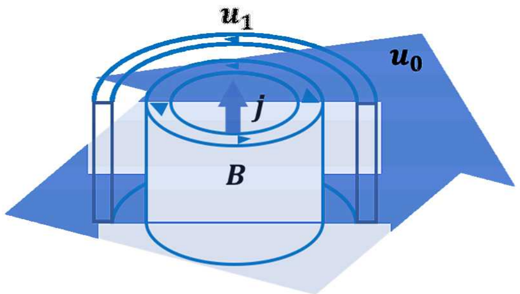
Two fluid plasma vortex in MHD limit

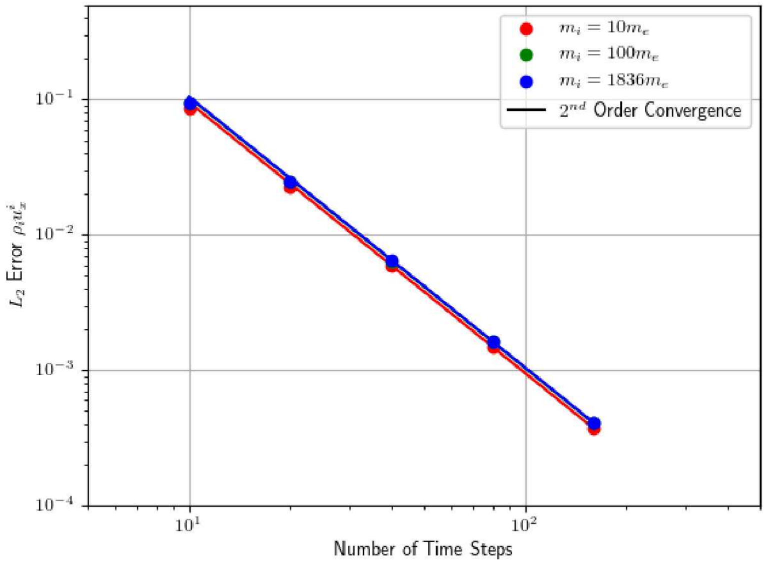
- IMEX time discretization
- Compatible spatial discretization

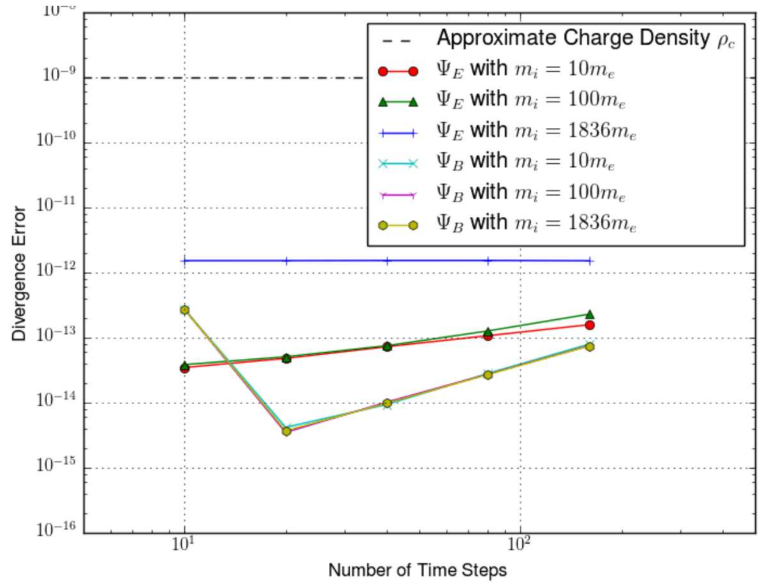
	Electrons	Ions
$\omega_p \Delta t$	**23 - 270**	**0.55 - 6.3**
$\omega_c \Delta t$	**1 - 12**	$\mathbf{5.5 \cdot 10^{-4} - 6.3 \cdot 10^{-3}}$
$v_s \frac{\Delta t}{\Delta x}$	0.25	$5.7 \cdot 10^{-3}$
$c \frac{\Delta t}{\Delta x}$	**6.3**	

Achieves 2nd order conv, satisfies involutions:

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





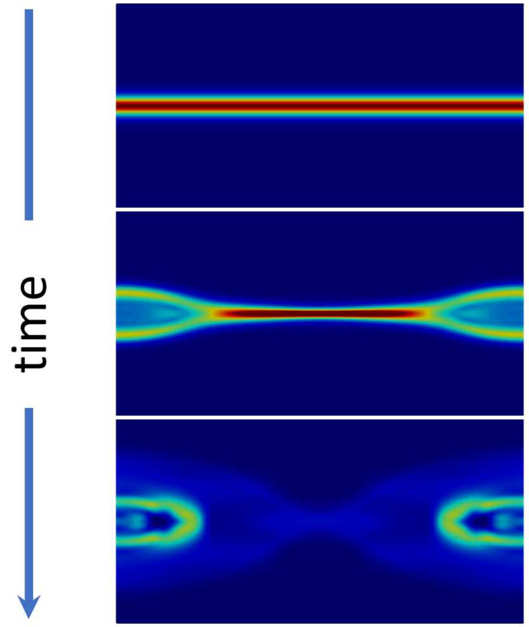


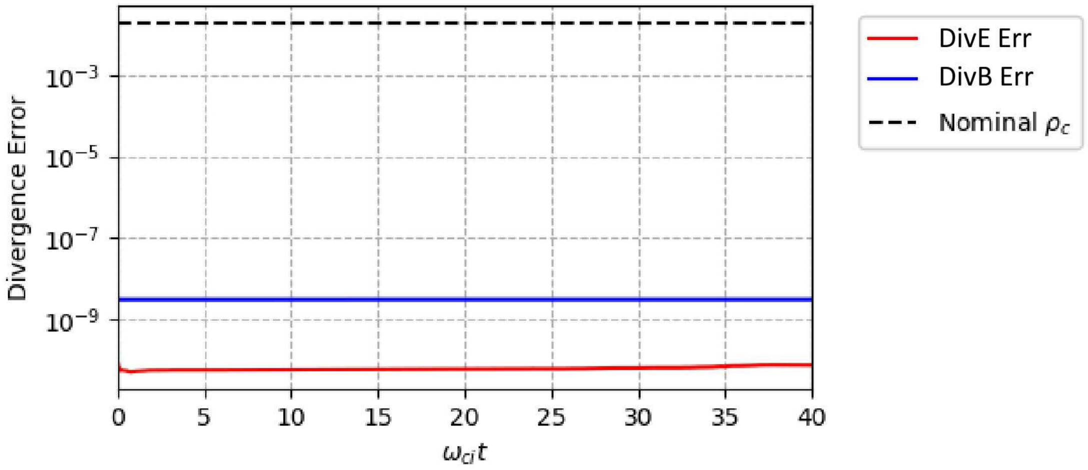
*See Miller, Cyr, Shadid, Kramer, Phillips, Conde, Pawlowski., IMEX and exact sequence discretization of the multi-fluid plasma model, in press JCP, 2019

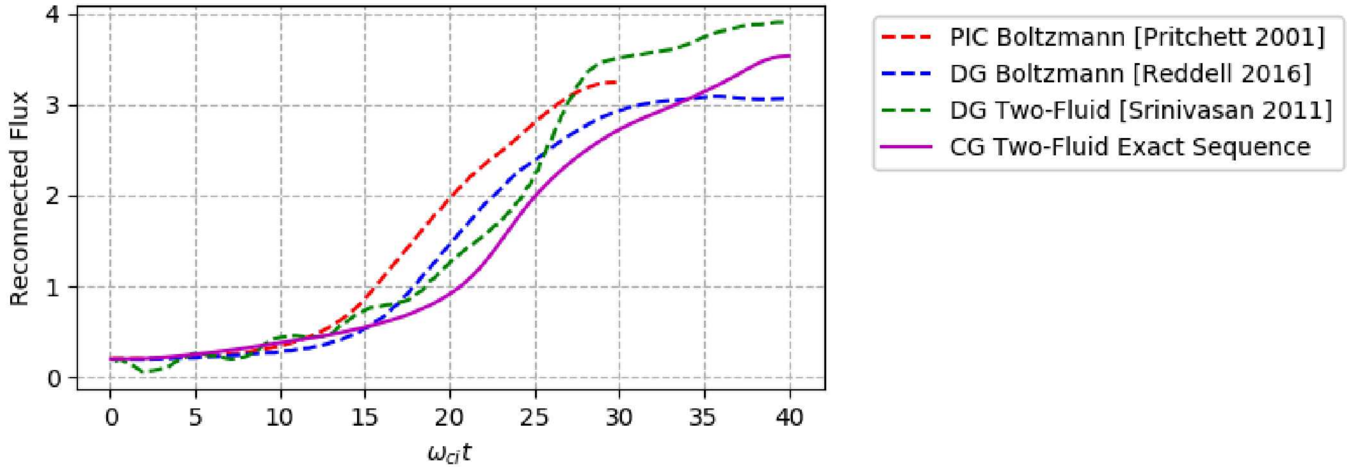
GEM Challenge Problem (from Drekar)*

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

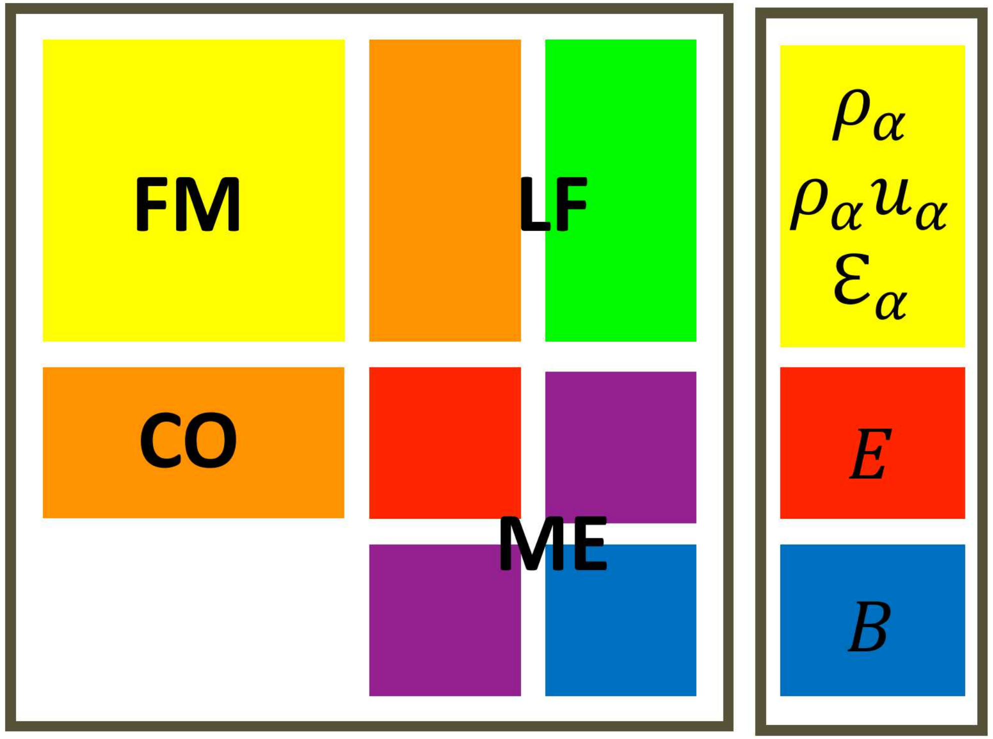
Nonlinear Algorithm

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

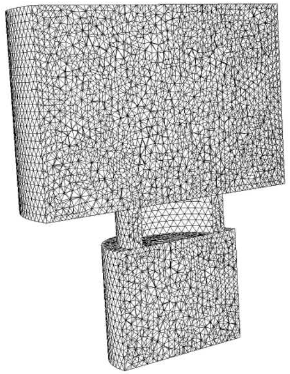
- Fluid matrix (mass like)
- Lorentz Force

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

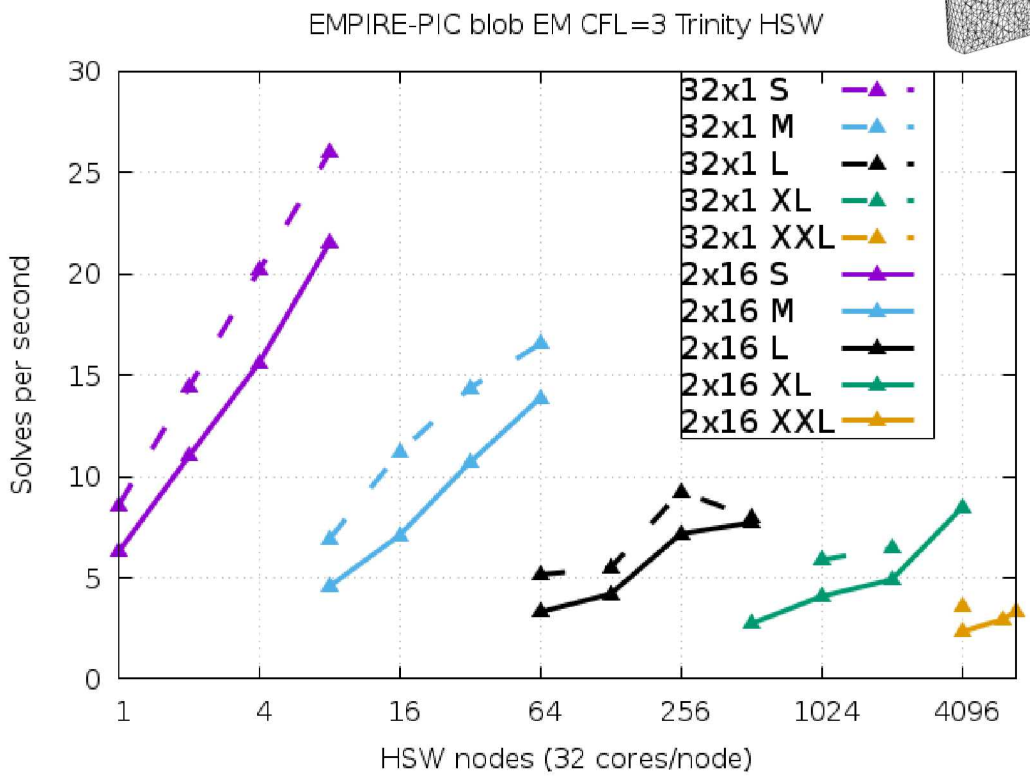


We (Sandia royal*) have made good progress in solving the Maxwell system

- 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

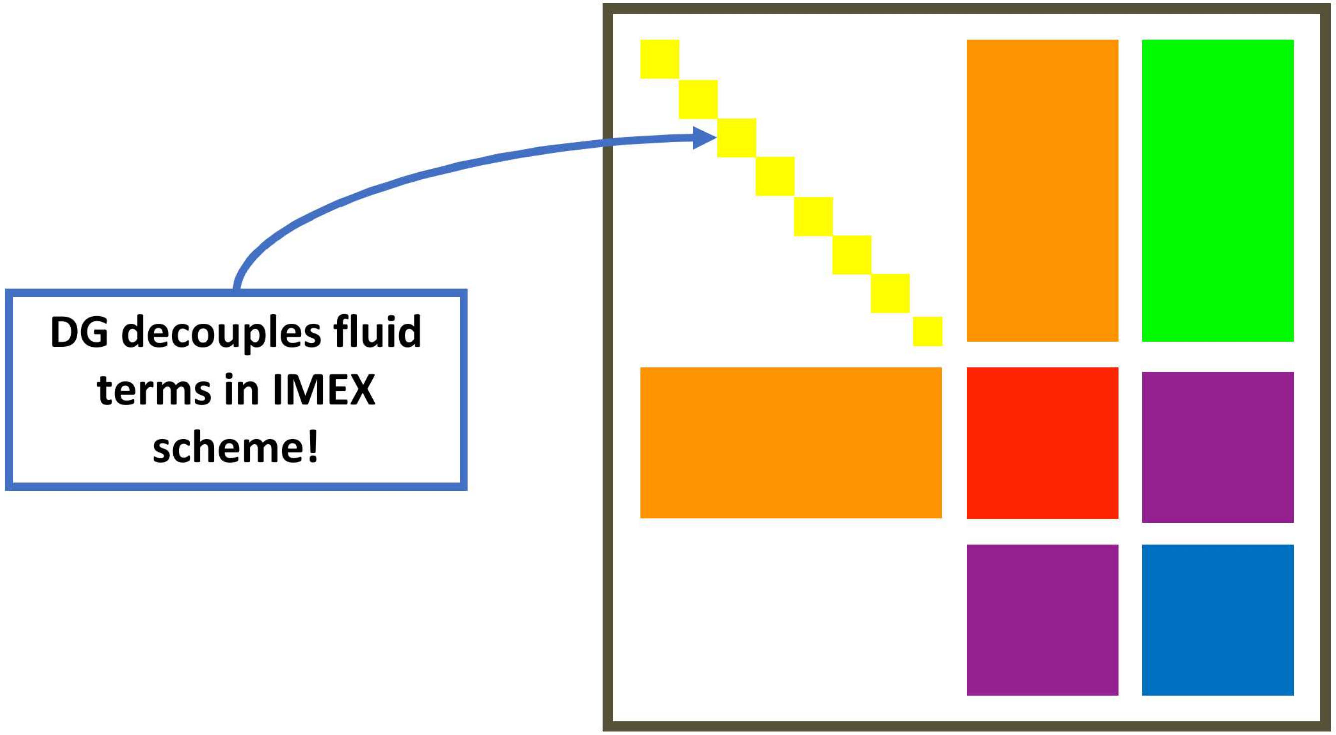
- Fluid matrix is mass matrix (CG fluids gives global coupling)
- Maxwell solver is effective (and should remain unperturbed)
  - Handles speed of light coupling
- Important to get plasma frequency and cyclotron frequency coupling
  - Handled by preconditioning
  - These are local (ODE-like) coupling 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

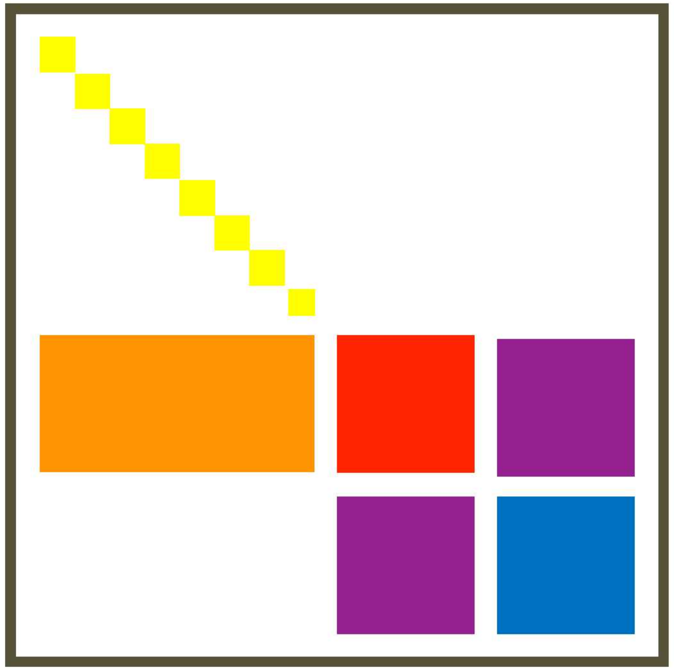
- DG Fluids will make the fluid contribution block diagonal on each element
  - Local nature of DG discretization
  - IMEX splitting choice
- Support for involutions still preserved
  - No Magnetic monopoles is the same
  - Weak enforcement of Gauss' law works (math is more complex)



Quasi-Newton Method

Typically I would do Newton-Krylov, but…

Block lower Gauss-Seidel



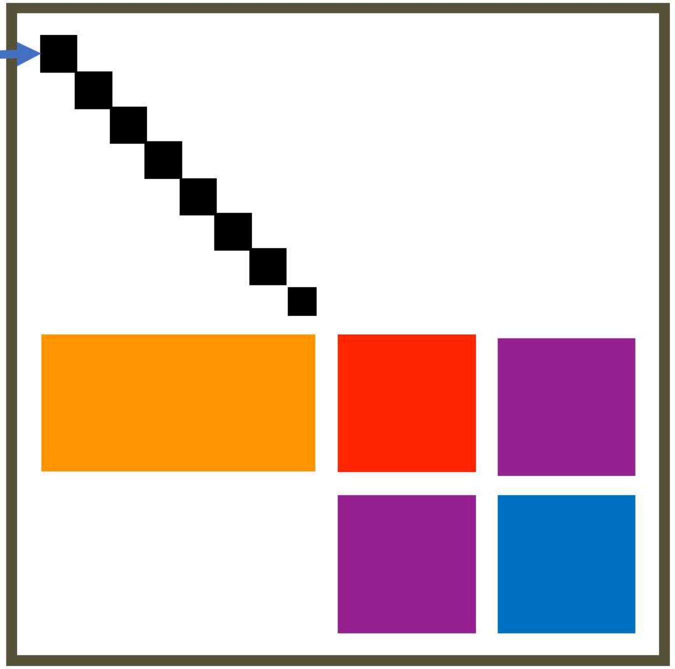
- ✓ Triangular solve
- ✓ Leverages Maxwell solver
- ✓ Block diagonal fluid solve
- ✓ Implicit cyclotron frequency
- ✗ Implicit plasma frequency

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.

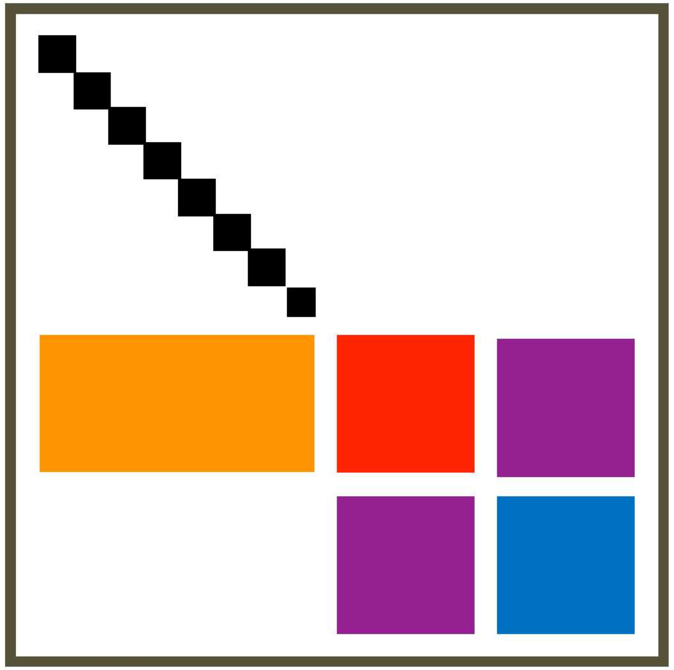
- Mode derived from coupling Ampere’s law and momentum equation

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

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

$$\frac{(\rho_\alpha \mathbf{u}_\alpha)}{\Delta t} + \underbrace{\Delta t \frac{1}{\epsilon_0}\frac{q_\alpha^2}{m_\alpha^2}\rho_\alpha(\rho_\alpha \mathbf{u}_\alpha)}_{\text{Correction}}$$

Block GS with Schur Complement

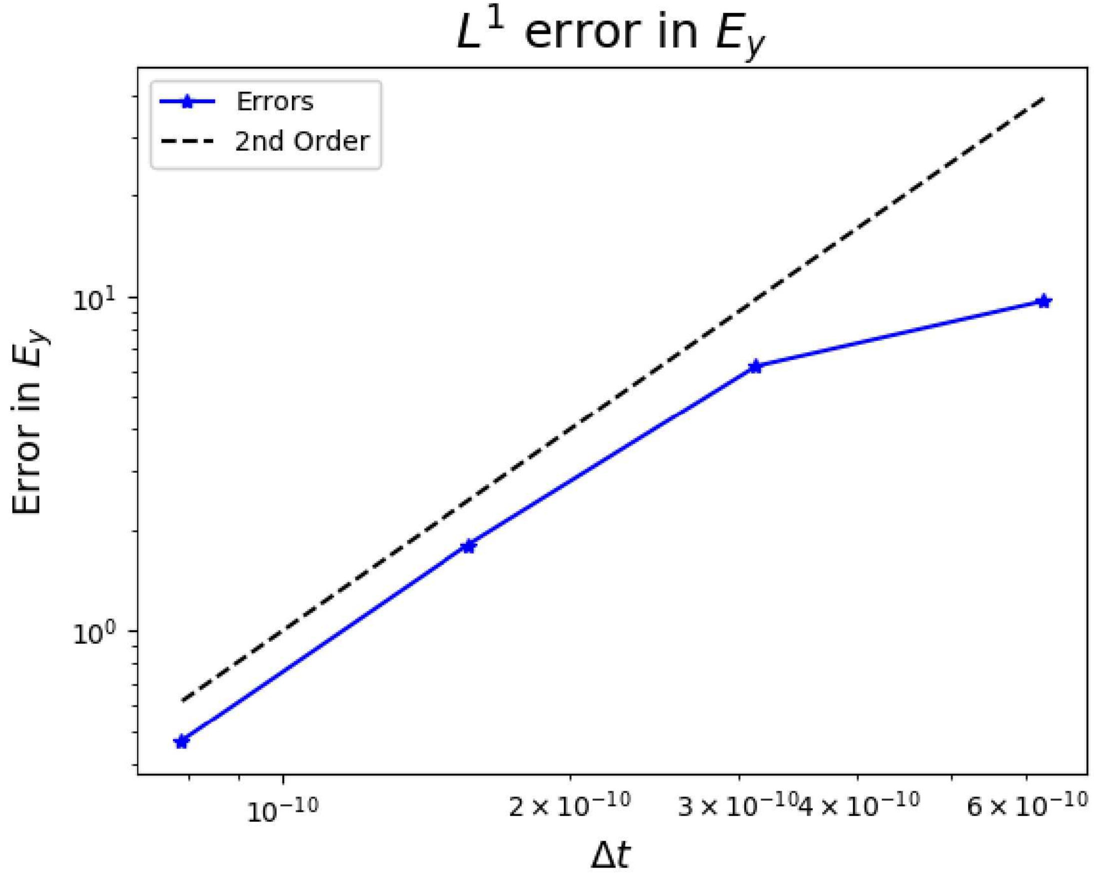


O-Wave Convergence Results (EMPIRE-Fluid)

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.

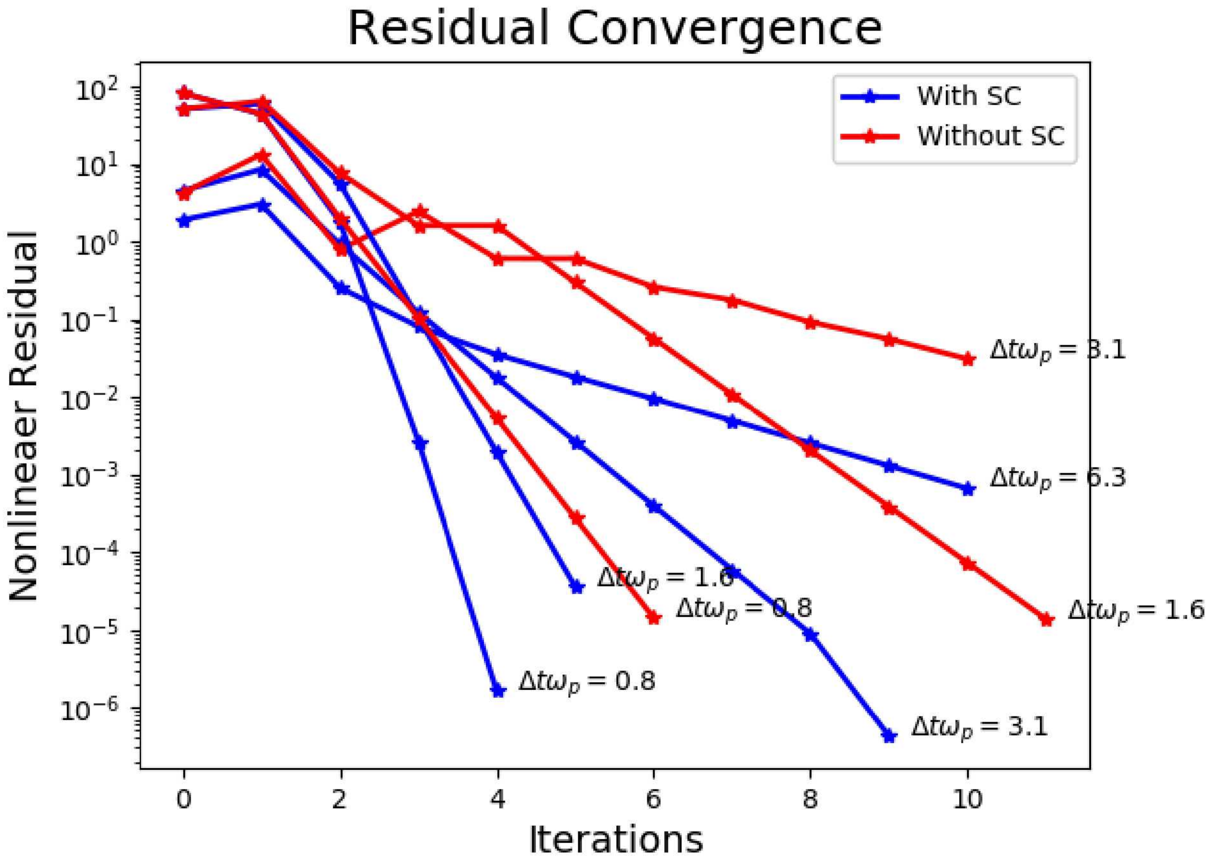
O-Wave Nonlinear Solver (EMPIRE-Fluid)

Adding Schur complement improves nonlinear convergence

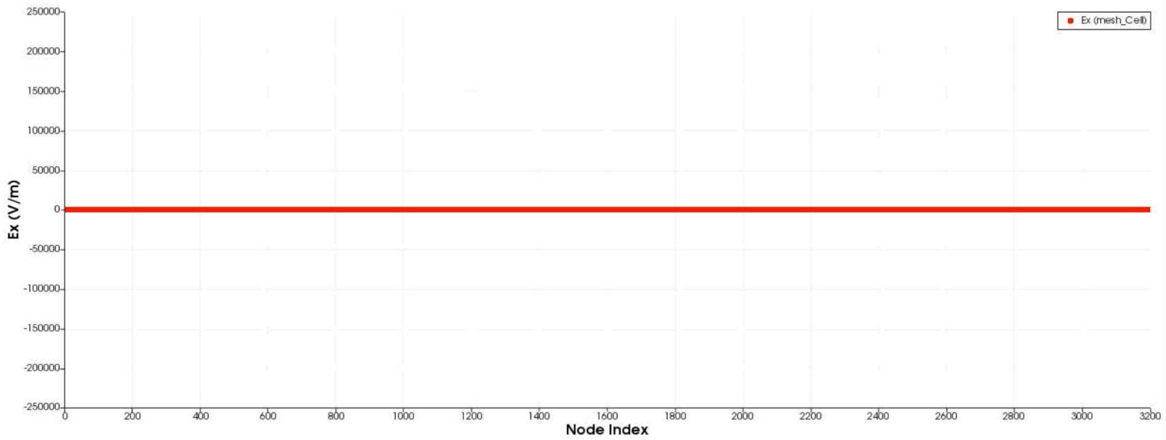
- Still has strong growth in iteration count with increasing time steps
- Cost/benefit tradeoff study against Newton-Krylov with similar preconditioner required

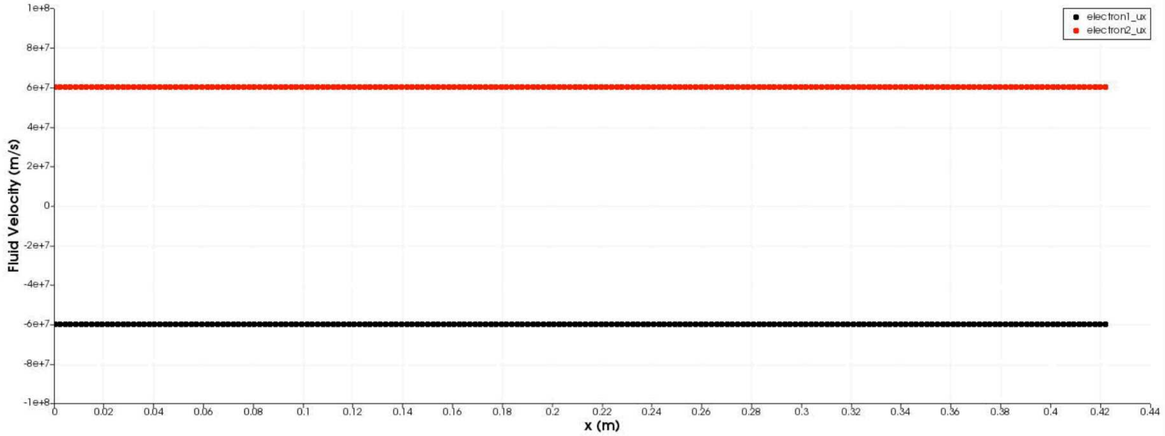
Each nonlinear iteration requires:

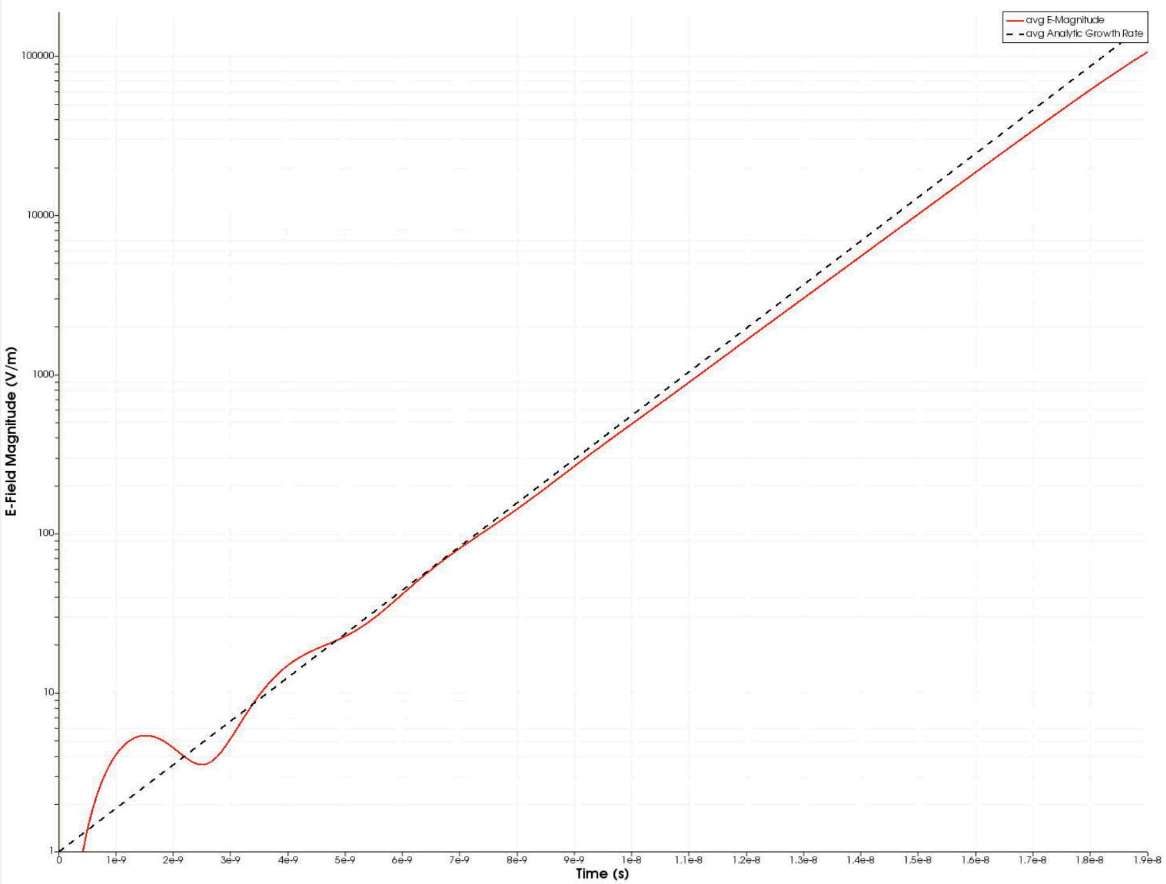
1. Reconstruction of fluid Jacobian inverse
2. Solve of Maxwell system



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 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 compare with Newton-Krylov?
2. How does quasi-Newton converge in other scenarios? (e.g. scalability)
3. How does stabilization interact with Exact-Sequence/IMEX discretization?