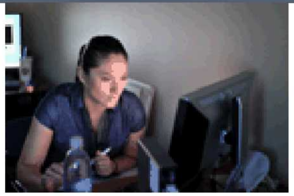
SAND2019-14579PE

Techniques for Simulating Multiple Timescales with Application to Plasmas



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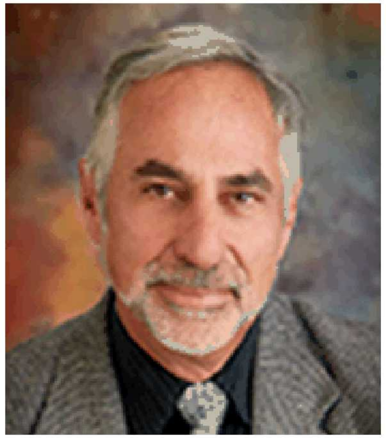

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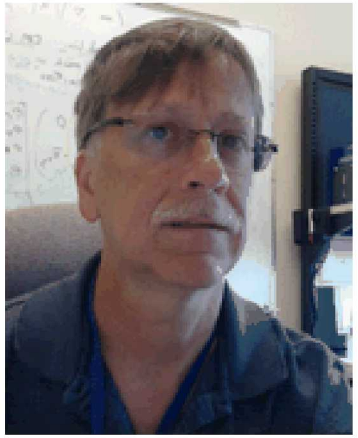

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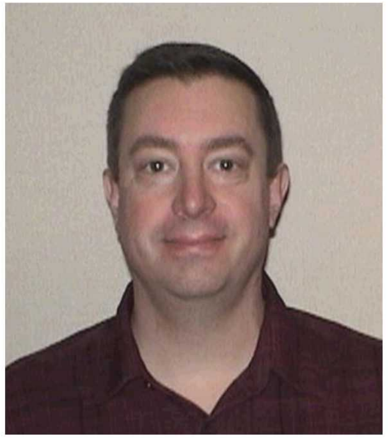

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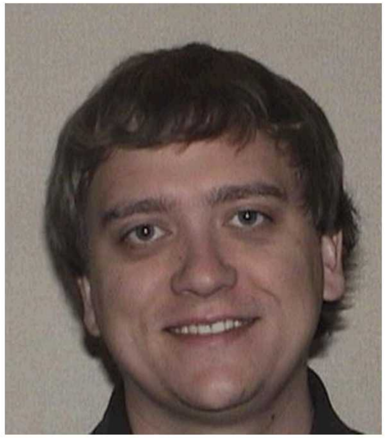

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Motivating Example: Multi-Fluid Plasma

5-Moment Fluid

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

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

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

Maxwell Equations

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

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

Multi-fluid plasmas:

- Evolve multiple charged fluids
- Interactions with electromagnetics
- Neutral fluid limit: Magnetohydrodynamics

Challenges:

- Lots of equations
- Handling involutions (divergence constraints)
- Multiple time scales

Multiple Time Scales

Fluid Time Scales:
- Advection
- Diffusion
- Sound speed*

Plasma Time Scales:
- Speed of light
- Plasma Oscillation
- Collisions
- Cyclotron frequency

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) = \mathbf{0}$$

$$\frac{\partial (\rho_\alpha \mathbf{u}_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha + p_\alpha I + \Pi_\alpha) = \mathbf{0}$$

- Fluid standard modes: u-c, u, u+c
- Plasma time scales are usually stiff
- Component time scales (advection, diffusion)
- Coupling time scales (sound speed, speed of light, etc…)

*I'm over simplifying the sound speed for the sake of presentation, usually an energy equation is required

Multiple Time Scales

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

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

$\propto \Delta t$

Flow velocity

$$u_\alpha$$

$\propto \frac{\Delta t}{\Delta x}$

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

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

$\propto \frac{\Delta t}{\Delta x^2}$

Thermal diffusivity

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

Take home: These plasmas are hard to simulate!

Multiple Time Scales: What is stiff?

What is stiff?

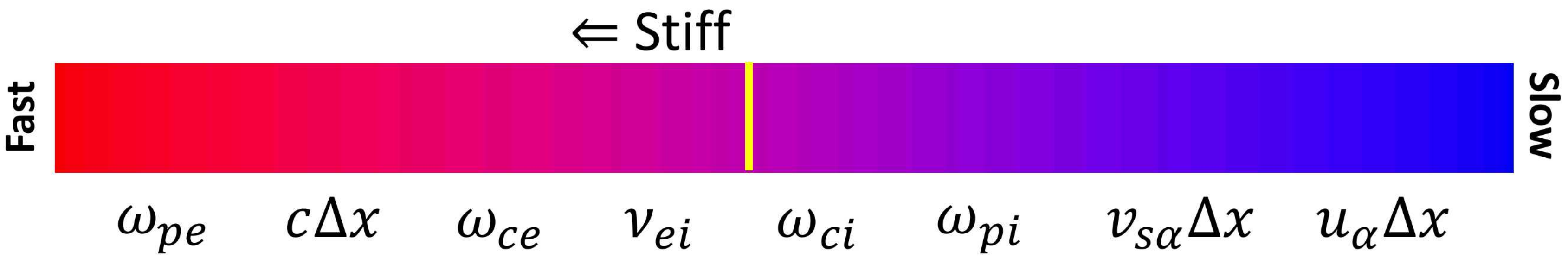
? "Is the air in this room stiff?" – Jed Brown (UC Boulder)

A It depends, what do you want to know?

1. Heat transfer, how effective is your heater? Probably stiff
2. How effective is the air mixing? Stiff sound speed
3. What is the impact of a gas explosion? Not stiff (exclude chemistry)

What are the consequences?

- Think of the "speed" of the mode to be the explicit Euler stability time step
- By defining the dynamics you want to resolve, you select which modes are stiff
- Stiff modes' explicit Euler stability limited is violated by the resolved time scale



What is this talk about?

Multi-physics problems often have multiple stiff modes depending on choice of resolved time scale:

- **This talk tries to answer the question of "How do we handle these stiff modes?"**

How do we handles these stiff modes?

1. For implicit time integration, we develop block preconditioners that try to account for the stiff modes in the Jacobian
2. We pursue Implicit-Explicit time integration to focus nonlinear solvers on handling only stiff physics, resolved physics can be integrated explicitly

This is summarized by looking at the multi-fluid plasma equations, and applying a combination of techniques to handle the complex range of time scales

Outline

1. A motivating example: Multi-Fluid Plasmas
    - Types of time scales
    - Quantifying stiffness
2. Fully implicit methods
    - Motivating example
    - Block preconditioners
3. Time integration
    - IMEX RK
    - ALE Methods
4. Multi-fluid plasmas
5. Final Thoughts

Outline

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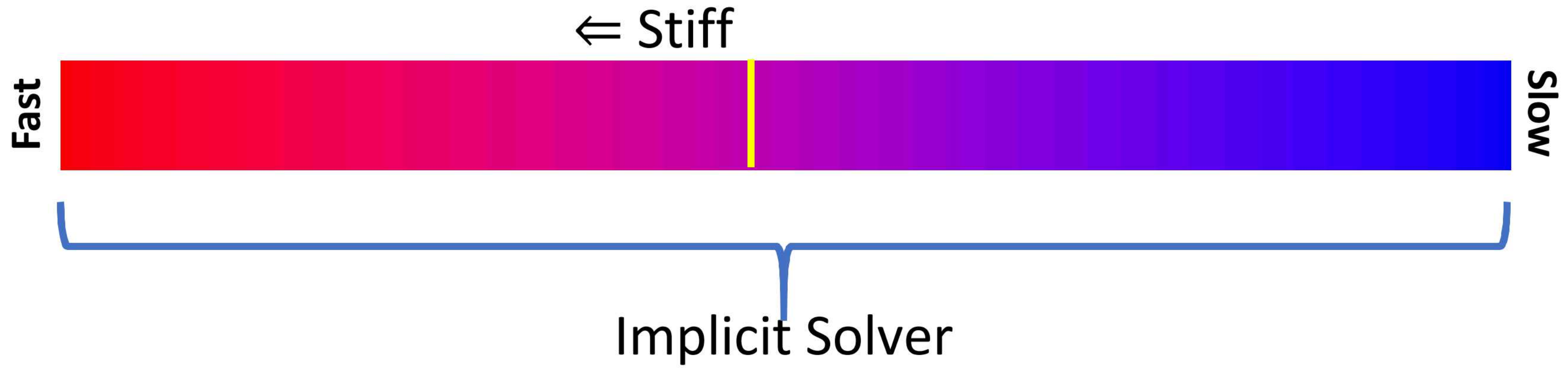
Implicit Time integration



- Implicit time integration overcomes stiffness
- We use Newton-Krylov to evolve implicit physics

$$\text{Solve } \mathbf{J}p_k = -F(x_k) \text{ where } \mathbf{J} = \partial F / \partial x$$

$$x_{k+1} = x_k + p_k$$

- Effective preconditioning is the key to parallel scalability of Newton-Krylov
- We pursue **block preconditioning** to handle multi-physics

A Simple Example*

Assume positive a_{**}, simplifies to a second order wave:

$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} a_{uu} & a_{uv} \\ a_{vu} & a_{vv} \end{bmatrix} \frac{\partial}{\partial x}\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Using a finite difference discretization, Jacobian is:

$$\begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} = \begin{bmatrix} \frac{1}{\Delta t} I + a_{uu} D & a_{uv} D \\ a_{vu} D & \frac{1}{\Delta t} I + a_{vv} D \end{bmatrix}$$

*From Chacón, L., "An optimal, parallel, fully implicit Newton–Krylov solver for three-dimensional viscoresistive magnetohydrodynamics," Physics of Plasmas, 2008.

A Segregated System

$$\begin{bmatrix} A_{00} & A_{01} & \cdots & A_{0N} \\ A_{10} & A_{11} & \cdots & A_{1N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N0} & A_{N1} & \cdots & A_{NN} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_N \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_N \end{bmatrix}$$

- Most of A_{ij} are "large sparse" matrices
- This structure is common:
  1. Multi-physics (the focus of this talk)
  2. Constraints
  3. Optimization
- "Effective preconditioners" are robust and scalable for these systems

“Classical” Block Preconditioners

$$M^{-1} = \begin{bmatrix} A_{00} & & & \\ & A_{11} & & \\ & & \ddots & \\ & & & A_{NN} \end{bmatrix}^{-1}$$

Jacobi

$$M^{-1} = \begin{bmatrix} A_{00} & A_{01} & \cdots & A_{0N} \\ & A_{11} & \cdots & A_{1N} \\ & & \ddots & \vdots \\ & & & A_{NN} \end{bmatrix}^{-1}$$

Gauss-Seidel

Benefits:

- Easy to implement!
- Nice convergence theory

When are they “effective”?

- Little coupling
- One directional coupling

Schur Complements for 2x2 Systems

Use a block LU factorization:

$$\begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} = \begin{bmatrix} I & \\ A_{10}A_{00}^{-1} & I \end{bmatrix} \begin{bmatrix} A_{00} & A_{01} \\ & S \end{bmatrix}$$

$$\text{where } S = A_{11} - A_{10}A_{00}^{-1}A_{01}$$

An important result:

M. F. Murphy, G. H. Golub, and A. J. Wathen, A note on preconditioning for indefinite linear systems, SISC, 21 (2000).

$$M_{SC} = \begin{bmatrix} A_{00} & A_{01} \\ & S \end{bmatrix}$$

Three Block Preconditioners

GMRES iterations averaged over 10 steps

$$\begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} = \begin{bmatrix} \frac{1}{\Delta t} I + a_{uu} D & a_{uv} D \\ a_{vu} D & \frac{1}{\Delta t} I + a_{vv} D \end{bmatrix}$$

- $h = 1/500, \Delta t = h$
- Three different preconditioners

Classical

$$M_{SC} = \begin{bmatrix} A_{00} & A_{01} \\ & S \end{bmatrix} \quad M_J = \begin{bmatrix} A_{00} & \\ & A_{11} \end{bmatrix}$$

Schur-Comp

$$M_{GS} = \begin{bmatrix} A_{00} & A_{01} \\ & A_{11} \end{bmatrix}$$

- Required inverses of A_{00}, A_{11}, and S computed directly

a_{uu}/a_{vv}	a_{uv}	a_{vu}	M_J	M_{GS}	M_{SC}	CFL
1	1	1	2	2	2	1
1	10	10	42	34	2	10
1	100	100	317	251	2	100
1	10	1	3.8	3	2	3
1	100	1	44	42	2	10
1	100	10	141	131	2	31
10	1	1	3	2	2	0.1
10	10	10	2	3	2	1
10	100	100	77	49	2	10
100	1	1	3	2	2	0.01
100	10	10	4	3	2	0.1
100	100	100	2	3	2	1

Recipe for Block Preconditioners

1. Consider the desired time step Δt
2. Look at *explicit* stability limit of all time scales:
   - Diffusion: $\nu\Delta t/\Delta x^2$
   - Advection: $|u|\Delta t/\Delta x$
   - Waves (typically from coupling): $|w|\Delta t/\Delta x$
3. Modes where the stability limit is “relatively large” for desired time step must be addressed in the preconditioner!

This is motivated by the ideas of “Physics-Based” preconditioning: See *Mousseau, Knoll, and Rider, JCP 2000*.

Incompressible Navier-Stokes

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} - \nabla \cdot \nu \nabla \mathbf{u} + \nabla p = f$$

$$\nabla \cdot \mathbf{u} = 0$$

Jacobian with LU Factorization:

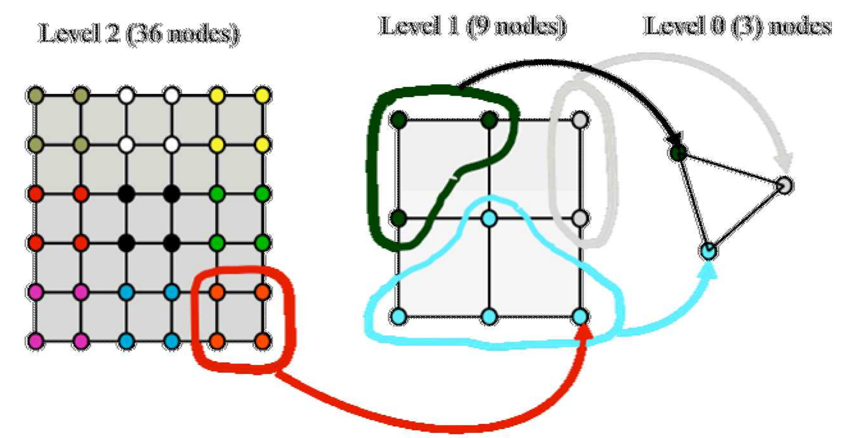
$$\begin{bmatrix} F & B^T \\ B & C \end{bmatrix} = \begin{bmatrix} I & \\ BF^{-1} & I \end{bmatrix} \begin{bmatrix} F & B^T \\ & S \end{bmatrix} \Rightarrow M = \begin{bmatrix} \hat{F} & B^T \\ & \hat{S} \end{bmatrix}$$

$$\text{where } \hat{S} \approx C - BF^{-1}B^T$$

- $F^{-1} \approx \hat{F}^{-1}$ using multigrid
- $S^{-1} \approx \hat{S}^{-1}$ using SIMPLEC, PCD or LSC

Three Types of Preconditioner

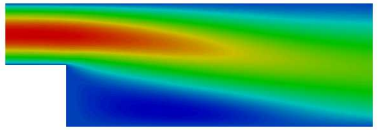
1. Domain Decomposition (**DD**)
   - ILU Factorization on each processor (with overlap)
2. Multilevel methods: ML Library (Tuminaro, Sala, Hu, Siefert, Gee)
   - Labeled Aggressive Coarsening (**AggC**)
   - Multiple unknowns per node
   - ILU solvers
3. Block Preconditioners: Block LU Fact.
   - Used multigrid for sub solves
   - Three different Schur complements
     1. **SIMPLEC**: $-B\,\mathbf{absRowSum}(F)^{-1}B^T$
     2. **PCD**: $-L_p F_p^{-1} Q_p$
     3. **LSC**: $-(BQ_u^{-1}B^T)(BQ_u^{-1}FQ_u^{-1}B^T)^{-1}(BQ_u^{-1}B^T)$



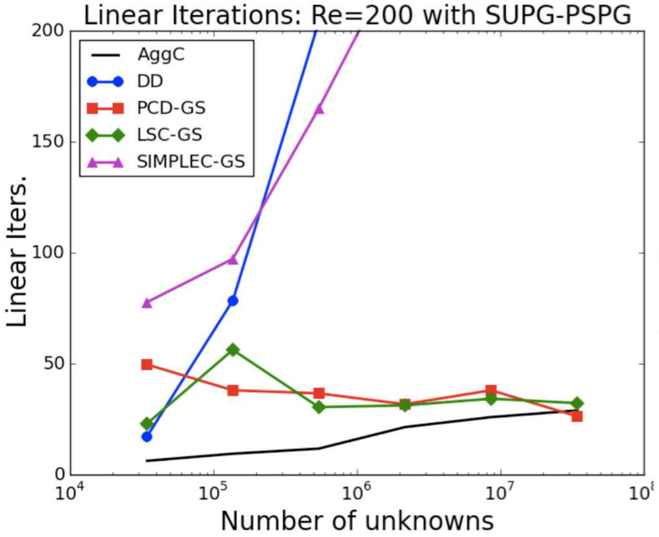
Visualization of effect of partition of matrix graph on mesh

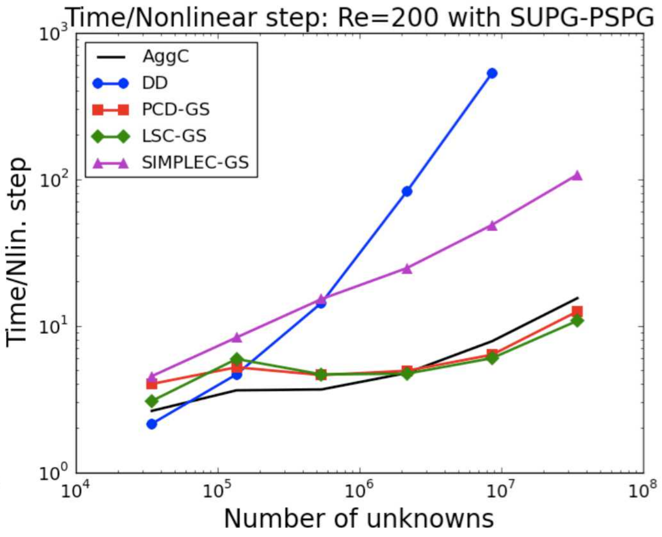
Aggregation based Multigrid: Vanek, Mandel, Brezina, 1996, Vanek, Brezina, Mandel, 2001, Sala, Formaggia, 2001

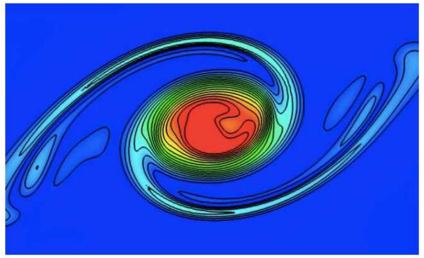
Navier-Stokes: Results



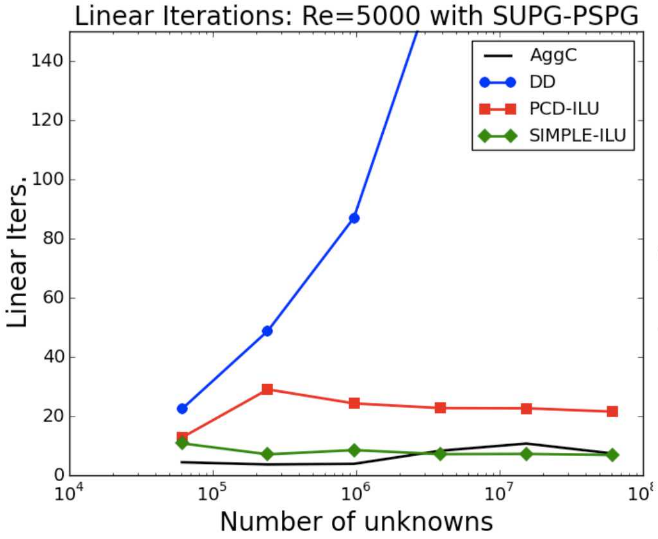
Backward Facing Step: Steady
- Re = 200
- 1 to 1024 Processors
- Stabilization: SUPG & PSPG

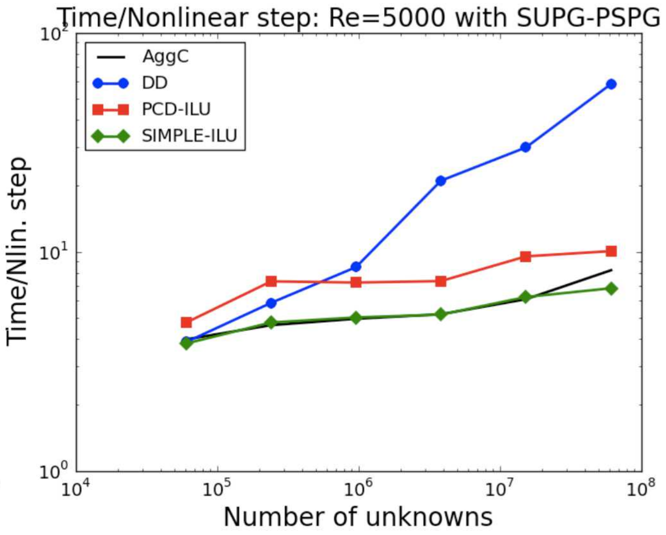






Kelvin Helmholtz: Transient
- Re = 5000
- 1 to 1024 Processors
- Stabilization: SUPG & PSPG
- CFL = 2.5





* E. C. Cyr, J. N. Shadid, R. S. Tuminaro, Stabilization and Scalable Block Preconditioning for the Navier-Stokes Equations, J. Comp. Phys., 231:345-363, 2011.

Incompressible MHD: B-Field Lagrange Multiplier Formulation

Magnetohydrodynamics (MHD) equations couple fluid flow to magnetics equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \nabla^2 \mathbf{u} + \nabla p - \frac{1}{\mu_0} (\nabla \times \mathbf{B}) \times \mathbf{B} = \mathbf{f}$$

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{u} \times \mathbf{B}) + \frac{\eta}{\eta_0} \nabla \times \nabla \times \mathbf{B} + \nabla r = \mathbf{0}$$

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

Using a stabilized finite element formulation

$$\mathcal{J}\mathbf{x} = \begin{bmatrix} F & B_p^T & Z & \\ B_p & C_u & & \\ Y & & D & B_r^T \\ & & B_r & C_B \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \\ \mathbf{B} \\ r \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ 0 \\ \mathbf{0} \\ 0 \end{bmatrix}$$

- Equal order basis functions, C_u and C_B are stabilization operators

Multiple Time Scales: MHD

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \nabla^2 \mathbf{u} + \nabla p - \frac{1}{\mu_0} (\nabla \times \mathbf{B}) \times \mathbf{B} =& \mathbf{f} \\ \nabla \cdot \mathbf{u} =& 0 \\ \frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{u} \times \mathbf{B}) + \frac{\eta}{\eta_0} \nabla \times \nabla \times \mathbf{B} + \nabla r =& \mathbf{0} \\ \nabla \cdot \mathbf{B} =& 0 \end{aligned}$$

Some time scales are obvious:

- Diffusion (fast, often implicit)
- Elliptic constraints (real fast, often implicit)
- Advection (fast or slow, explicit or implicit)

Others are not so obvious (to me anyway)

Multiple Time Scales: MHD

$$\frac{\partial \delta \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \delta \mathbf{u} + \nabla \delta p - \frac{1}{\mu_0} (\nabla \times \delta \mathbf{B}) \times \mathbf{B} = \mathbf{0}$$

$$\nabla \cdot \delta \mathbf{u} = 0$$

$$\frac{\partial \delta \mathbf{B}}{\partial t} - \nabla \times (\delta \mathbf{u} \times \mathbf{B}) + \nabla \delta r = \mathbf{0}$$

$$\nabla \cdot \delta \mathbf{B} = 0$$

A linearization about (**u**,**B**), dropped diffusive terms

- Particulars of linearization important to fixed point convergence

Alfvén Wave generated by coupling

- Highlighted coupling gives wave speed:
- Secondary gives wave "character": anisotropic

$$v_A = \frac{|\mathbf{B}|}{\sqrt{\rho \mu_0}}$$

Splitting for MHD

Two split block factorization preconditioners

A $$\mathcal{M}_{Split\text{-}3\times 3} = \begin{bmatrix} F & & \hat{Z} \\ & I & \\ \hat{Y} & & \hat{D} \end{bmatrix} \begin{bmatrix} F^{-1} & & \\ & I & \\ & & I \end{bmatrix} \begin{bmatrix} F & B^T & \\ B & C & \\ & & I \end{bmatrix}$$

- Coupled multigrid for magnetics ($\hat{D}$)
- Block LU with SIMPLEC for Magnetics-Velocity (Alfvén)
- Block LU with PCD or SIMPLEC for Fluids

B $$\mathcal{M}_{Split\text{-}4\times 4} = \begin{bmatrix} F & & Z & \\ & I & & \\ Y & & D & \\ & & & I \end{bmatrix} \begin{bmatrix} F^{-1} & & & \\ & I & & \\ & & D^{-1} & \\ & & & I \end{bmatrix} \begin{bmatrix} F & B_u^T & & \\ B_u & C_u & & \\ & & D & B_b^T \\ & & B_b & C_b \end{bmatrix}$$

- Block LU with SIMPLEC for Magnetics-Velocity (Alfvén)
- Block LU with PCD or SIMPLEC for Fluids
- Block LU with SIMPLEC for magnetics

Do these splittings work?

Structurally small perturbation:

$$\mathcal{M}_{Split\text{-}3\times 3} = \begin{bmatrix} F & B^T & \hat{Z} \\ B & C & \\ \hat{Y} & \boxed{YF^{-1}B^T} & \hat{D} \end{bmatrix}$$

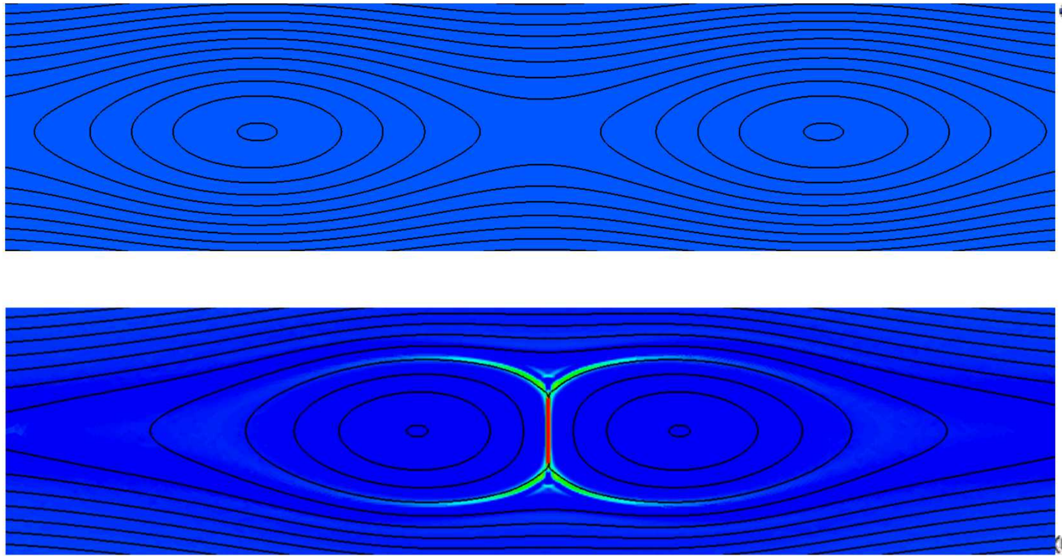
Favorable spectrum:

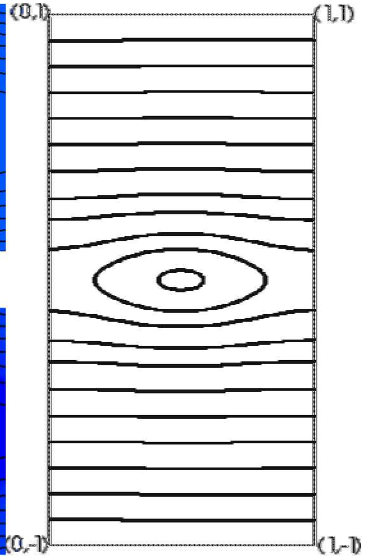
$$\mathcal{J}\mathcal{M}_{Split\text{-}3\times 3}^{-1} = \begin{bmatrix} I & & \\ & I & \\ A_1 & A_2 & (D - YF^{-1}K_u Z)\hat{P}^{-1} \end{bmatrix}$$

$$A_1 = YF^{-1}K_u$$
$$A_2 = -YF^{-1}B^T S_u^{-1}$$

$$S_u = C - BF^{-1}B^T$$
$$K_u = I + B^T S_u^{-1} B F^{-1}$$
$$\hat{P} = D - YF^{-1}Z$$

Island Coalescence: 2D Vector Potential





Simulation on half domain

- Symmetry BC
- Perturbed Harris-Sheet

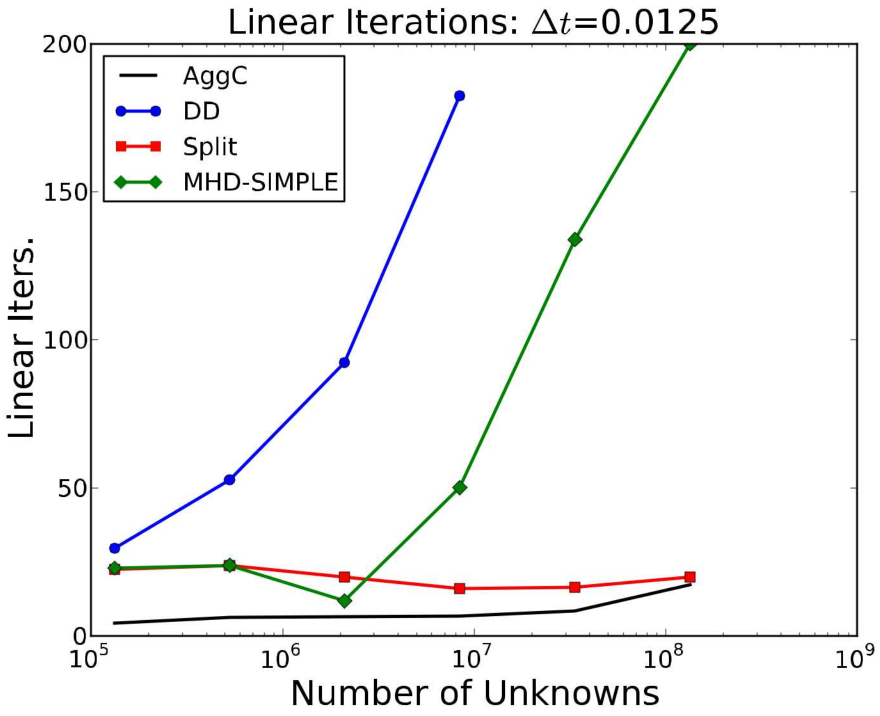
$$A_z^0(x,y,0) = \delta \; ln \left[\cosh\left(\frac{y}{\delta}\right) + \epsilon \; \cos\left(\frac{x}{\delta}\right)\right]$$

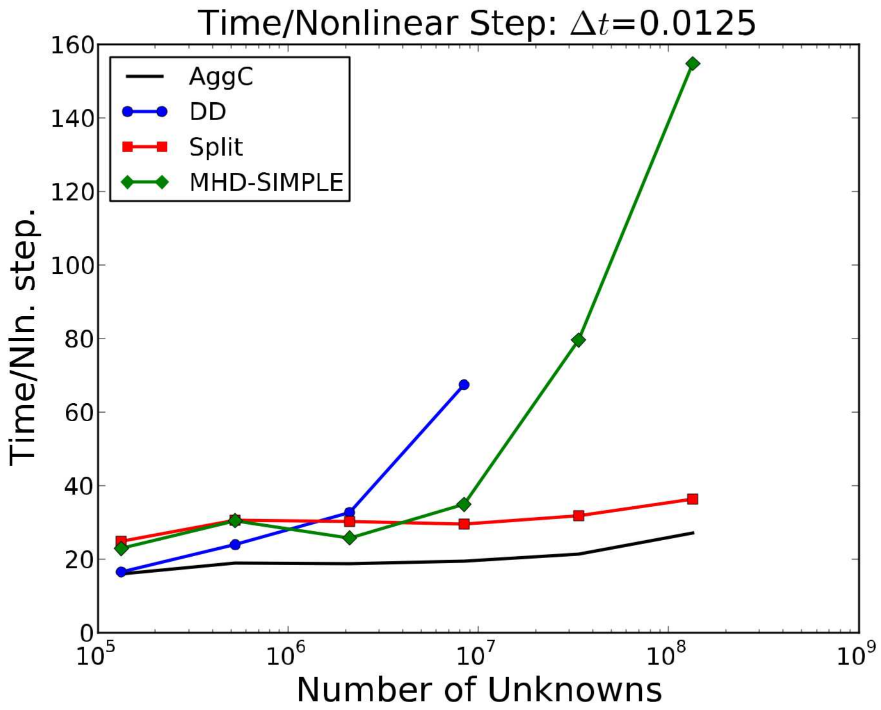
-1

Results details (an initial study):

- Lundquist number: 10^4
- Starting time right before reconnection: 5.75s
- Results averaged over 45 uniform time steps
- Run on 1, 4, 16, 64, 256, and 1024 processors (~33000 unks/core)

Island Coalescence: Weak Scaling





Fully coupled Algebraic

AggC: Aggressive Coarsening Multigrid

DD: Additive Schwarz Domain Decomposition

Block Preconditioners

Split: New Operator split preconditioner

SIMPLEC: Extreme diagonal approximations

Take home: Split preconditioner scales algorithmically, more relevant for mixed discretizations

References

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1. Perot, J. Blair. An analysis of the fractional step method. *Journal of Computational Physics* 108, no. 1 (1993): 51-58.
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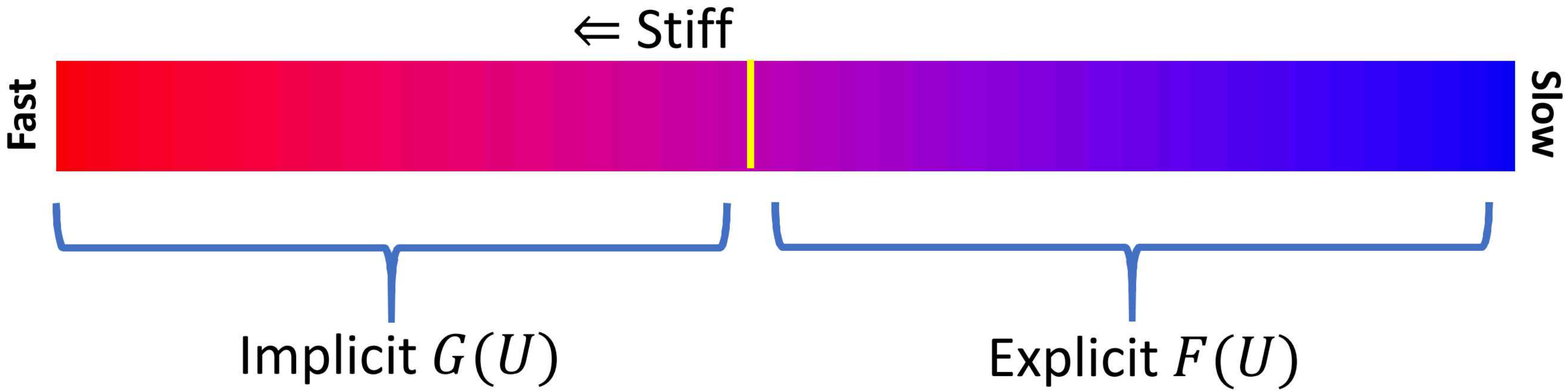
Outline

1. A motivating example: Multi-Fluid Plasmas
    - Types of time scales
    - Quantifying stiffness
2. Fully implicit methods
    - Motivating example
    - Block preconditioners
3. Time integration
    - IMEX RK
    - ALE Methods
4. Multi-fluid plasmas
5. Final Thoughts

Implicit-Explicit (IMEX) Time integration



- IMEX assumes additive splitting into fast (G) and slow (F) modes

$$\dot{\mathcal{U}} + F(\mathcal{U}) + G(\mathcal{U}) = 0$$

- Focuses implicit algorithm on only the modes that require it
- We again use Newton-Krylov to evolve implicit physics

IMEX Runge Kutta (IMEX-RK) Methods

Again, an ODE where "F" is slow and "G" is fast:

$$\dot{\mathcal{U}} + F(\mathcal{U}) + G(\mathcal{U}) = 0$$

- Implicit-Explicit (IMEX) methods evolve "F" explicitly and "G" implicitly
- There are multi-step (BDF) and multi-stage (RK) versions of these methods
- Our focus is on IMEX-Runge Kutta (IMEX-RK) methods

IMEX-RK Methods

We start with an ODE:

$$\dot{\mathcal{U}} + F(\mathcal{U}) + G(\mathcal{U}) = 0$$

- Two Butcher tableaus are used:

$$\begin{array}{c|c} c & A \\ \hline & b^t \end{array}$$ is for implicit terms, $$\begin{array}{c|c} \hat{c} & \hat{A} \\ \hline & \hat{b}^t \end{array}$$ is for explicit terms

- An s-stage IMEX-RK method satisfies ('c' defines time node)

$$\mathcal{U}^{(i)} = \mathcal{U}^n - \Delta t \sum_{j=1}^{i-1} \hat{A}_{ij} F(\mathcal{U}^{(j)}) - \Delta t \sum_{j=1}^{i} A_{ij} G(\mathcal{U}^{(j)}) \qquad \text{for } i = 1 \ldots s,$$

$$\mathcal{U}^{n+1} = \mathcal{U}^n - \Delta t \sum_{i=1}^{s} \hat{b}_i F(\mathcal{U}^{(i)}) - \Delta t \sum_{i=1}^{s} b_i G(\mathcal{U}^{(i)})$$

Monolithic ALE Equations

Monolithic ALE scheme solves (x is the moving frame):

$$\left.\frac{\partial \mathbf{x}}{\partial t}\right|_{\boldsymbol{Y}} - \hat{\mathbf{v}} = \mathbf{0},$$

$$\left.\frac{\partial \boldsymbol{\mathcal{U}}}{\partial t}\right|_{\boldsymbol{Y}} + \nabla_{\mathbf{x}} \cdot \boldsymbol{\mathcal{F}} - [\nabla_{\mathbf{x}} \boldsymbol{\mathcal{U}}]\hat{\mathbf{v}} + \boldsymbol{\mathcal{S}} = \mathbf{0}$$

Depending on the choice of coordinate velocity we can recover:

Eulerian	(no mesh motion)
Lagrangian	(material velocity)
ALE	(prescribed mesh)

IMEX Monolithic ALE ODE Form

Treat mesh motion explicitly

$$\left.\frac{\partial \mathbf{x}}{\partial t}\right|_{\boldsymbol{Y}} - \hat{\mathbf{v}} = \mathbf{0},$$

$$\left.\frac{\partial \boldsymbol{\mathcal{U}}}{\partial t}\right|_{\boldsymbol{Y}} - [\nabla_{\mathbf{x}}\, \boldsymbol{\mathcal{U}}]\hat{\mathbf{v}} + \nabla_{\mathbf{x}} \cdot \boldsymbol{\mathcal{F}}_{\boldsymbol{I}} + \boldsymbol{\mathcal{S}}_{\boldsymbol{I}} + \nabla_{\mathbf{x}} \cdot \boldsymbol{\mathcal{F}}_{\boldsymbol{E}} + \boldsymbol{\mathcal{S}}_{\boldsymbol{E}} = \mathbf{0}$$

Implicit and Explicit

Rules of the game:

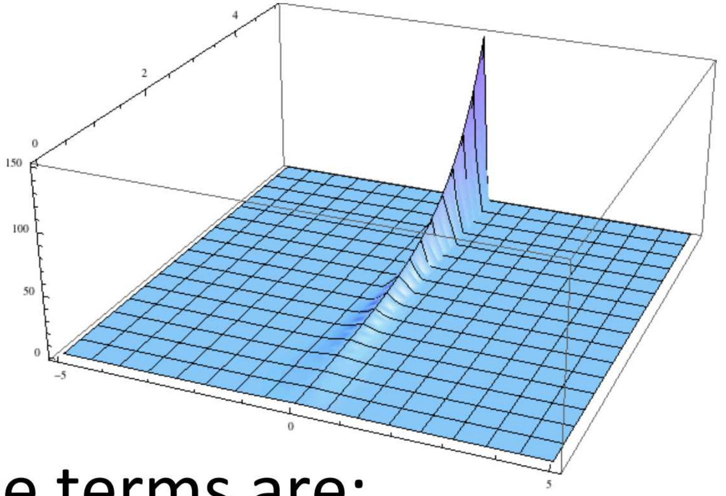
1. Mesh motion is treated explicitly
2. Other flux and source terms are handled implicitly or explicitly depending on “speed”
3. For ALE, we use a nonlinear elasticity formulation for mesh relaxation
4. Up to Lagrangian mesh nodes, mesh motion is linear within a IMEX Runge-Kutta step

Compressive CDR Problem

Transient nonlinear convection-diffusion-reaction (CDR) problem with an exact solution:

$$\frac{\partial e}{\partial t} + \frac{\partial}{\partial x}\left(ue - \lambda \frac{\partial e}{\partial x}\right) + S_e = 0$$

$$e = \left(1.0 + exp(t/\tau)\ sech\left[\frac{(1.0+t^2)x}{\delta}\right]\right)$$



Where the compressive velocity and nonlinear source terms are:

$$u = -U\ tanh\left[\frac{x}{\delta}\right]$$

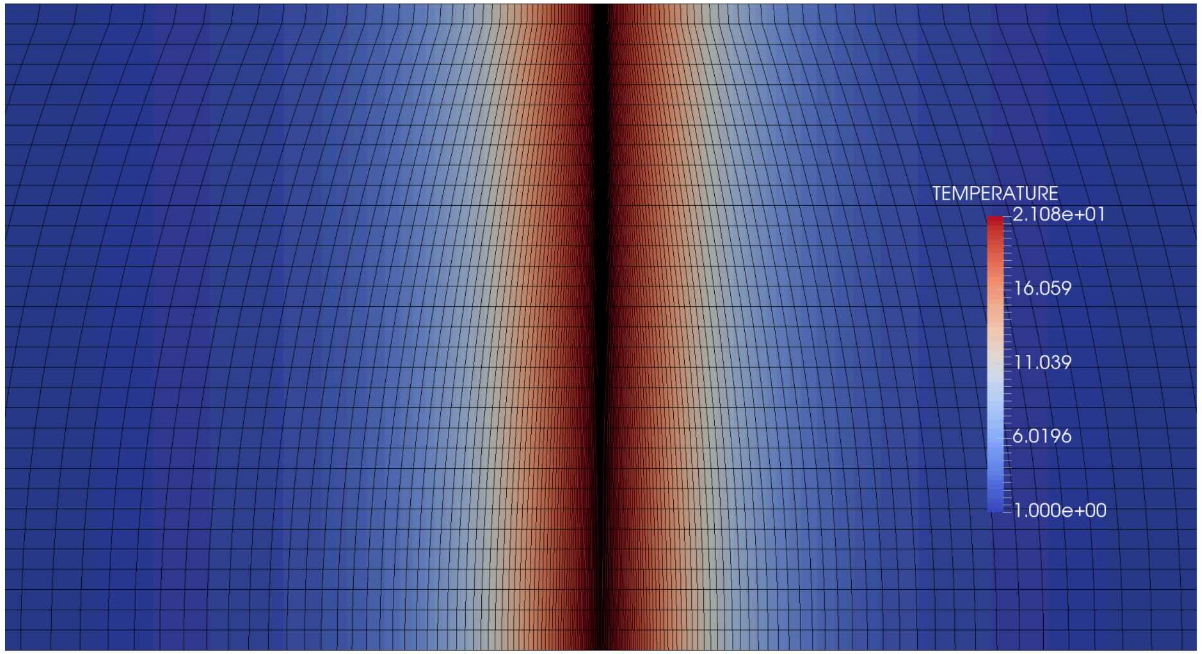
$$f_1 = \delta\ \tau\ U(1.0 - (u/U)^2)$$

$$f_2 = -(1.0+t^2)^2\ \lambda\ \tau + \delta^2 - f1$$

$$f_3 = \tau\ \delta\ (2\ t\ x + (1.0+t^2)\ u)\ tanh\left[\frac{((1.0+t^2)x}{\delta}\right]$$

$$S_e = \frac{\left[f_1 + (1.0-e) * \left(f_2 + \ 2\ \lambda\ \tau(1.0+t^2)^2\ [exp(-t/\tau)]^2(1.0-e)^2 - f_3\right)\right]}{\delta^2\ \tau}$$

Compression Problem: IMEX ALE

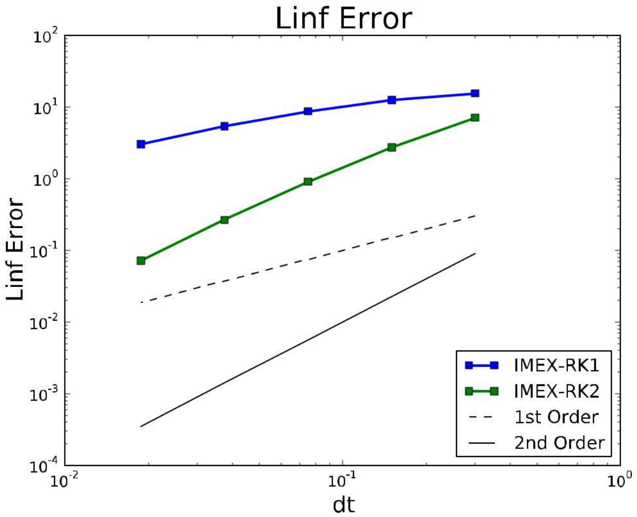


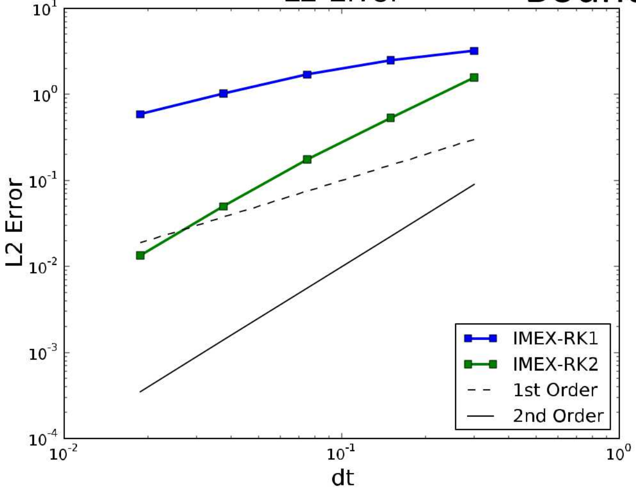
Lagrangian Boundary

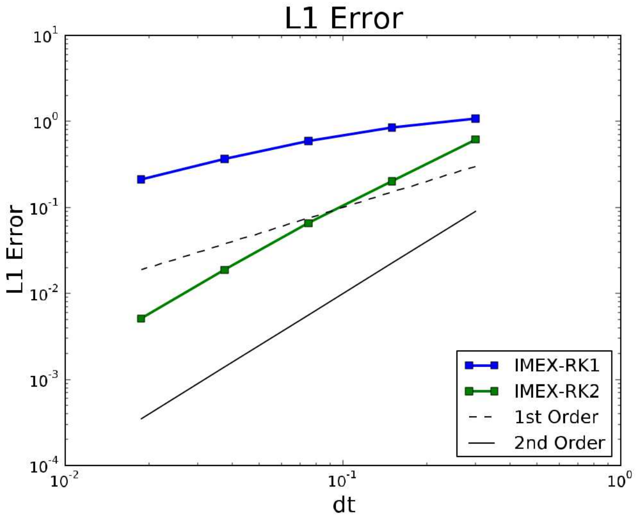
ALE Volume

Eulerian Boundary

Nx	Ny	Nt
16	2	10
32	4	20
64	8	40
128	16	80
256	32	160







Euler Equations: ALE Form

Our early efforts have focused on making mesh motion explicit

- Other terms are handled implicitly

$$\partial_t \mathbf{x} = \hat{\mathbf{v}}$$

$$\partial_t \rho = -\nabla \cdot (\rho \mathbf{u}) + (\nabla \rho)\hat{\mathbf{v}}$$

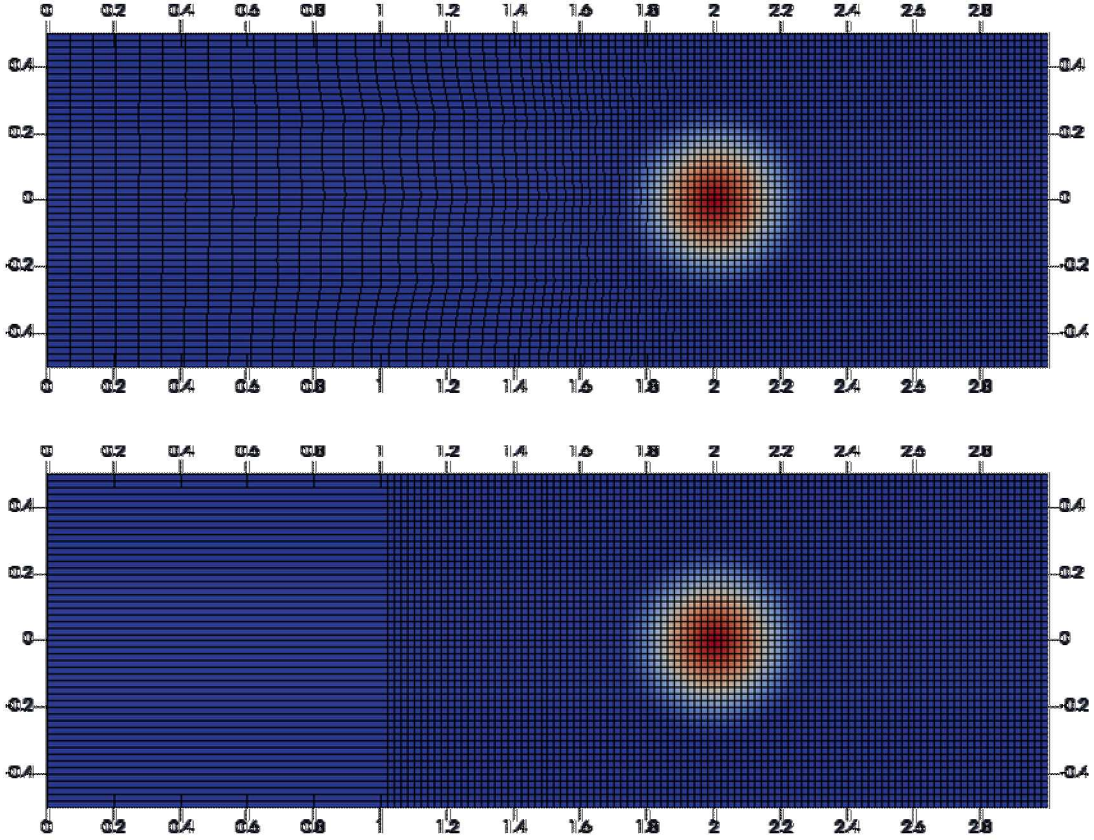
$$\partial_t (\rho \mathbf{u}) = -\nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} - \mathbf{T}) + (\nabla (\rho \mathbf{u}))\hat{\mathbf{v}}$$

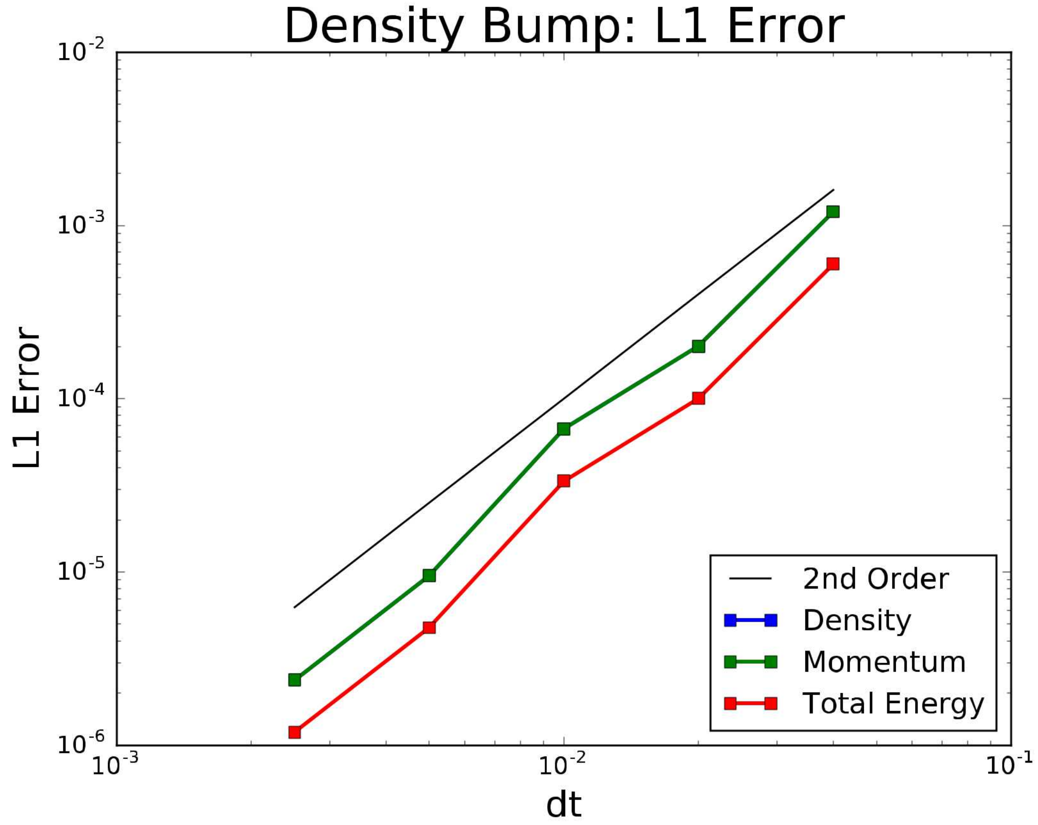
$$\partial_t E = -\nabla \cdot (E\mathbf{u} - \mathbf{T}^T + \mathbf{q}) + (\nabla E)\hat{\mathbf{v}}$$

ALE Convergence results: Mach 1.333

Euler equations advection of a smooth density hump in a constant velocity field

- No natural dissipation



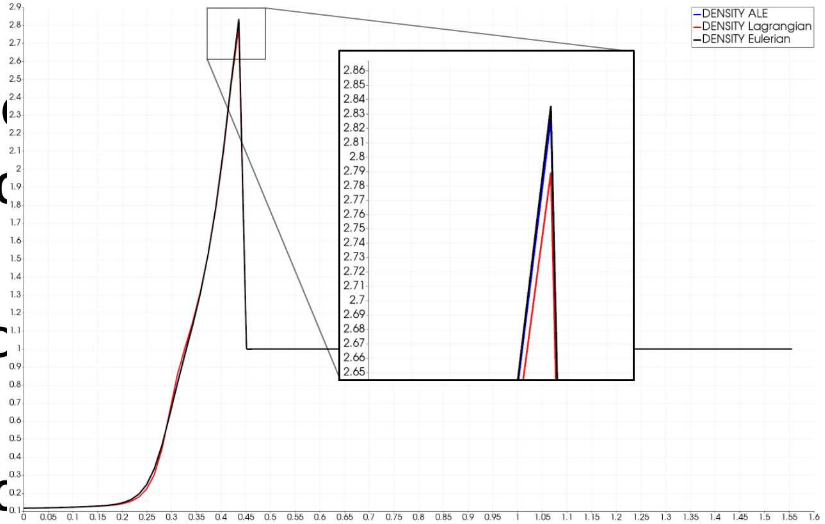


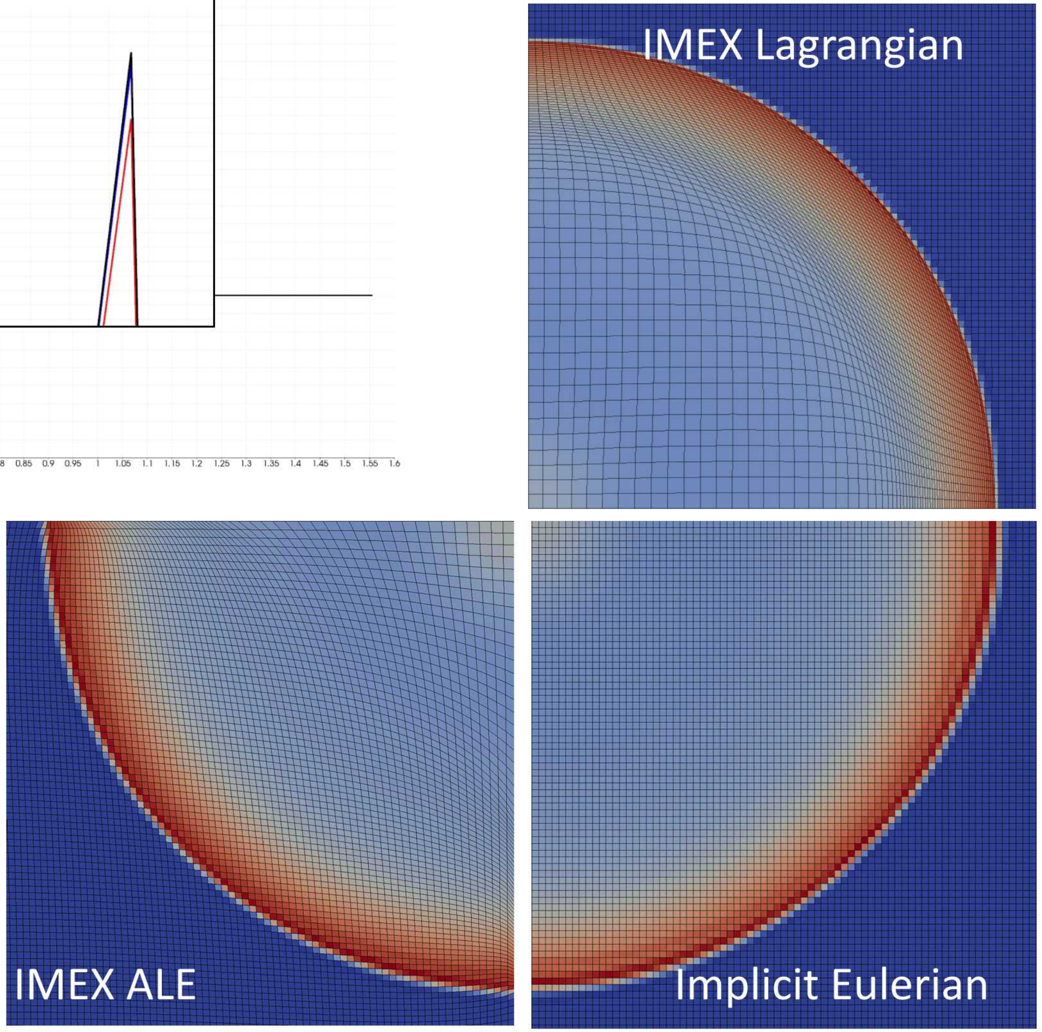
For smooth profiles IMEX expected convergence rate is achieved

Sedov type problem

This is a diffusive Euler pr

- Viscosity=Thermal Conc
- Lagrangian has explicit and implicit ALE convec
- ALE: 75% of Lagrangian the top and right bounc relax in interior





Take Home: IMEX ALE schemes can be applied to complex mesh motion problems (more work still required)

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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

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

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

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 (not discussed today, I can talk off line)
2. **Implicit-Explicit (IMEX) time integration to handle multiple time scales**

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$\sim |\mathrm{B}| \Delta t$

Plasma: Electrons and Electromagnetics

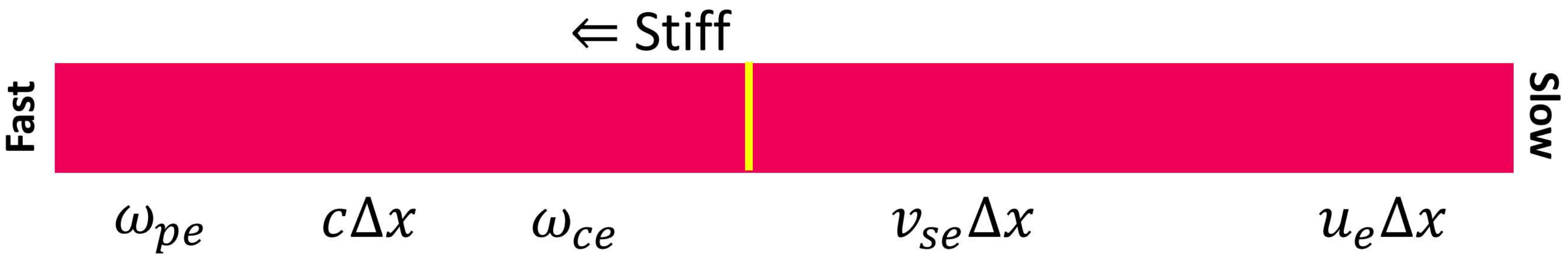
- Use IMEX to integrate fast electromagnetic time scales with an implicit solver, and slow fluid time scales with an explicit solver.

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) = 0$$

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

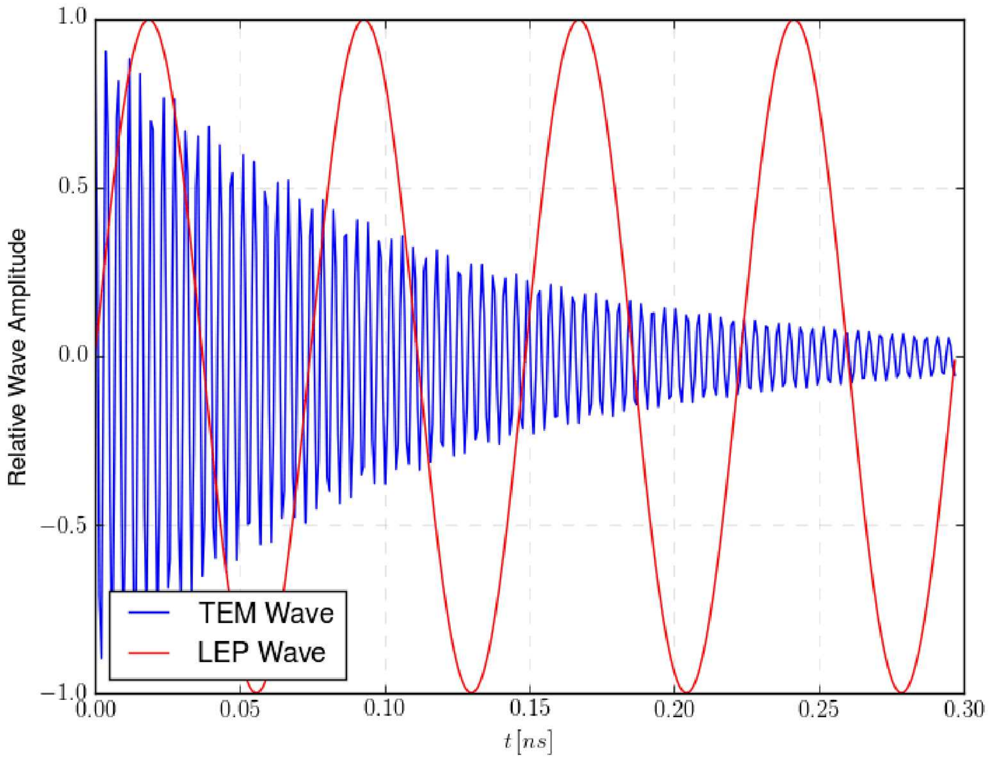
$$\frac{\partial \mathbf{E}}{\partial t} - c^2 \nabla \times \mathbf{B} = -\frac{1}{\epsilon_0} \sum_\alpha \frac{q_\alpha}{m_\alpha} \rho_\alpha \mathbf{u}_\alpha$$

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



Plasma: IMEX damps fast time scales

- L-stable implicit time integrator in IMEX stabilizes fast, under-resolved modes.



Transverse Electromagnetic (TEM) waves

Fast (speed of light)

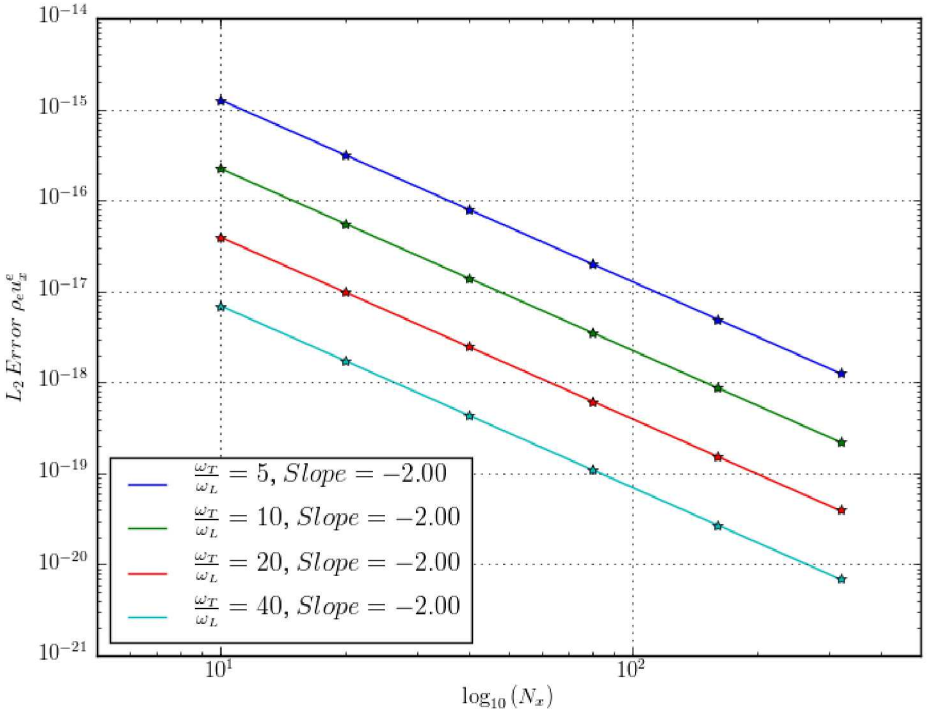
Longitudinal Electron Plasma (LEP) waves

Slow (speed of sound)

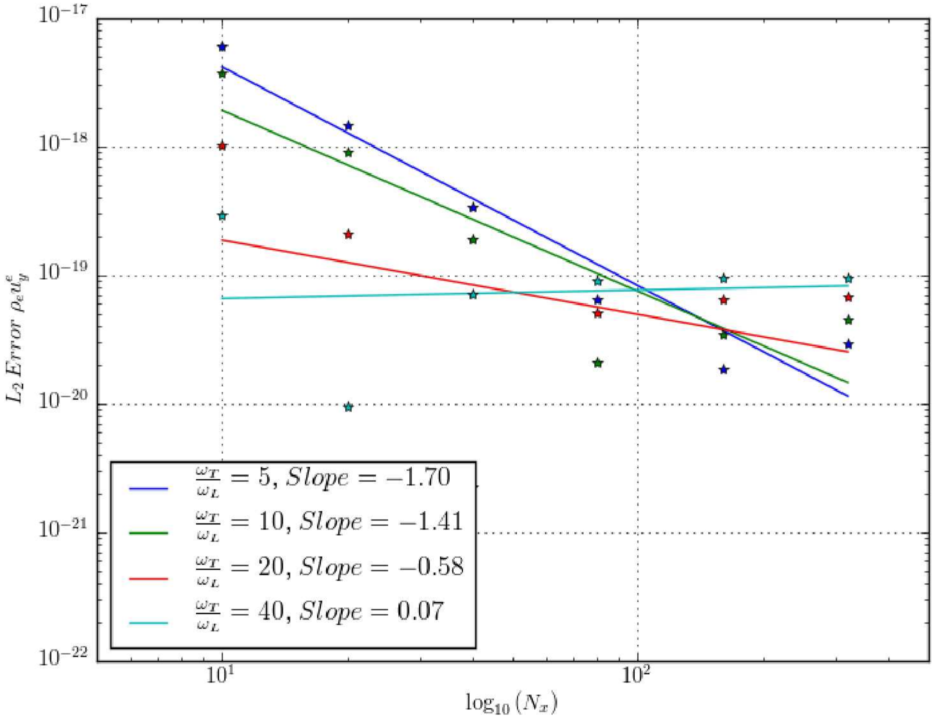
- Under-resolved fast modes may not impact dynamics of interest, and can therefore be ignored.

Plasma: Convergence

Resolved explicit modes converge at proper order for IMEX integrator



Under resolved implicit components may not converge due to phase and amplitude distortion



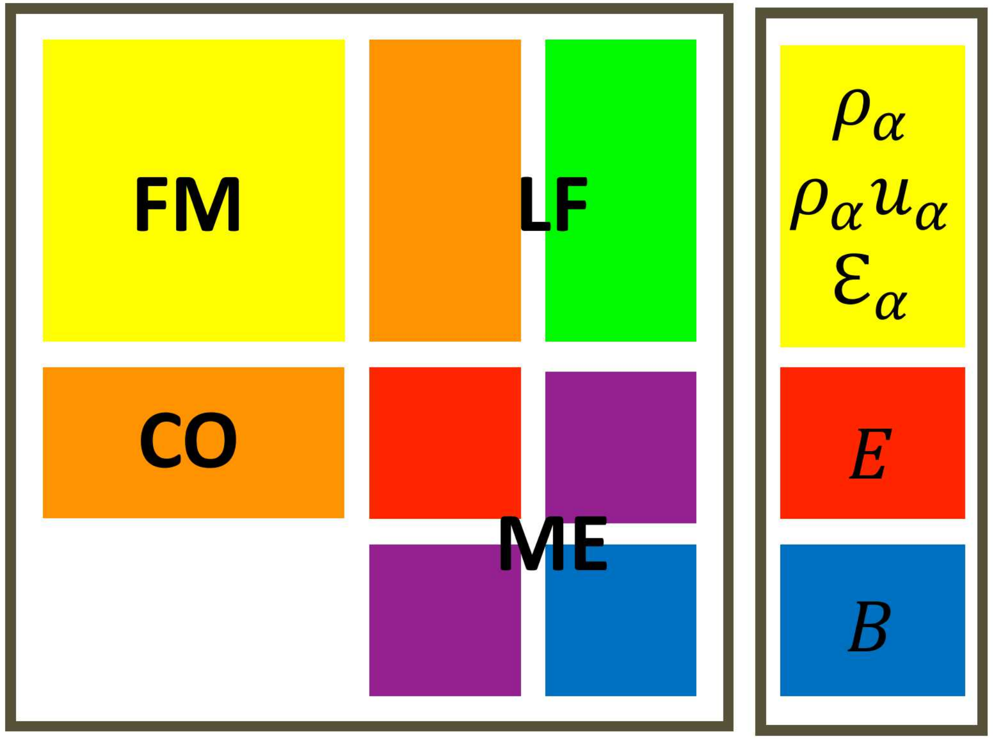
Nonlinear Algorithm

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.

Examining the IMEX Scheme

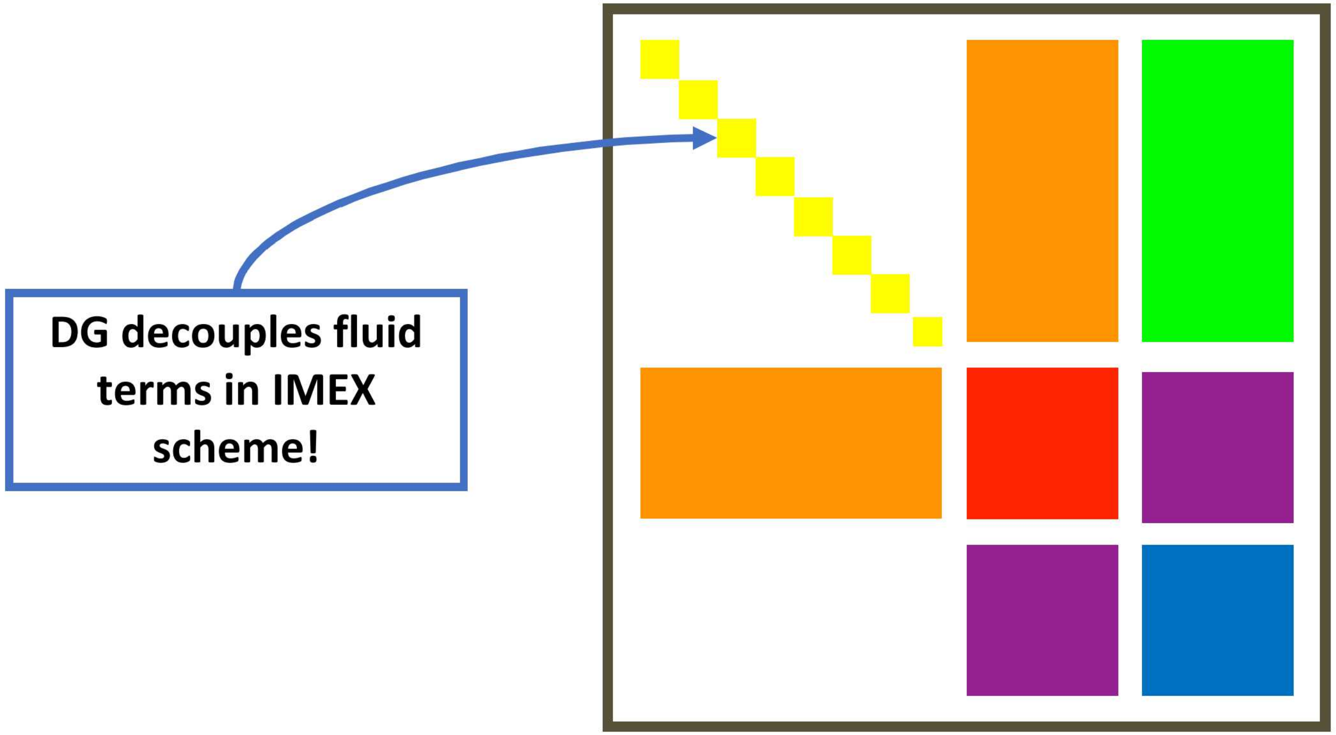
- Fluid matrix is mass matrix (CG fluids gives global coupling)
- Maxwell solver is effective (and should remain unperturbed)
  - Handles speed of light coupling
- Important to get plasma frequency and cyclotron frequency coupling
  - Handled by preconditioning
  - These are local (ODE-like) coupling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

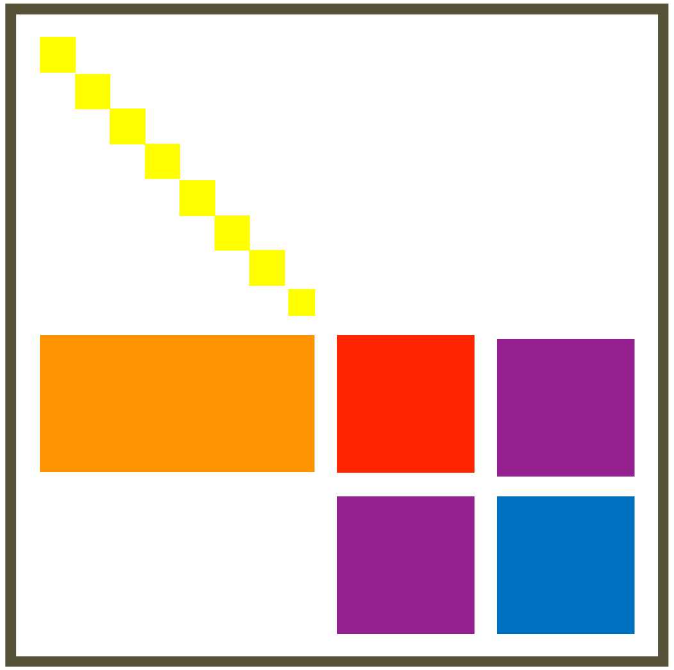
- DG Fluids will make the fluid contribution block diagonal on each element
  - ➢ Local nature of DG discretization
  - ➢ IMEX splitting choice
- Support for involutions still preserved
  - ➢ No Magnetic monopoles is the same
  - ➢ Weak enforcement of Gauss' law works (math is more complex)



Quasi-Newton Method

Typically I would do Newton-Krylov, but…

Block lower Gauss-Seidel



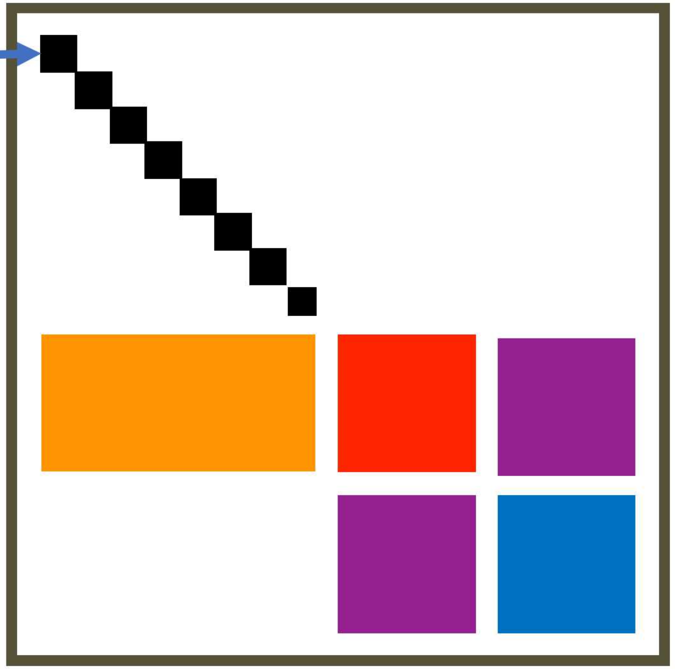
- ✓ Triangular solve
- ✓ Leverages Maxwell solver
- ✓ Block diagonal fluid solve
- ✓ Implicit cyclotron frequency
- ✗ Implicit plasma frequency

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.

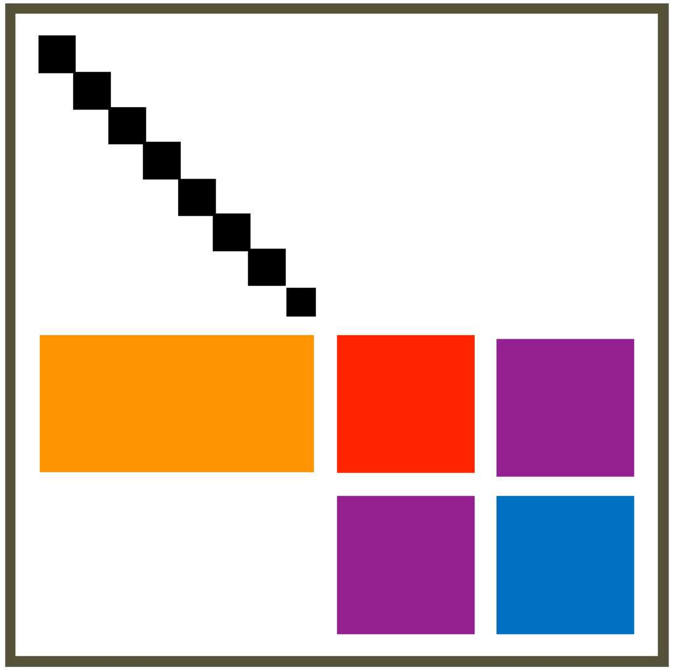
- Mode derived from coupling Ampere's law and momentum equation

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

- 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



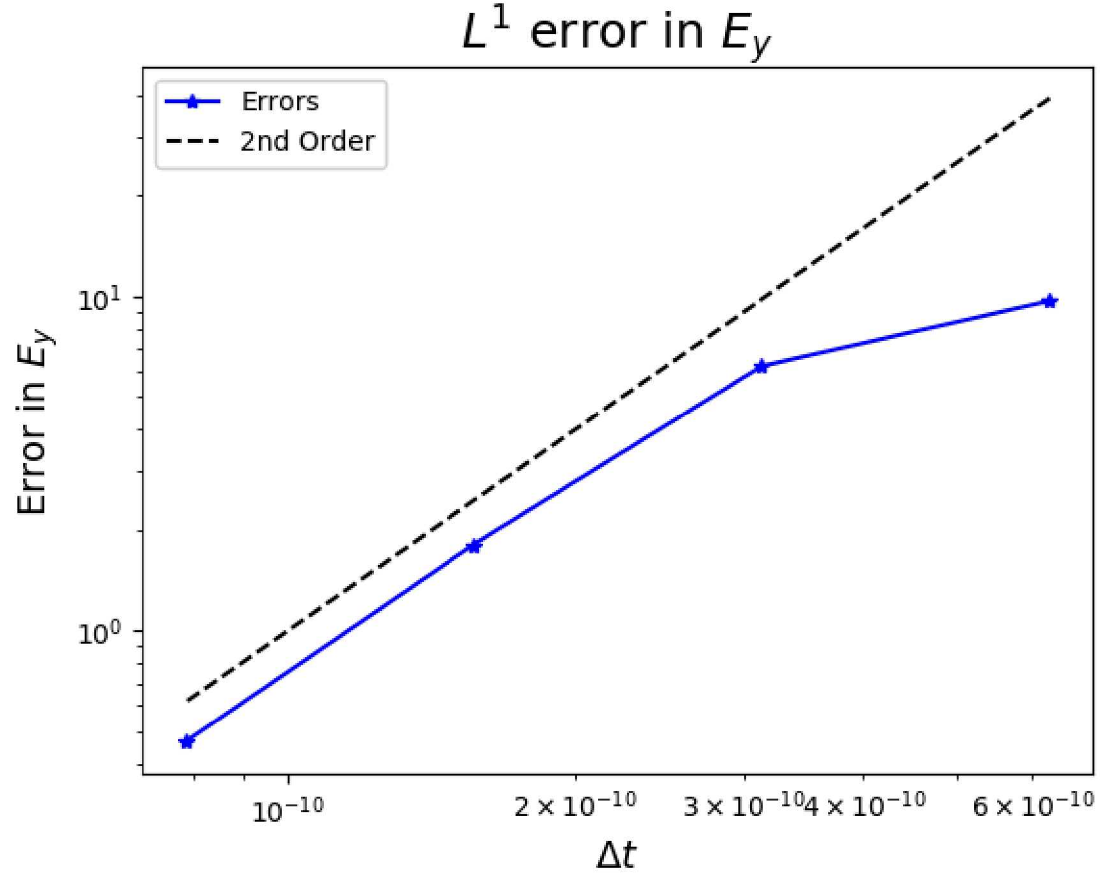
(Unlike the "analysis" above, we use the full current in the Schur complement correction)

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.

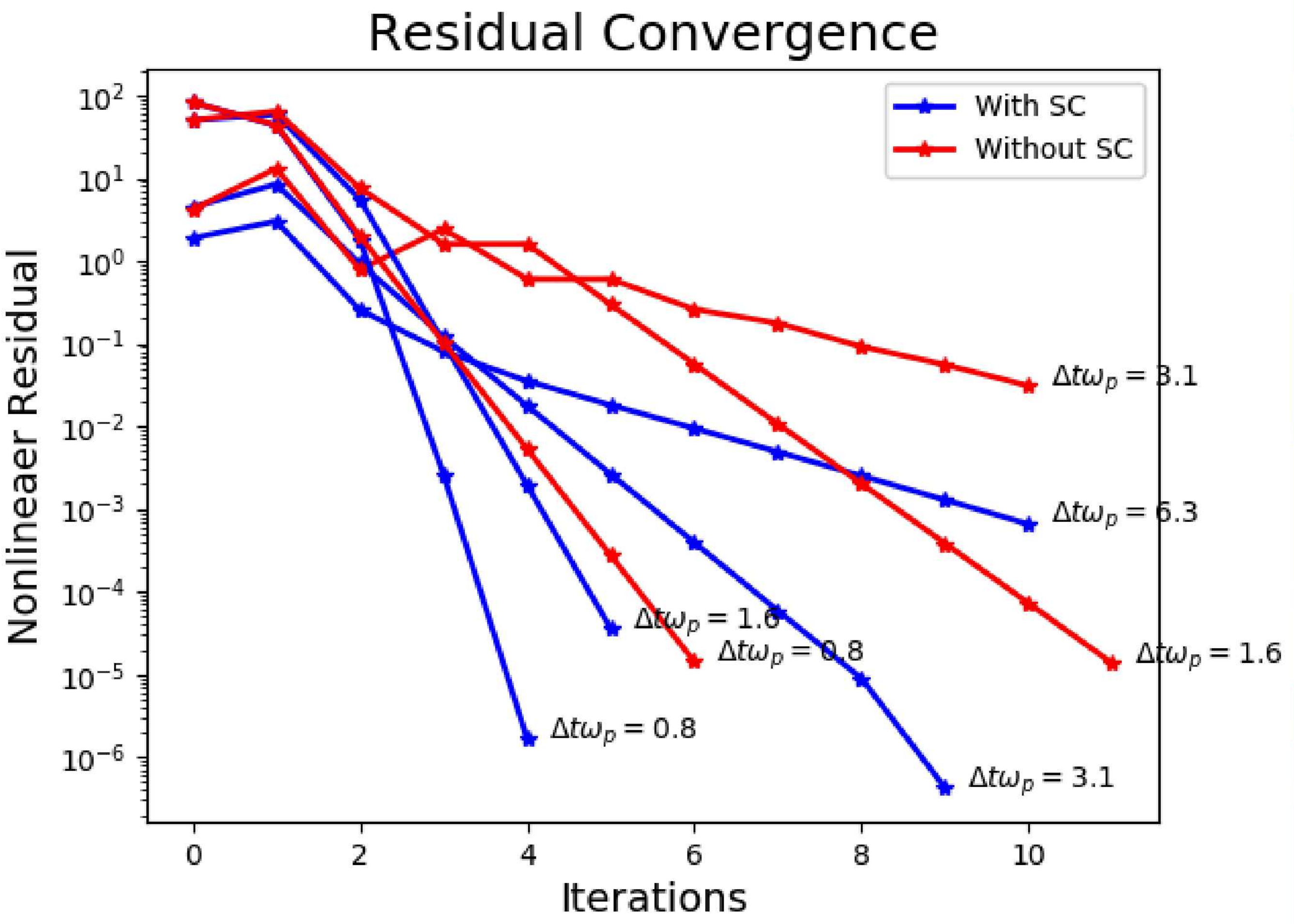
O-Wave Nonlinear Solver (EMPIRE-Fluid)

Adding Schur complement improves nonlinear convergence

- Still has strong growth in iteration count with increasing time steps
- Schur complement assembly takes a small fraction longer than without
- 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 $x_{k+1} = g(x_k) - \mathcal{G}_k \gamma^{(k)}$.

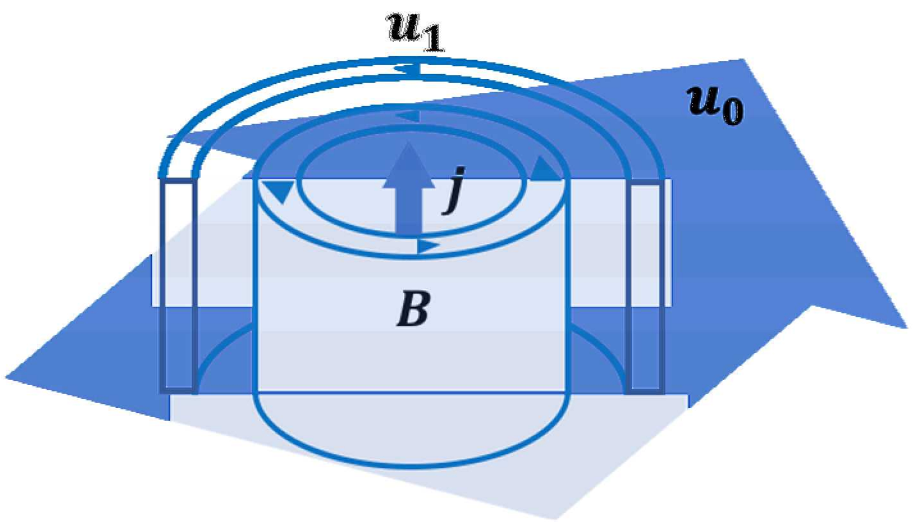
$f_i = g(x_i) - x_i$
$\mathcal{F}_k = (\Delta f_{k-m_k}, \ldots, \Delta f_{k-1})$ with $\Delta f_i = f(x_{i+1}) - f(x_i)$.
$\mathcal{G}_k = (\Delta g_{k-m_k}, \ldots, \Delta g_{k-1})$ with $\Delta g_i = g(x_{i+1}) - g(x_i)$.

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!

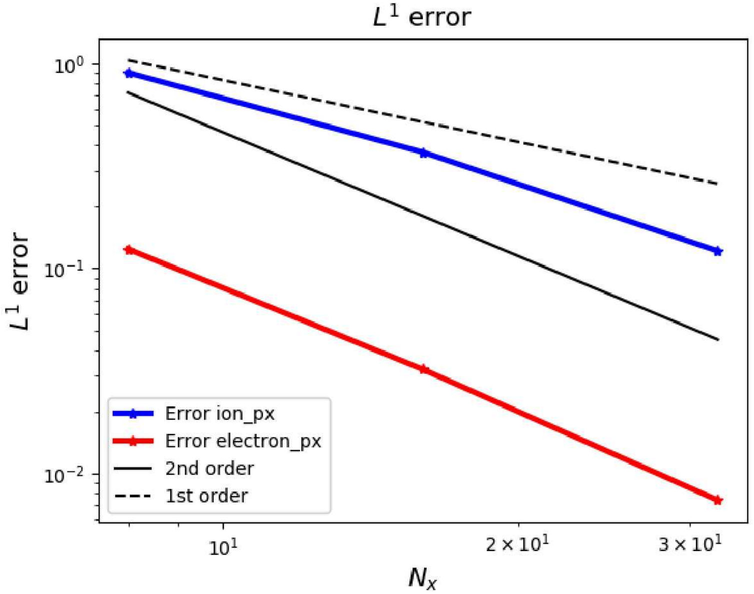
Two Fluid Plasma Vortex

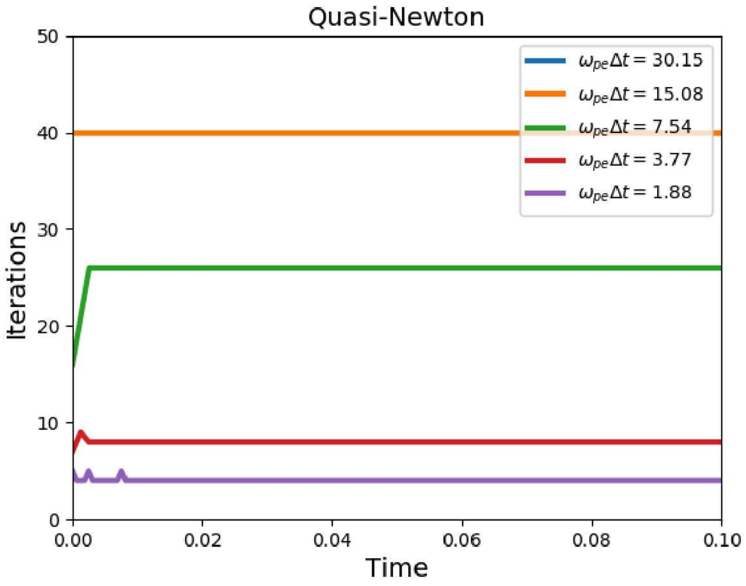
Two fluid plasma vortex in MHD limit
- IMEX time discretization, DG fluid discretization, CG Maxwell discretization
- Using Schur-Complement in all simulations

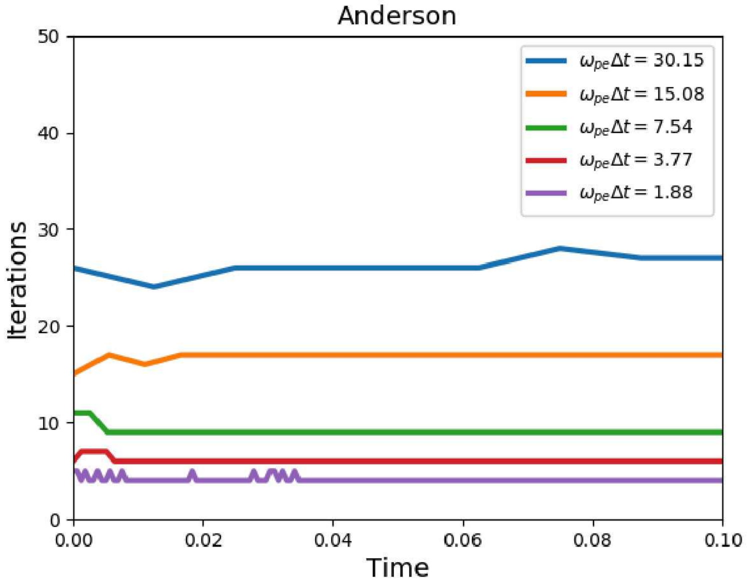


Convergence study:
- N_x x N_x x N_x =[8x8x8, 16x16x16, 32x32x32]
- N_t = [10,20,40]
- Speed of light: C dt/dx = 8

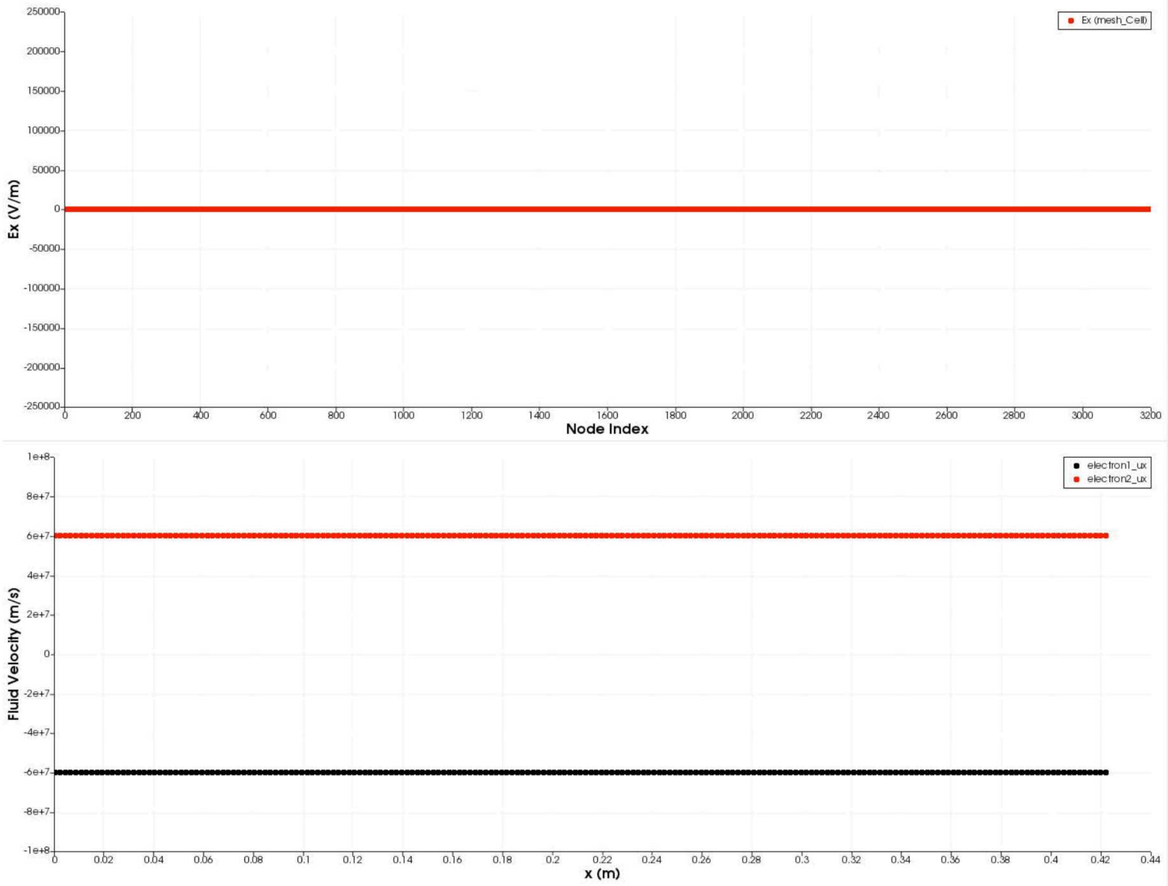
Iteration study: 8x8x8 grid

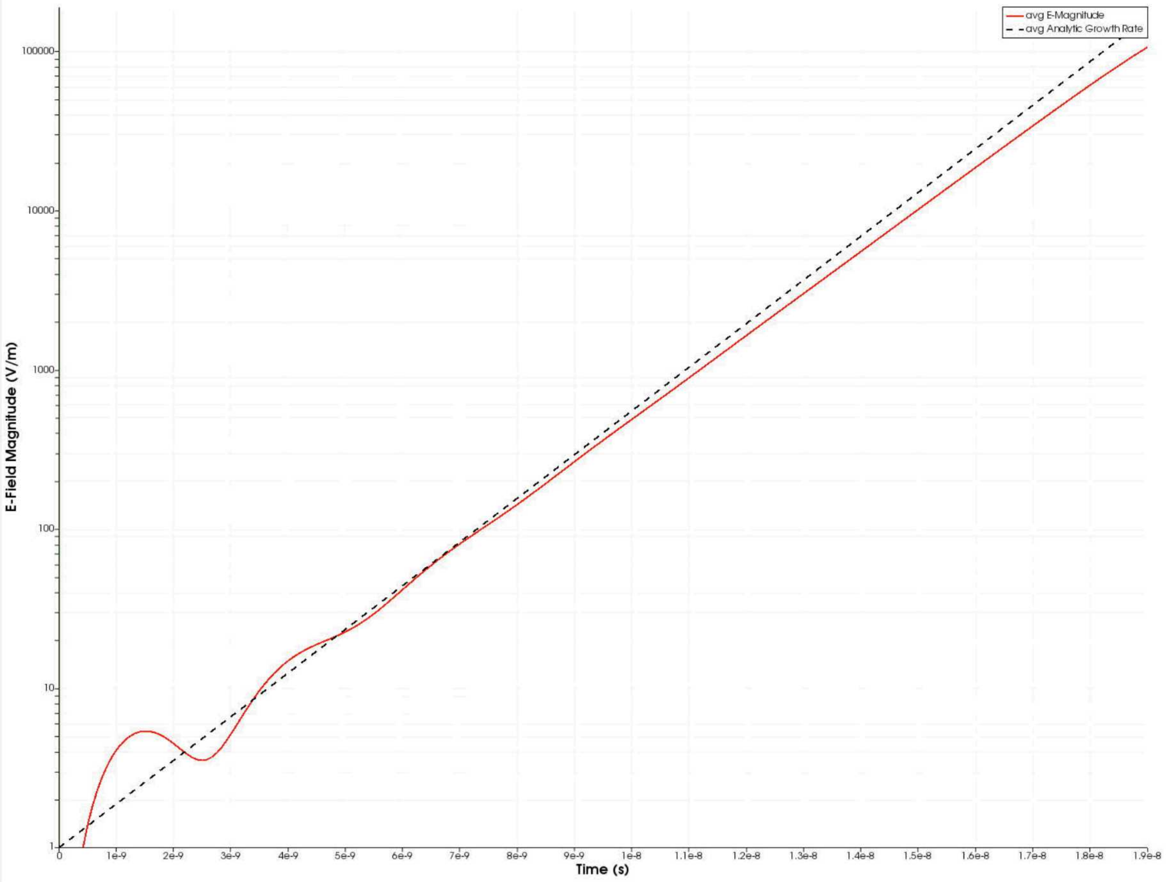






Two Stream Instability*





* We run this only through the linear growth regime

Outline

Final Thoughts

1. Stiffness is as much a function of the question asked of the model, as the model itself
2. Preconditioners for multi-physics can target stiff physics and ignore non-stiff physics and still scale
3. Time integration targeting implicit evolution of only stiff physics can simplify preconditioner construction and still yield high-order: IMEX
4. Combining different techniques, physics-based/block-preconditioning, IMEX time integration and carefully chosen spatial discretization leads to methods with attractive computational characteristics
5. Considering moving beyond Newton-Krylov framework where appropriate using quasi-Newton and Anderson can simplify Jacobian/preconditioner construction and still achieve efficiencies (preliminary!)

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