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Block Preconditioning Informed by Plasma Timescales

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OVERVIEW

- Interested in large multiphysics systems with multiple length- and time-scales
- When time-scales of interest are much slower than the fastest time-scales in the system, implicit or IMEX time integration is a good option when efficient linear solvers are available

- Multifluid plasma equations as motivating example

- Take a physics-based approach to preconditioning
  - Block preconditioners segregated by physical degrees of freedom
  - Use properties known at a high level about the physics to improve and automatically tune the preconditioner to different use cases

- Illustrate this preconditioning strategy by analyzing multifluid plasma system

- Results and conclusions

MULTIFLUID PLASMA MODEL

CONTINUUM PLASMA MODELS

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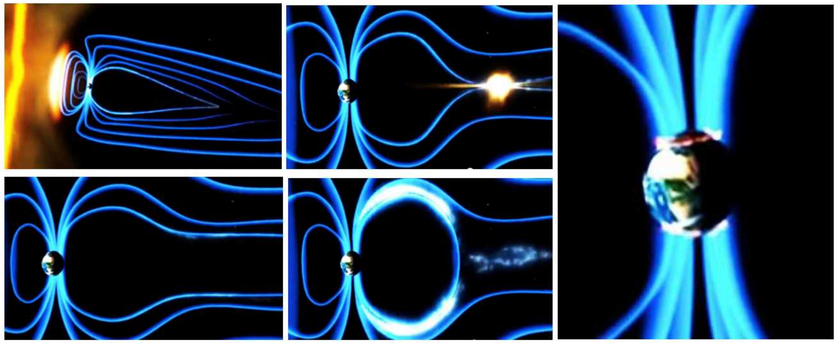
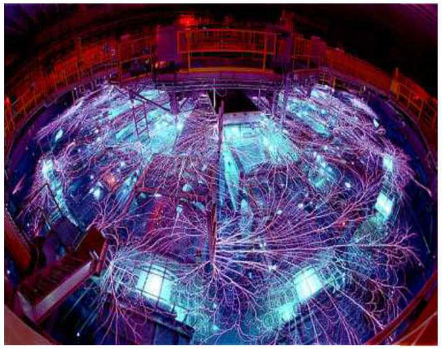
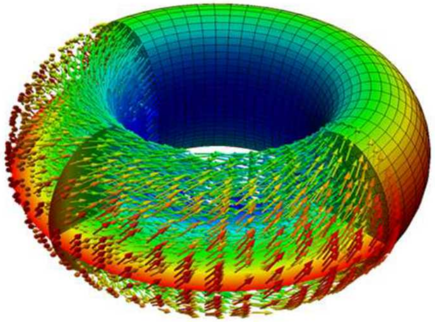
- Obtained from moments of a Boltzmann equation (5-moment, 13-moment models) + Maxwell equations
- Valid for dense plasmas where PIC models are prohibitively expensive
- Valid for finite charge separation where MHD approximations do not hold
- Set of hydrodynamic equations for each species (e.g. electrons, ions, neutrals) coupled through currents in Maxwell equations and Lorentz forces



NASA Magnetic Reconnection Animation (https://www.youtube.com/watch?v=i_x3s8ODaKg)



Z Machine



MHD Tokamak Equilibrium

ELECTRON-ION PLASMA SIMULATION

- 2D electron/ion plasma driven by an external current pulse with background magnetic field and density gradient
- Plasma scales:

$$c = 3.0e8$$
$$||\mathbf{u}_e|| = 2.0e5$$
$$||\mathbf{u}_i|| = 2.0e2$$
$$||\omega_{p,e}|| = 5.1e7$$
$$||\omega_{p,i}|| = 1.6e6$$
$$||\omega_{c,e}|| = 2.6e7$$
$$||\omega_{c,i}|| = 2.6e4$$
$$\frac{1}{\tau_{source}} = 2.0e5$$

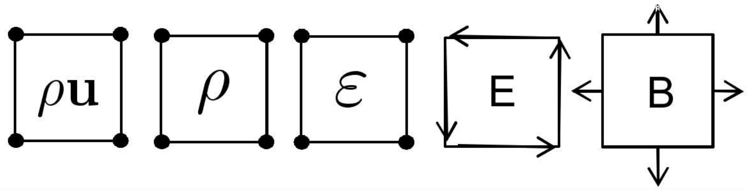
Electron momentum

Ion momentum

MULTIFLUID 5-MOMENT PLASMA MODEL

Density	$$\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a) = \sum_{b \neq a} (n_a \rho_b \bar{\nu}^+_{ab} - n_b \rho_a \bar{\nu}^-_{ab})$$
Momentum	$$\frac{\partial (\rho_a \mathbf{u}_a)}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a \otimes \mathbf{u}_a + p_a I + \Pi_a) = q_a n_a (\mathbf{E} + \mathbf{u}_a \times \mathbf{B}) - \sum_{b \neq a} [\rho_a (\mathbf{u}_a - \mathbf{u}_b) n_b \bar{\nu}^M_{ab} + \rho_b \mathbf{u}_b n_a \bar{\nu}^+_{ab} - \rho_a \mathbf{u}_a n_b \bar{\nu}^-_{ab}]$$
Energy	$$\frac{\partial \varepsilon_a}{\partial t} + \nabla \cdot ((\varepsilon_a + p_a)\mathbf{u}_a + \Pi_a \cdot \mathbf{u}_a + \mathbf{h}_a) = q_a n_a \mathbf{u}_a \cdot \mathbf{E} + Q^{src}_a - \sum_{b \neq a} \left[(T_a - T_b) k \bar{\nu}^E_{ab} - \rho_a \mathbf{u}_a \cdot (\mathbf{u}_a - \mathbf{u}_b) n_b \bar{\nu}^M_{ab} - n_a \bar{\nu}^+_{ab} \varepsilon_b + n_b \bar{\nu}^-_{ab} \varepsilon_a \right]$$
Charge and Current Density	$$q = \sum_k q_k n_k \qquad \mathbf{J} = \sum_k q_k n_k \mathbf{u}_k$$
Maxwell's Equations	$$\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} + \mu_0 \mathbf{J} = \mathbf{0} \qquad \nabla \cdot \mathbf{E} = \frac{q}{\epsilon_0}$$ $$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0} \qquad \nabla \cdot \mathbf{B} = 0$$

Nodal discretization for fluids, Compatible discretization for electromagnetics



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TIME INTEGRATION FOR MULTIFLUID PLASMAS

Eigen-values for 5M Euler Eqn for each species

$$\lambda_\alpha = (u_\alpha, u_\alpha \pm \sqrt{\gamma T_\alpha / m_\alpha})$$

Time-scales from Maxwell Eqn. & EM source terms

$$\tau_{EM} = \Delta x / c; \quad \tau_{\omega_{p\alpha}} = \frac{1}{\sqrt{\frac{n_\alpha q_\alpha^2}{\epsilon_0 m_\alpha}}}; \quad \tau_{\omega_{c\alpha}} = \frac{1}{\frac{q_\alpha B}{m_\alpha}}$$

A possible ordering of time-scales:

$$\tau_{EM} \le \tau_{\omega_{pe}} \le \tau_{\omega_{ce}} \le \tau_{\omega_{pi}} \le \tau_{\omega_{ci}} \le \tau_{ue} \le \tau_{ce} \le \tau_{ui} \le \tau_{ci}$$

Δt_{dyn} (at τ_{EM}): Fully EXPLICIT

Need linear solvers that can handle integrating over fast time-scales. Must be flexible about time-scale ordering.

Δt_{dyn} (at τ_{ce}): ← IMPLICIT | EXPLICIT →

Δt_{dyn} (at τ_{ci}): Fully IMPLICIT

Of course stablilty *does not imply accuracy*.

TIME-SCALES AND OPERATORS IN THE PLASMA EQUATIONS

Plasma Osc. $CFL_{p,\alpha} = \Delta t \sqrt{\frac{q_\alpha^2}{m_\alpha^2} \frac{\rho}{\varepsilon}}$

Density	$=$
Momentum	$+ \quad + \Pi_a) = \quad + \quad)$ $-$
Energy	$+ \Pi_a \cdot \mathbf{u}_a + \mathbf{h}_a) = \quad + Q_a^{src}$ $-$
Charge and Current Density	$q = \sum_k q_k n_k \qquad \mathbf{J} = \sum_k q_k n_k \mathbf{u}_k$
Maxwell's Equations	$+ \quad = \mathbf{0} \qquad \nabla \cdot \mathbf{E} = \frac{q}{\epsilon_0}$ $= \mathbf{0} \qquad \nabla \cdot \mathbf{B} = 0$

PHYSICS-BASED PHILOSOPHY FOR BLOCK PRECONDITIONING

BLOCK PRECONDITIONING IN CFD

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- Navier-Stokes

$$\begin{pmatrix} F & B^t \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} I & 0 \\ BF^{-1} & I \end{pmatrix} \begin{pmatrix} F & B^t \\ 0 & S \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix}$$

$$= -BF^{-1}B^t$$

- Blocks precond ... pproximations

$$\mathcal{P} = \begin{pmatrix} F & B^t \\ 0 & \hat{S} \end{pmatrix}$$

oximation; easy
dominant

- Commutator-b
  - PCD: req ... e pressure Laplace s
  - LSC: requ ... solves
  - Both worl ... vection CFL

Knowing which approximations work in which regimes, can we always use the cheapest preconditioner that will be effective for a given problem?

How much physics does the preconditioner need to know to achieve this?

- Augmented Lagrangian

$$\mathcal{P} = \begin{pmatrix} F + B^t W^{-1} B & B^t \\ 0 & \hat{S}_{aug} \end{pmatrix}$$

  - Works well for strong advection
  - More difficult solve in the (0,0) block although simpler Schur complement can be used

Block preconditioners inherit parallel scalability of multilevel subsolves

PHYSICS-BASED PHILOSOPHY FOR BLOCK PRECONDITIONING

- Time-scales dictate preconditioner parameters
  - Which Schur complement approximations to use
  - Subsolve settings
- Fast physics require more advanced Schur complement approximations (if off-diagonal) and/or more heavyweight solvers/smoothers
- Use cheapest settings possible $\rightarrow$ use lower fidelity approximations and simpler smoothers for slow physics
- Most solver details can be hidden from physics driver and user
  - The preconditioner only needs to know which time-scales are fast/slow)
  - Can be quantified with CFL numbers which can be automatically computed

APPLICATION TO NAVIER-STOKES

$$\begin{pmatrix} F & B^t \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} I & 0 \\ BF^{-1} & I \end{pmatrix} \begin{pmatrix} F & B^t \\ 0 & S \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix}$$

$$S = -BF^{-1}B^t$$

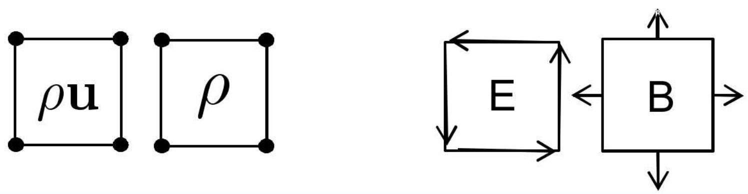
- Slow advection and diffusion (CFL_d < tol, CFL_a < tol)
  - Use SIMPLEC Schur complement approximation
  - Use cheap smoother (e.g. 2 sweeps of Gauss-Seidel) for velocity solve
- Slow advection, fast diffusion (CFL_a < tol)
  - Ignore advection $\longrightarrow$ time-dependent Stokes: use simplified version of PCD
- Fast advection (CFL_a > tol)
  - Use at least PCD for Schur complement (combine with AL for very fast advection)
  - Use more expensive smoother (e.g. ILU with overlap or Krylov smoothing) for velocity solve

MULTIFLUID PLASMA PRECONDITIONER

COLLISIONLESS, COLD SIMPLIFICATION

Density	$\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a) = \mathbf{0}$
Momentum	$\frac{\partial (\rho_a \mathbf{u}_a)}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a \otimes \mathbf{u}_a \quad) = q_a n_a (\mathbf{E} + \mathbf{u}_a \times \mathbf{B})$
Energy	
Charge and Current Density	$q = \sum_k q_k n_k \qquad \mathbf{J} = \sum_k q_k n_k \mathbf{u}_k$
Maxwell's Equations	$\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} + \mu_0 \mathbf{J} = \mathbf{0} \qquad \nabla \cdot \mathbf{E} = \frac{q}{\epsilon_0}$ $\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0} \qquad \nabla \cdot \mathbf{B} = 0$

Nodal discretization for fluids,
Compatible discretization for
electromagnetics

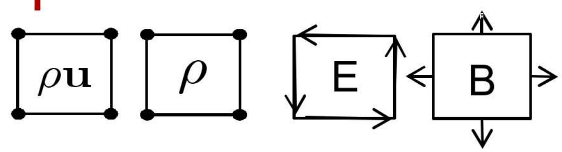


DISCRETE TWO-FLUID SYSTEM

- Fully discrete (cold, collisionless) two-fluid system:

$$
\left(\begin{array}{cc|cc|c|c}
A_e & G_e & 0 & 0 & Q_E^e & Q_M^e \\
B & Q_\rho & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & A_i & G_i & Q_E^i & Q_B^i \\
0 & 0 & B & Q_\rho & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & Q_B & K \\
\hline
Q_e^E & 0 & Q_i^E & 0 & -\hat{K}^t & Q_E
\end{array}\right)
\left(\begin{array}{c}
\rho_e \mathbf{u}_e \\
\rho_e \\
\rho_i \mathbf{u}_i \\
\rho_i \\
\mathbf{B} \\
\mathbf{E}
\end{array}\right)
$$

Block each fluid species, E, and B separately. Segregates DOFs by discretization type, and allows faster species to be treated differently from slow species.



- …pling and can range over many orders
- Disparate discretizations make it difficult to apply monolithic multigrid solvers

ANALYZE SPECIES BY SPECIES

$$\begin{pmatrix} D_\alpha & Q_B^\alpha & Q_E^\alpha \\ 0 & Q_B & K \\ Q_\alpha^E & -\hat{K}^t & Q_E \end{pmatrix} \begin{pmatrix} \mathbf{F}_\alpha \\ \mathbf{B} \\ \mathbf{E} \end{pmatrix}$$

- F contains moment $\rho_\alpha)$
- Different factorizat ner forms, with different Schur con

Let the time-scales dictate which factorization to use for each species

$$\mathcal{P}_1 = \begin{pmatrix} S_\alpha & 0 & 0 \\ 0 & Q_B & K \\ Q_\alpha^E & 0 & S_E \end{pmatrix} \qquad \mathcal{P}_2 = \begin{pmatrix} D_\alpha & Q_B^\alpha & Q_E^\alpha \\ 0 & Q_B & K \\ 0 & 0 & S_{E,\alpha} \end{pmatrix}$$

$$S_E = Q_E + \hat{K}^t Q_B^{-1} K$$

$$S_\alpha = D_\alpha - (Q_E^\alpha - Q_B^\alpha Q_B^{-1} K) S_E^{-1} Q_\alpha^E$$

$$S_{E,\alpha} = S_E - Q_\alpha^E F_\alpha^{-1} Q_E^\alpha + Q_\alpha^E F_\alpha^{-1} Q_B^\alpha Q_B^{-1} K$$

DETAILED ANALYSIS OF SLOW LIGHT WAVE

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$$CFL_c = c\frac{\Delta t}{\Delta x} = \frac{1}{\sqrt{\varepsilon\mu}}\frac{\Delta t}{\Delta x} < \tau$$

- Fully resolved electromagnetic effects
- Although no physical speeds exceed the speed of light, the numerical time-scale associated with the plasma frequency can be faster at large length-scales

$$CFL_{p,\alpha} = \Delta t\sqrt{\frac{q_\alpha^2}{m_\alpha^2}\frac{\rho_\alpha}{\varepsilon}}$$

- Advection should always be slow in this setting

$$CFL_{a,\alpha} = ||\mathbf{u}_\alpha||\frac{\Delta t}{\Delta x}$$

- Electromagnetic Schur complement dramatically simplifies

$$||\hat{K}^t Q_B^{-1} K|| \approx \frac{\Delta t}{\mu\Delta x^2} < \tau^2\frac{\varepsilon}{\Delta t} \approx \tau^2||Q_E||$$

$$S_E = Q_E + \hat{K}^t Q_B^{-1} K \approx Q_E$$

SLOW LIGHT WAVE AND FLUID-EM COUPLING

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$$S_E \approx Q_E \longrightarrow \; S_\alpha \approx D_\alpha - (Q_E^\alpha - Q_B^\alpha Q_B^{-1} K) Q_E^{-1} Q_\alpha^E$$

- Diagonal approximations of mass operators work well embedded in Schur complements
  - Replace Q_B and Q_E with diagonal approximations
- Fluid Schur complement simplifies further

$$CFL_{a,\alpha} < \tau \;\longrightarrow\; ||Q_B^\alpha Q_B^{-1} K Q_E^{-1} Q_\alpha^E|| < \tau ||Q_E^\alpha Q_E^{-1} Q_\alpha^E||$$

$$S_\alpha \approx D_\alpha - Q_E^\alpha Q_E^{-1} Q_\alpha^E$$

Hardest part of fluid subsolve if cyclotron frequency is fast

$$\hat{S}_\alpha(\rho_\alpha \mathbf{u}_\alpha) \sim \frac{\partial \rho_\alpha \mathbf{u}_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha) - \qquad + \underbrace{\frac{\Delta t}{\varepsilon} \frac{q_\alpha^2}{m_\alpha^2} \rho_\alpha (\rho_\alpha \mathbf{u}_\alpha)}$$

- Mass-like operator should make fluid subsolve easier
- Negligible when plasma frequency is slow

SLOW LIGHT WAVE PRECONDITIONER

$$\mathcal{P} = \begin{pmatrix} \hat{S}_\alpha & 0 & 0 \\ 0 & Q_B & K \\ Q_\alpha^E & 0 & Q_E \end{pmatrix}$$

- Block Gauss-Seidel in 2x2 electromagnetics block
  - Cheap smoothers or no AMG at all (Jacobi?) for mass solves
- Mass-like augmentation of fluid block
  - Or no augmentation (block Gauss-Seidel) when plasma frequency is slow
  - Use block Gauss-Seidel to decouple momentum and density solves since pressure wave speed must be slow
- Use expensive smoother (ILU) for momentum solve only if cyclotron frequency is fast (strong off-diagonal contributions)
  - Otherwise, Gauss-Seidel or Chebyshev suffice

SLOW LIGHT WAVE NUMERICAL EXPERIMENT

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Variation of left-handed circularly polarized wave 1D two-fluid problem (slow ions, fast electrons, resolving speed of light)

Time-scale	CFL
Light Wave	1.0e-1
Advection (e)	1.0e-1
Advection (i)	3.0e-3
Plasma Freq (e)	3.3e+1
Plasma Freq (i)	4.6e-1
Cyclotron Freq (e)	1.0e+2
Cyclotron Freq (i)	2.0e-2

Prec	Avg Its	Setup (s)	Solve (s)
Slow light, slow i, fast e	15.61	0.1397	0.2753
Slow light, slow i + p,i, fast e	15.61	0.1747	0.2793
Slow light, fast i, fast e	15.47	0.2130	0.2952
Fast light, fast i, fast e	13.24	0.5116	0.5117

No convergence with slow smoother settings applied to electron fluid solve

FAST LIGHT WAVE CASES

- Electromagnetic Schur complement is a transient curl-curl diffusion operator

$$S_E = Q_{\mathbf{E}} + \hat{K}^t Q_{\mathbf{B}}^{-1} K \sim \frac{\varepsilon}{\Delta t} I + \frac{\Delta t}{\mu} \nabla \times \nabla \times$$

- Close to singular when CFL_c is large (all gradients in null-space of curl-curl operator)
- Use a solver designed for curl-curl operator at long time-scales
  - Specialized multigrid (auxiliary space, refMaxwell, etc)
  - Augmentation-based with traditional multigrid

$$S_E^{-1} \approx T_E^{-1} Z_E Q_E^{-1}$$

$$T_E = S_E + G Q_\rho^{-1} G^t$$
$$Z_E = Q_E + G Q_\rho^{-1} G^t$$

- Special cases for fluid-electromagnetics coupling
  - Slow plasma frequency (use block Gauss-Seidel)
  - Slow advection and cyclotron frequencies

$$D_\alpha \approx Q_\alpha \ \rightarrow S_{E,\alpha} \approx S_E - Q_\alpha^E Q_\alpha^{-1} Q_E^\alpha$$

MULTIFLUID PLASMA PRECONDITIONER ALGORITHM

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- Take as input list of which time-scales are slow and fast
- Slow light wave -> special case (discussed above)
- Loop through fluid species
  - Slow plasma frequency -> no contribution to Schur complements
  - Slow advection and cyclotron frequencies -> add plasma frequency operator to S_E
  - Otherwise, add species to leftover list
- Compute S_α for each leftover species, using a diagonal approximation for augmented S_E operator in embedded inverses
- Setup subsolves using expensive smoothers if the time-scales dictate
- Setup outer block structure

FULL PRECONDITIONER 1D RESULTS

Time-scale	CFL
Light Wave	1.0e+3
Advection (e)	1.7e0
Advection (i)	3.4e-1
Plasma Freq (e)	3.3e+1
Plasma Freq (i)	3.3e0
Cyclotron Freq (e)	3.1e-1
Cyclotron Freq (i)	3.1e-3

Prec	Avg Its	Setup (s)	Solve (s)
Fast light, slow i, fast e	49.35	0.3729	1.542
Fast light, slow i, slow e	48.31	0.2145	1.473
Fast light, slow plasma freqs	65.36	0.1917	2.067
Fast light, fast i, fast e	65.52	0.5064	2.243

No convergence without fast light approximation

A MORE REALISTIC TEST PROBLEM

- 2D electron/ion plasma driven by an external current pulse with background magnetic field and density gradient
- Simulation resolves current source

Time-scale	CFL max
Light Wave	2.0e+1
Advection (e)	1.3e-2
Advection (i)	1.3e-5
Plasma Freq (e)	2.6e+1
Plasma Freq (i)	8.1e-1
Cyclotron Freq (e)	1.3e+1
Cyclotron Freq (i)	1.3e-2

Procs	DOFS	Avg Its	Setup (s)	Solve (s)
1	2.6e4	16.26	0.5122	0.7833
4	1.0e5	16.45	0.8571	1.031
16	4.0e5	17.95	1.064	2.141
64	1.3e6	27.74	1.213	3.923
256	6.3e6	32.68	1.344	5.078

NEXT STEPS

- Subsolve settings
  - Fluid subsolves can be improved – currently using SIMPLEC for fast sound speed
  - Not aware of much research on block preconditioners for compressible flow, especially including Lorentz force term
- Structural changes when physics are added
  - Collisional terms – need to analyze interactions between fluids
  - Diffusive terms – all diagonal, but can make embedded inverses harder to approximate. Can also ameliorate issues with strong advection
  - Energy equation for warm plasmas – introduces sound speed physics
- Reuse for efficiency
  - Take advantage of linear parts of the system (e.g. Maxwell) where operators do not change throughout nonlinear iteration
  - Can also assume that slow physics are essentially unchanging on a time-step

CONCLUSION

- Time-scales dictate what operators are stiff in a linear system
- Time-scales can inform a preconditioner's choice of Schur complement approximations and subsolvers

- Motivated a physics-based block preconditioner for multifluid plasma systems
- Using cheaper approximations and solves for slow physics results in more efficient preconditioners although iteration counts may be slightly higher
- Showed preliminary parallel performance for a difficult plasma application