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Block Preconditioning for Multi-physics: From Jacobi to Schur Complements

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A Segregated System

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

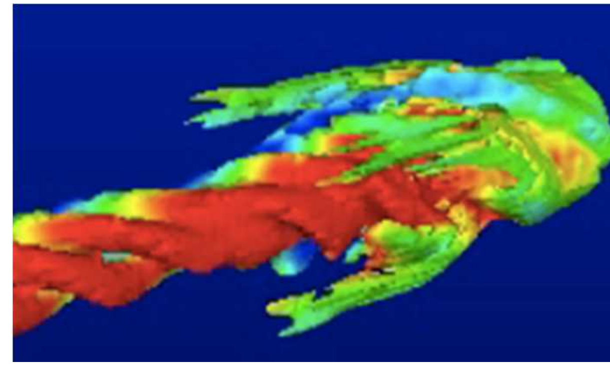
- Most of A_{ij} are “large sparse” matrices
- This structure is common:
  1. Multi-physics (the focus of this talk)
  2. Constraints
  3. Optimization
- “Effective preconditioners” are robust and scalable for these systems

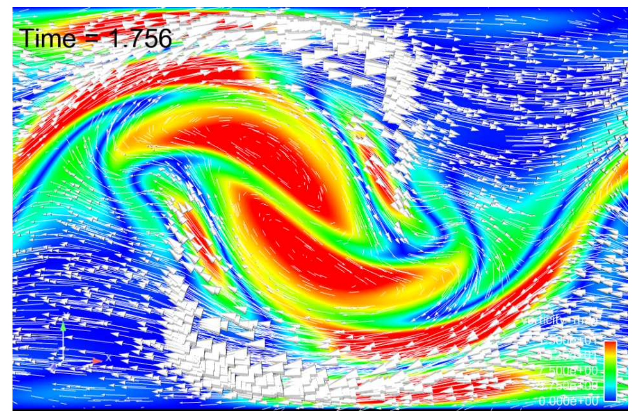
Multi-Physics PDEs

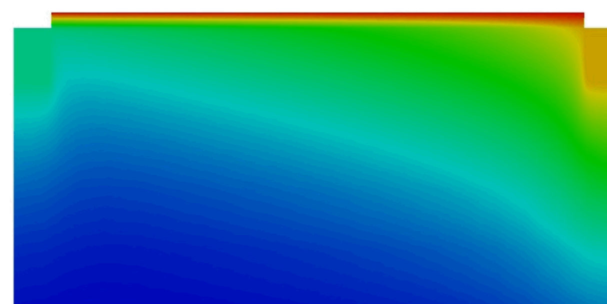
My working definition: Multi-physics PDEs are characterized by multiple interacting time and spatial scales arising from coupling between many distinct physical fields and mechanisms.

For example

1. Fluid-dynamics
2. Magnetohydrodynamics
3. Semiconductor modeling
4. Many more…



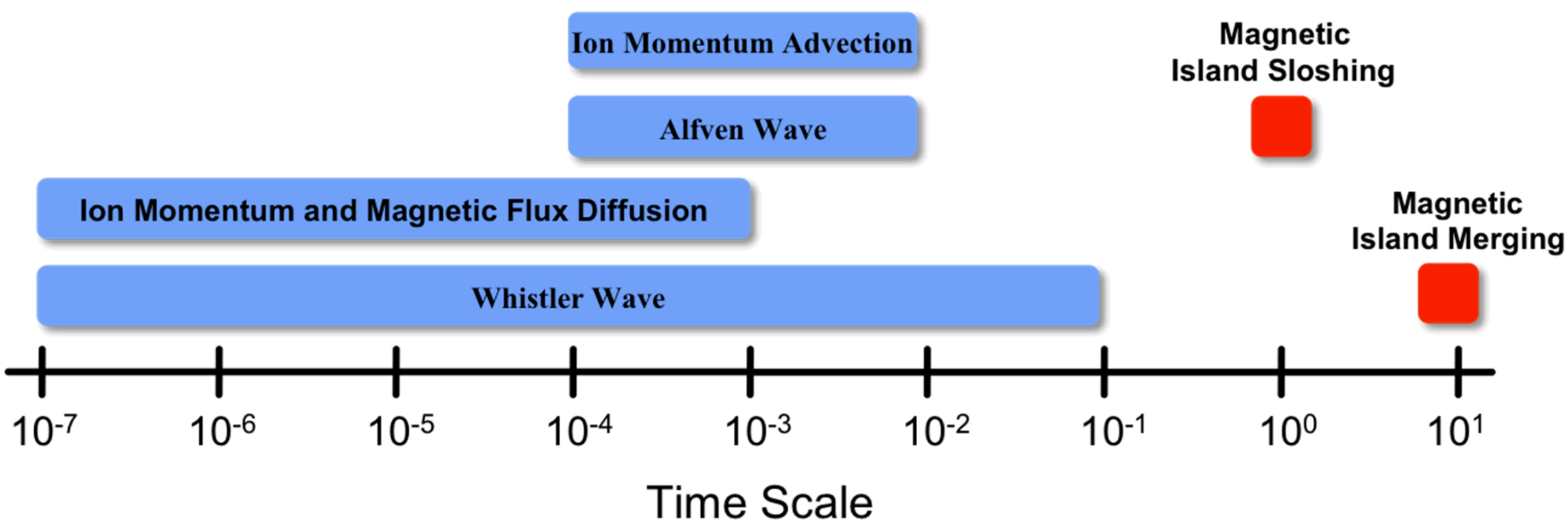




MHD example: Multiple Time Scales

MHD has multiple interacting time scales

- Often much faster than target mechanism
- Interaction makes operator splitting more challenging (time scales not well separated)
- We will use implicit time stepping with block preconditioners targeting each time scale



Some "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:

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

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).

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

A First-Order PDE

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:

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

Three Block Preconditioners

$$M_J = \begin{bmatrix} A_{00} & \\ & A_{11} \end{bmatrix}$$

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

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

- $h=1/500$, $\Delta t=h$
- GMRES iterations averaged over 10 steps
- 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

My "Algorithm" for Block Preconditioner Development

A quick and dirty (i.e. non-rigorous) approach to understanding what is included in a block preconditioner:

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. Everything where the stability limit is "relatively large" for the desired time step must be addressed in the preconditioner!

Incompressible Navier-Stokes

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

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

Segregated Jacobian is (C=0 implies stable discretization):

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

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

Navier-Stokes: SIMPLEC Schur Complement

Use Neumann series expansion (assume)

$$F^{-1} = M^{-1} \sum_{i=0}^{\infty} \left(I - FM^{-1}\right)^i$$

Truncate after K terms

$$\hat{S} = C - B \left(M^{-1} \sum_{i=0}^{K-1} (I - FM^{-1})^i \right) B^T$$

For $K=0$: explicitly compute approximate Schur complement

- M^{-1} = **diag**$(F)^{-1}$ is SIMPLE
- M^{-1} = **absRowSum**$(F)^{-1}$ is SIMPLEC

SIMPLE-like methods restricted by assumptions on Neumann series

- ➢ CFL like constraint on time step for effective preconditioner

Navier-Stokes: Commuting

To avoid CFL restriction, try another approach: Assume

$$\nabla \cdot \left(\frac{\partial}{\partial t} + \mathbf{w} \cdot \nabla - \ \nu \nabla^2 \right)_u \approx \left(\frac{\partial}{\partial t} + \mathbf{w} \cdot \nabla - \ \nu \nabla^2 \right)_p \nabla \cdot$$

motivates discrete commuting

$$B Q_u^{-1} F \approx F_p Q_p^{-1} B$$

which gives an approximate Schur complement (for *C=0*)

$$S = -B F^{-1} B^T \approx -Q_p F_p^{-1} \left(B Q_u^{-1} B^T \right) := \hat{S}$$

F_p is a discrete convection-diffusion operator on pressure

Navier-Stokes: PCD Approximation

$$S^{-1} \approx -(BQ_u^{-1}B^T)^{-1}F_pQ_p^{-1}$$

Pressure Laplacian: $(BQ_u^{-1}B^T)$

Pressure Conv-Diff: F_p

Pressure Mass: Q_p

Need to approximate

1. Inverse of pressure Laplacian
2. Application of pressure convection-diffusion operator
3. Pressure mass inverse (just use a lumped inverse!)

Pressure Convection-Diffusion (PCD) method

- Explicit construction Laplacian and conv-diff operators

$$-\nabla\cdot\nabla \sim A_p \qquad \frac{\partial}{\partial t} + \mathbf{w}\cdot\nabla - \nu\nabla\cdot\nabla \sim F_p$$

- Gives PCD schur complement approximation

$$S^{-1} \approx S_{PCD}^{-1} := A_p^{-1}F_pQ_p^{-1}$$

Navier-Stokes: LSC Approximation

PCD works well – but not algebraic!

- requires extra infrastructure to construct A_p and F_p

Lease-Squares Commutator (LSC) addresses this

$$(F_p Q_p^{-1})^T \approx \underset{X}{\operatorname{argmin}} \|B^T X - F^T Q_u^{-1} B^T\|$$

Substituting LS approximation of F_p into S gives

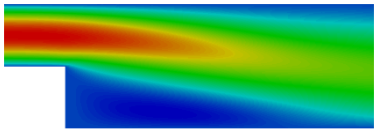
$$S^{-1} \approx S_{LSC}^{-1} := -(BQ_u^{-1}B^T)^{-1}(BQ_u^{-1}FQ_u^{-1}B^T)(BQ_u^{-1}B^T)^{-1}$$

Approximated with AMG ← $(BQ_u^{-1}B^T)^{-1}$; $(BQ_u^{-1}FQ_u^{-1}B^T)$ → Easy to evaluate

Navier-Stokes: Schur Complement Summary

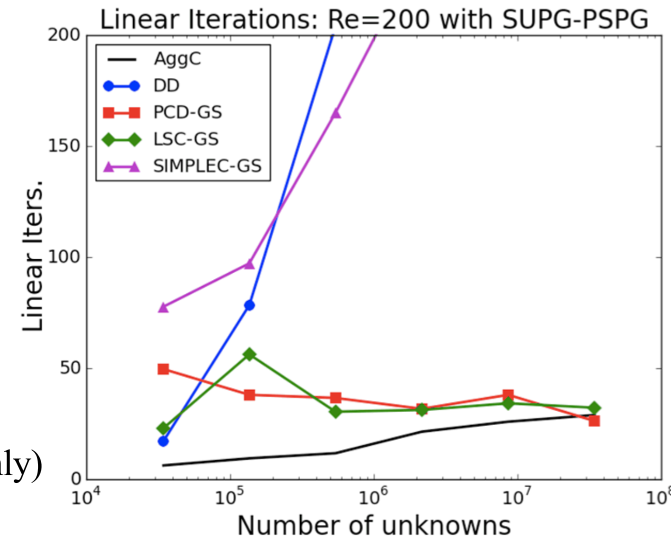
	$S = -BF^{-1}B^T$	Inverses Required
SIMPLEC	$-B\,\mathbf{AbsRowSum}(F)^{-1}B^T$	$-B\,\mathbf{AbsRowSum}(F)^{-1}B^T$
PCD	$Q_p F_p^{-1} A_p$	A_p^{-1}
LSC	$-(BQ_u^{-1}B^T)(BQ_u^{-1}FQ_u^{-1}B^T)^{-1}(BQ_u^{-1}B^T)$	$(BQ_u^{-1}B^T)^{-1}$

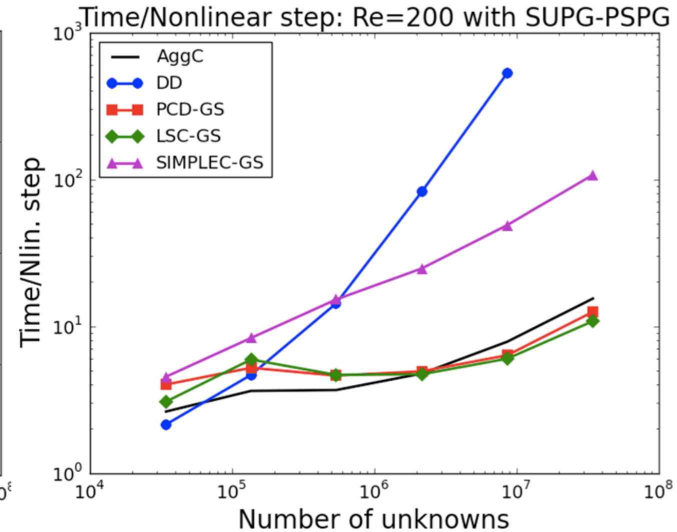
Navier-Stokes: Results

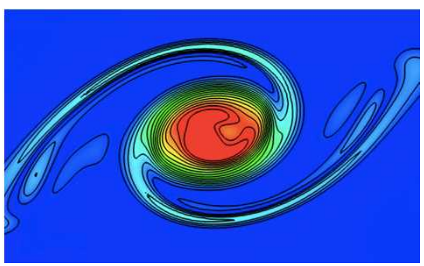


Backward Facing Step: Steady

- Re = 200
- 1 to 1024 Processors
- Stabilization:
  - Pressure: PSPG
  - Velocity: SUPG (residual only)

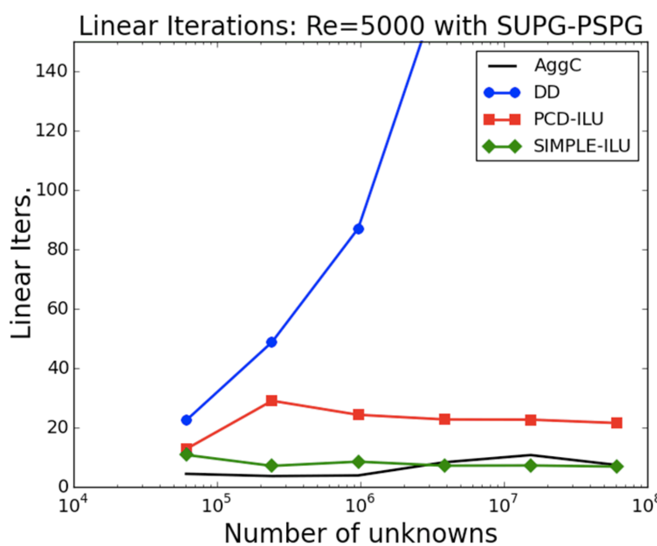


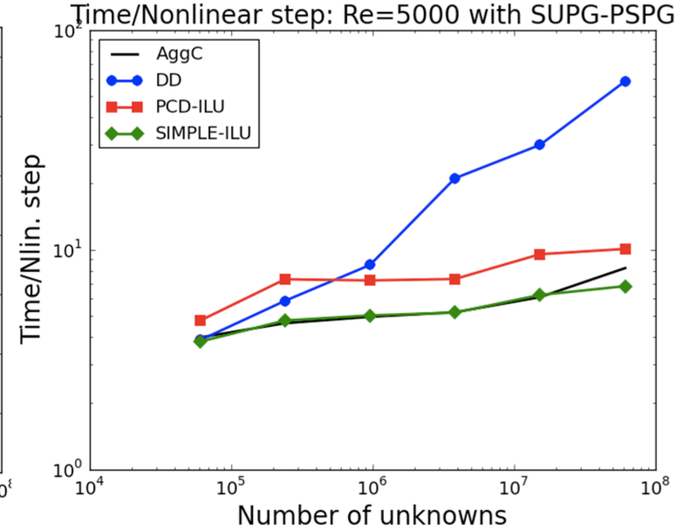




Kelvin Helmholtz: Transient

- Re = 5000
- 1 to 1024Processors
- 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 for all fields, C_u and C_B are nonzero stabilization operators

Multiple Time Scales: MHD

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

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

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

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

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

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

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

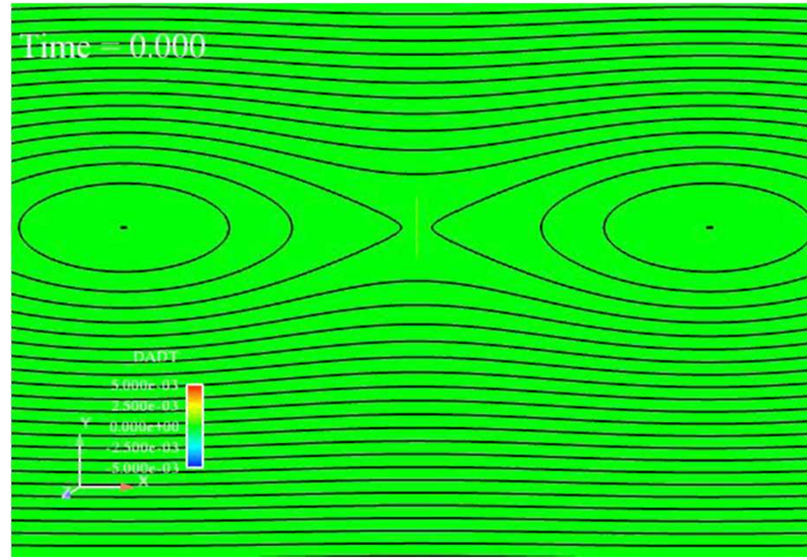
$$\frac{\partial \delta \mathbf{B}}{\partial t} - \nabla \times (\delta \mathbf{u} \times \mathbf{B}) + \nabla \delta r = \mathbf{0}$$

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

- A linearization about (**u**,**B**), dropped diffusive terms
  - Particulars of linearization important to fixed point convergence
- Alfvén Wave generated by coupling
  - Highlighed coupling gives wave speed: $v_A = \frac{|\mathbf{B}|}{\sqrt{\rho \mu_0}}$
  - Secondary gives wave “character”: anisotropic

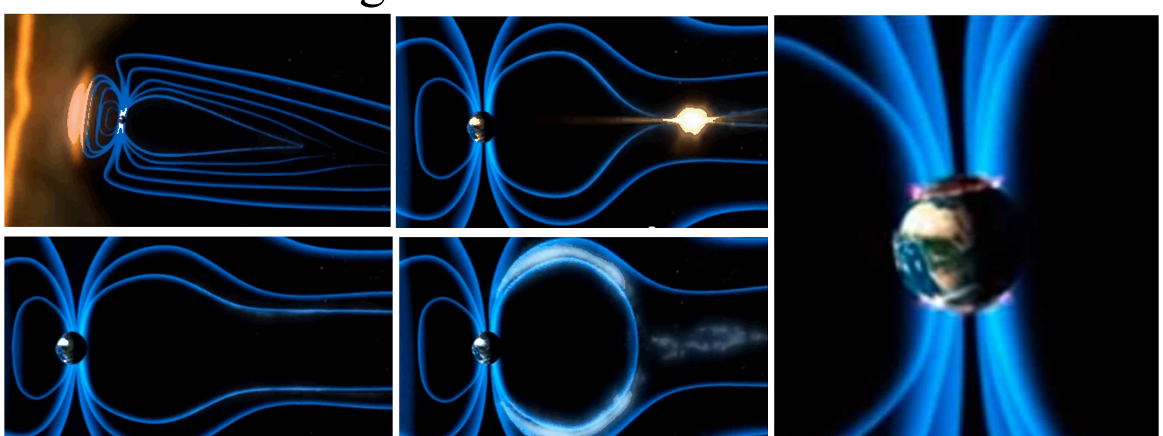
Can I see the Alfvén wave?

Magnetic Reconnection Simulation



Yep! Alfvén wave effects can be seen clearly in magnetic reconnection

NASA Magnetic Reconnection Animation



https://www.youtube.com/watch?v=i_x3s8ODaKg

Aurora Borealis

http://en.wikipedia.org/wiki/File:Northern_Lights_2.jpg

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

Shameless plug - previous splitting for 2D vector potential MHD formulation in: *Cyr, et al., "A new approximate block factorization for 2D incompressible (reduced) resistive MHD", SISC 2013*

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:

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

$$A_1 = YF^{-1}K_u$$

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

$$S_u = C - BF^{-1}B^T$$

$$K_u = I + B^T S_u^{-1} BF^{-1}$$

$$\hat{P} = D - YF^{-1}Z$$

Do these splittings work?

Structurally small perturbation:

$$\mathcal{M}_{Split\text{-}4\times 4} = \begin{bmatrix} F & B_u^T & Z & \boxed{ZD^{-1}B_r^T} \\ B_u & C_u & & \\ Y & \boxed{YF^{-1}B_u^T} & D & B_r^T \\ & & B_r & C_r \end{bmatrix}$$

Favorable (?) spectrum:

$$\mathcal{J}\mathcal{M}^{-1}_{Split\text{-}4\times 4} = \begin{bmatrix} I & & A_1 & A_2 \\ & I & & \\ A_3 & A_4 & (D - YF^{-1}K_uZ)\hat{P}^{-1} & \\ & & & I \end{bmatrix}$$

$$A_1 = Z(-I + D^{-1}K_bD)\hat{P}^{-1}$$

$$A_2 = -ZD^{-1}B_b^TS_b^{-1}$$

$$A_3 = YF^{-1}K_u$$

$$A_4 = -YF^{-1}B^TS_u^{-1}$$

$$S_u = C - BF^{-1}B^T$$

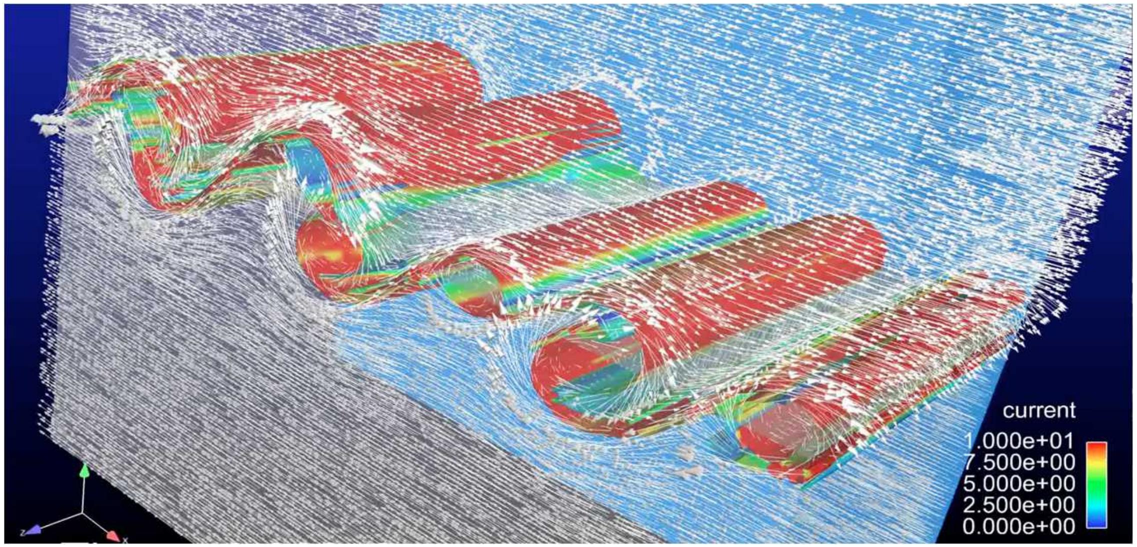
$$S_b = C - BD^{-1}B^T$$

$$\hat{P} = D - YF^{-1}Z$$

$$K_u = I + B^TS_u^{-1}BF^{-1}$$

$$K_b = I + B^TS_b^{-1}BD^{-1}$$

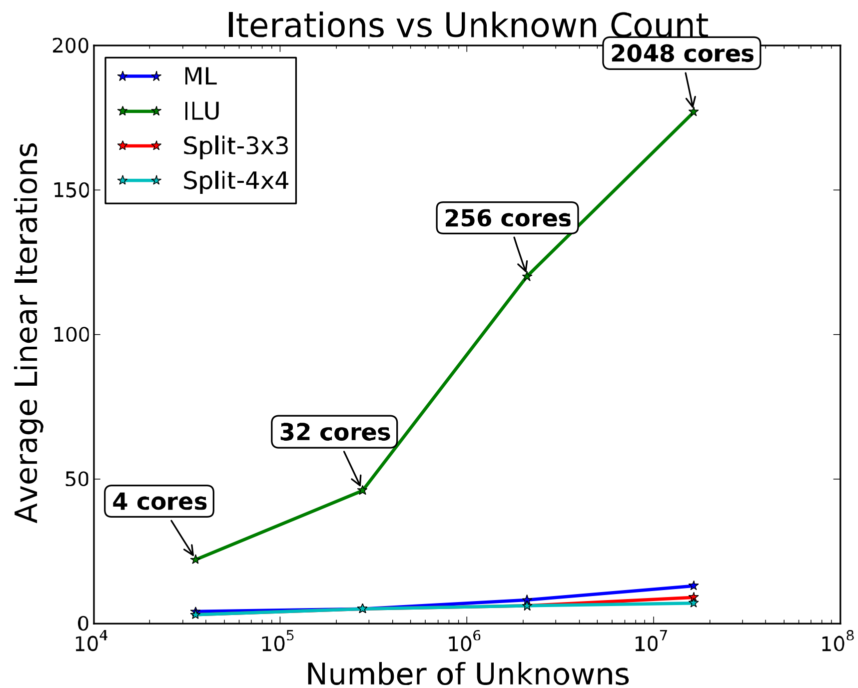
Hydromagnetic Kelvin Helmholtz (HMKH)

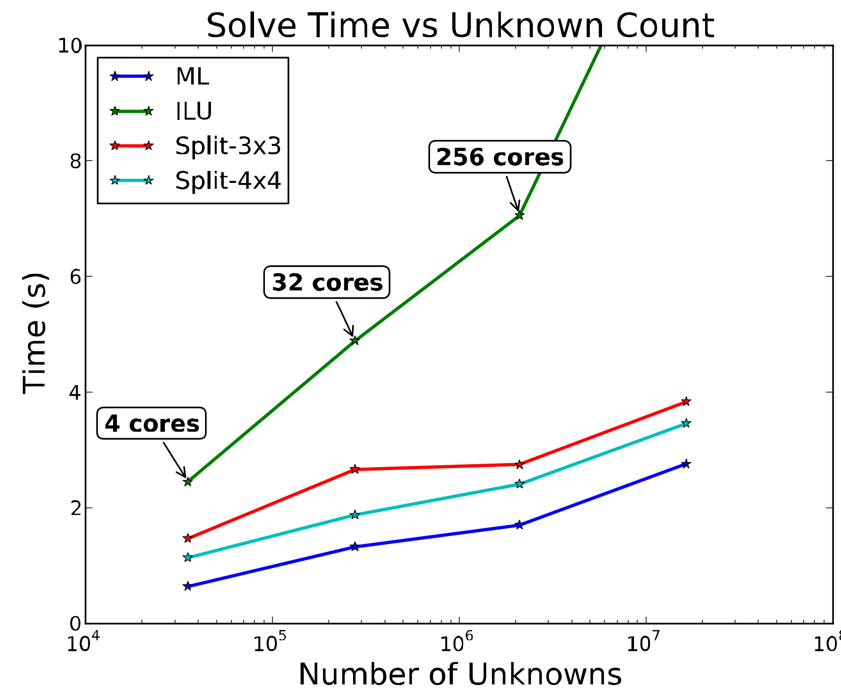


Results details:

- Magnetically stabilized 3D shear layer transient simulation
- Run to 5 time units with 2nd order BDF
- Uniform mesh (bilinear elements, 8 unknowns/node)
- Run on 4, 32, 256, 2048 processors (~8,000 unks/core)

HMKH: Weak Scaling (CFL~0.125)





<u>Fully coupled Algebraic</u>

ML: Uncoupled AMG with repartitioning

DD: Additive Schwarz Domain Decomposition

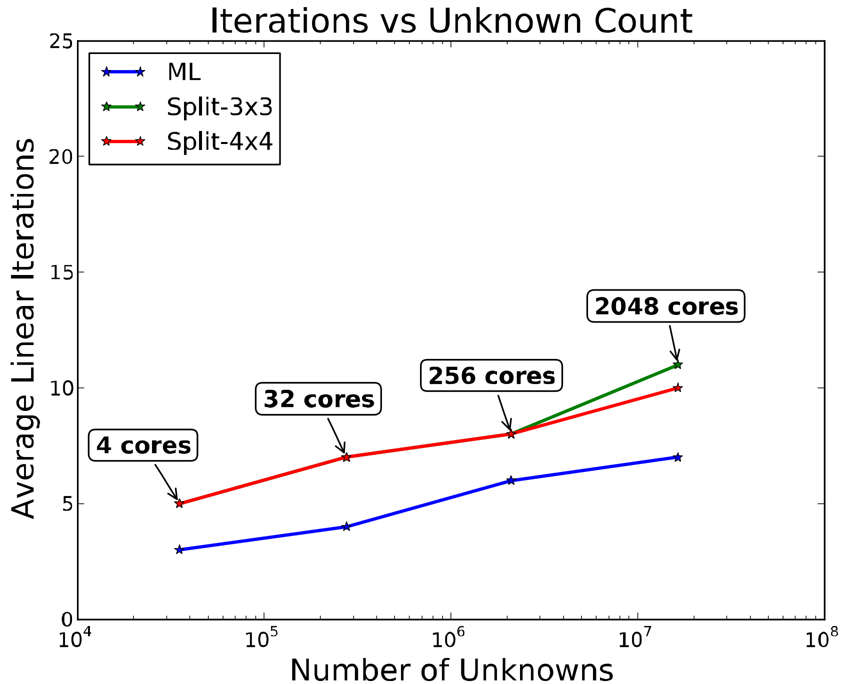
<u>Block Preconditioners</u>

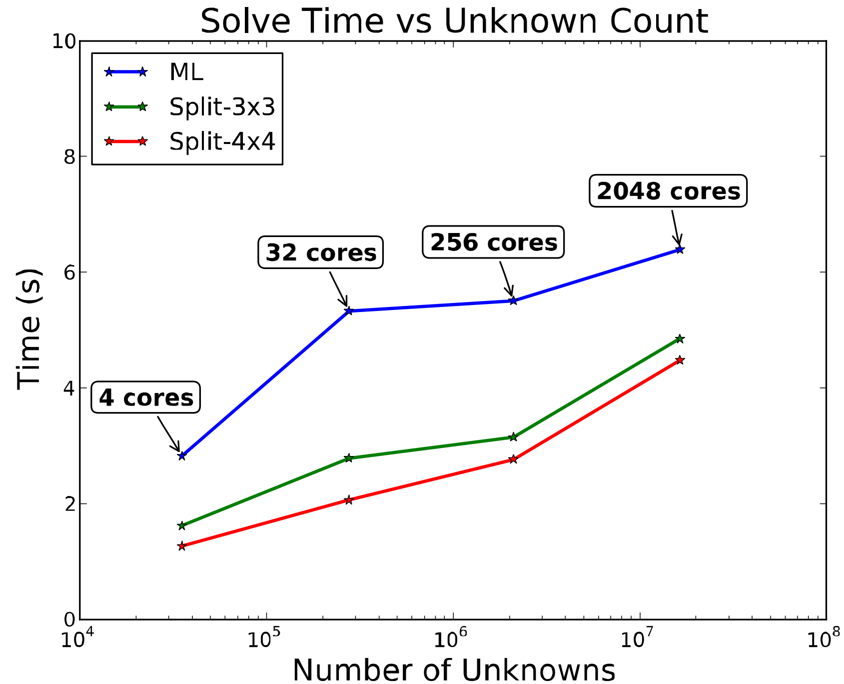
<u>Split-3x3</u>: 3x3 Splitting (SIMPLEC everywhere)

<u>Split-4x4</u>: 4x4 Splitting (SIMPLEC everywhere)

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

HMKH: Weak Scaling (CFL~1.125)





Fully coupled Algebraic

ML: Uncoupled AMG with repartitioning

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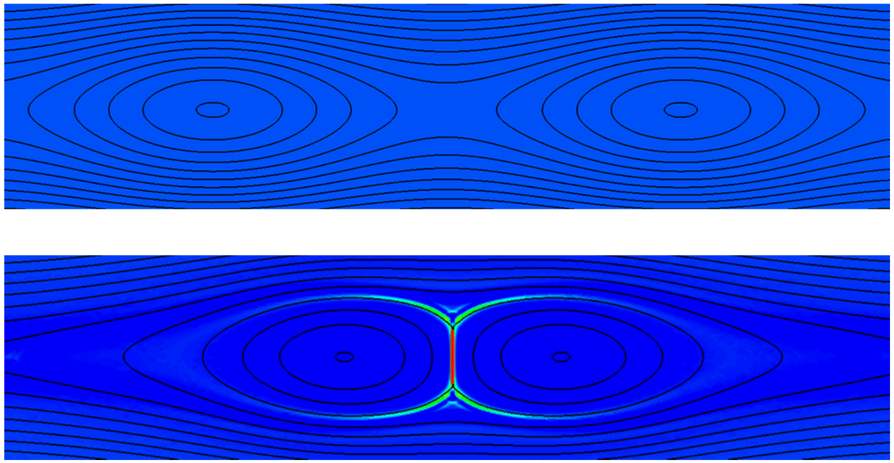
Block Preconditioners

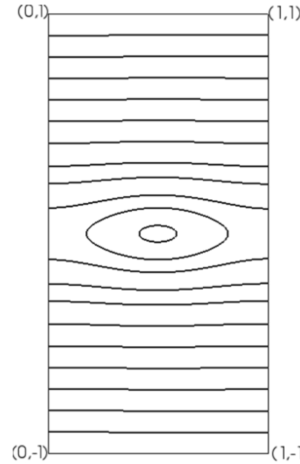
Split-3x3: 3x3 Splitting (SIMPLEC everywhere)

Split-4x4: 4x4 Splitting (SIMPLEC everywhere)

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

Island Coalescence (IC): 2D Vector Potential





Simulation on half domain

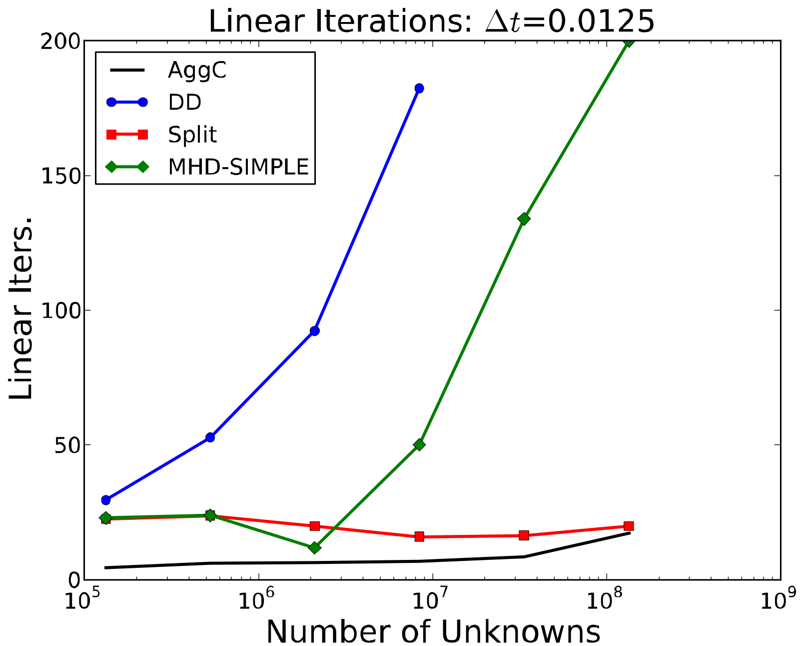
- Symmetry BC
- Perturbed Harris-Sheet

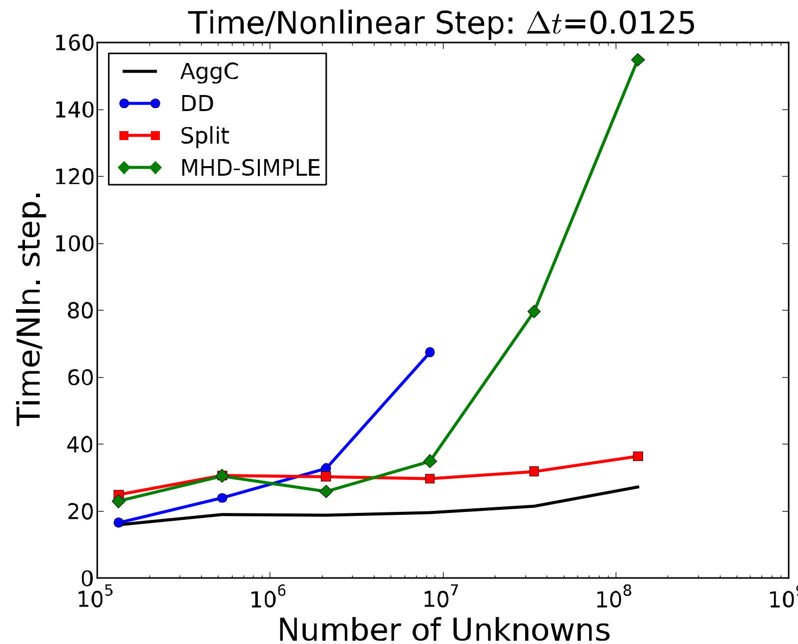
$$A_z^0(x,y,0) = \delta \; ln \left[\cosh\left(\frac{y}{\delta}\right) + \epsilon \;\cos\left(\frac{x}{\delta}\right)\right]$$

Results details (an initial study):

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

IC: 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

* E. C. Cyr, J. N. Shadid, R. S. Tuminaro, R. P. Pawlowski, L. Chacon, A New Approximate Block Factorization Preconditioner for Two Dimensional Incompressible (Reduced) Resistive MHD", SIAM Journal on Scientific Computing, 2013.

Final Thoughts

Discussed block preconditioning

- Multi-physics has broad range of time and spatial scales
- Block Jacobian segregated by physical field
- For tightly coupled physics must handle coupling
- Coupling in Schur complement
- Scalability attained by leveraging multigrid

Showed Results for Navier-Stokes

- Presented SIMPLE, PCD and LSC approximations
- Showed scaling results for stabilized discretizations

Show results for 2D MHD

- Developed operator-split preconditioner
  - Focuses on elliptic incompressibility and Alfven wave
- Showed results indicating good performance