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Approximate Block Factorization Preconditioner for 2D Incompressible Resistive MHD

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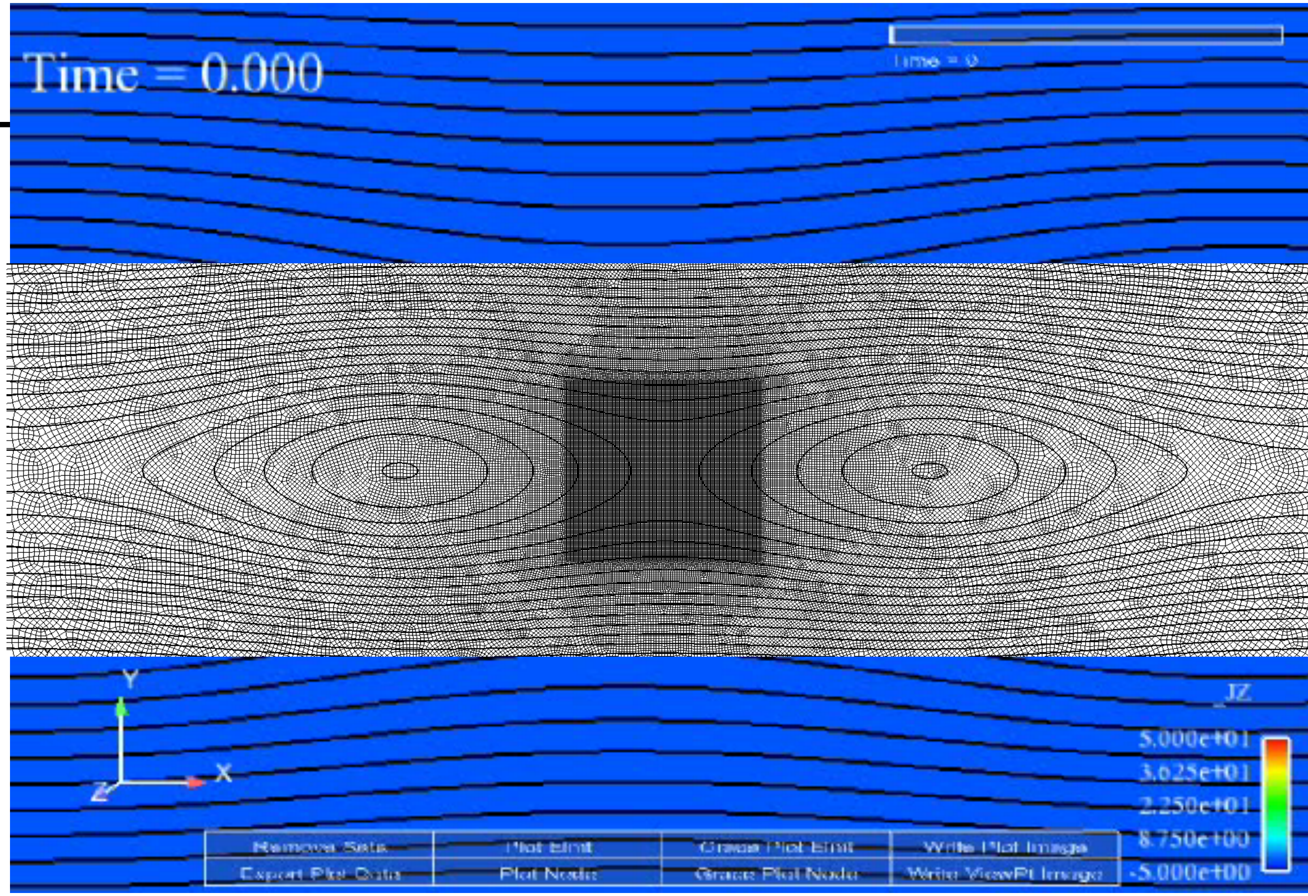
Multiple-time-scale systems: E.g. Driven Magnetic Reconnection with a Magnetic Island Coalescence Problem* (Incompressible)



<u>Approx. Computational Time Scales:</u>

- Incompressible or anelastic eq. state
    - => infinite speed fast and slow magneto-sonic waves
- Ion Momentum Diffusion: 10^{-7} to 10^{-3}
- Magnetic Flux Diffusion: 10^{-7} to 10^{-3}

- Ion Momentum Advection: 10^{-4} to 10^{-2}
- Alfven Wave $\left(\tau_A = \frac{h\sqrt{\rho\mu_0}}{B_O}\right)$ 10^{-4} to 10^{-2}
- XMHD Whistler Wave $\left(\tau_w = \frac{h^2}{V_A d_i}\right)$: 10^{-7} to 10^{-1}
- Magnetic Island Sloshing: 10^0
- Magnetic Island Merging: 10^1

[*Driven Island Coalescence Problem: Finn and Kaw 1977; Chacon and Knoll Phys. 2006]

Multiple Time Scales

MHD times scales difficult for explicit, operator-split, and semi-implicit integration

- Fast modes prohibit explicit simulation for long dynamical time-scales
  - × Stability restrictions imply small time steps: non-scalable with mesh resolution
  - × For long time integration accuracy becomes problematic
- Interacting time-scales make semi-implicit and operator-split methods challenging and fragile in terms of stability

Stable long time scale integration can be enabled by implicit time stepping

- However must solve challenging linear system: Newton's Method

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

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

Our approach is to solve using preconditioned Newton-Krylov methods

- Effective preconditioning is key to parallel scalability

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What must a preconditioner do?

- What must a preconditioner do?
  1. Handle ill conditioning of system due to:

     Fast waves, advection, elliptic operators, …

     Multiphysics systems strongly couple mechanisms, producing multiple time- and length-scales
  2. Must optimally scale with increasing:
     - problem size
     - processor count
- For incompressible MHD specifically
  1. Pressure-Velocity coupling: incompressibility constraint
  2. Alfven Wave: Velocity-Magnetics coupling
  3. Material advection (flow velocity)
  4. Dissipative operators (momentum, magnetics)

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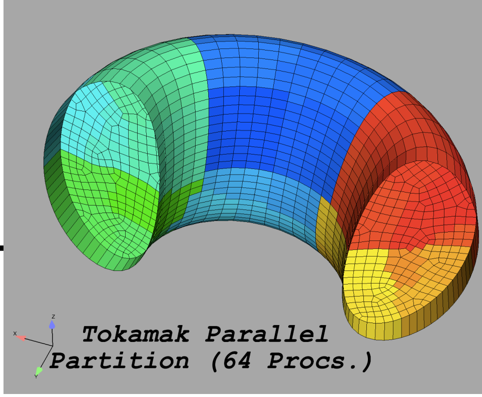
Three Types of Preconditioning



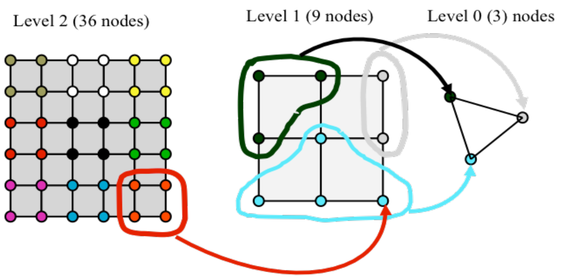
1. Domain Decomposition (Trilinos/Aztec & IFPack)

- 1 –level Additive Schwarz DD
- ILU(k) Factorization on each processor (with variable levels of overlap)
- High parallel efficiency, non-optimal algorithmic scalability

2. Multilevel Methods for Systems: ML pkg (Tuminaro, Sala, Hu, Siefert, Gee)

Fully-coupled Algebraic Multilevel methods

- Consistent set of DOF at each node (e.g. stabilized FE)
- Uses block non-zero structure of Jacobian
- Aggregation techniques and coarsening rates can be set
- Jacobi, GS, ILU(k) as smoothers
- Can provide optimal algorithmic scalability



Visualization of effect of partition of matrix graph on mesh

3. Approximate Block Factorization / Physics-based (Trilinos/Teko package)

- Applies to mixed interpolation (FE), staggered (FV), physics compatible discretization approaches using segregated unknown blocking
- Applied to systems where coupled AMG is difficult or might fail
- Can provide optimal algorithmic scalability

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Block preconditioning: CFD example

Consider discretized Navier-Stokes equations

$$\left.\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} - \nu\nabla^2\mathbf{u} + \nabla p = f \\ \nabla\cdot\mathbf{u} = 0\end{aligned}\right\} \Leftrightarrow \begin{bmatrix} F & B^T \\ B & C \end{bmatrix}\begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}$$

Fully Coupled Jacobian

$$\mathcal{A} = \begin{bmatrix} F & B^T \\ B & C \end{bmatrix}$$

Block Factorization

$$\mathcal{A} = \begin{bmatrix} I & \\ BF^{-1} & I \end{bmatrix}\begin{bmatrix} F & B^T \\ & S \end{bmatrix}$$

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

- Coupling in Schur-complement

Preconditioner

$$\mathcal{A}^{-1} \approx \mathcal{M}^{-1} = \begin{bmatrix} \hat{F} & B^T \\ & \hat{S} \end{bmatrix}^{-1}$$

Required operators:

- $F^{-1} \approx \hat{F}^{-1} \rightarrow$ Multigrid
- $S^{-1} \approx \hat{S}^{-1} \rightarrow$ PCD, LSC, SIMPLEC

Properties of block factorization

1. Important coupling in Schur-complement
2. Better targets for AMG $\rightarrow$ leveraging scalability

Properties of approximate Schur-complement

1. "Nearly" replicates physical coupling
2. Invertible operators $\rightarrow$ good for AMG

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Brief Overview of Block Preconditioning Methods for Navier-Stokes:
(A Taxonomy based on Approximate Block Factorizations, JCP – 2008)

Discrete N-S	Exact LDU Factorization	Approx. LDU
$\begin{pmatrix} F & B^T \\ \hat{B} & -C \end{pmatrix} \begin{pmatrix} \Delta u_k \\ \Delta p_k \end{pmatrix} = \begin{pmatrix} g_u^k \\ g_p^k \end{pmatrix}$	$\begin{pmatrix} I & 0 \\ \hat{B}F^{-1} & I \end{pmatrix} \begin{pmatrix} F & 0 \\ 0 & -S \end{pmatrix} \begin{pmatrix} I & F^{-1}B^T \\ 0 & I \end{pmatrix}$ $S = C + \hat{B}F^{-1}B^T$	$\begin{bmatrix} I & 0 \\ \hat{B}H_1 & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & -\hat{S} \end{bmatrix} \begin{bmatrix} I & H_2B^T \\ 0 & I \end{bmatrix}$

Precond. Type	H_1	H_2	$\hat{S}$	References
Pres. Proj; 1st Term Neumann Series	$\mathbf{F}^{-1}$	$(\mathbf{\Delta t I})^{-1}$	$\mathbf{C} + \mathbf{\Delta t \hat{B} B^T}$	Chorin(1967);Temam (1969); Perot (1993): Quateroni et. al. (2000) as solvers
SIMPLEC	$\mathbf{F}^{-1}$	$(\mathbf{diag}(\sum \lvert\mathbf{F}\rvert))^{-1}$	$\mathbf{C} + \mathbf{\hat{B}}(\mathbf{diag}(\sum \lvert\mathbf{F}\rvert))^{-1}\mathbf{B^T}$	Patankar et. al. (1980) as solvers; Pernice and Tocci (2001) as smothers/MG
Pressure Convection / Diffusion	0	$\mathbf{F}^{-1}$	$\mathbf{A_p F_p^{-1}}$	Kay, Loghin, Wathan, Silvester, Elman (1999 - 2006); Elman, Howle, S., Shuttleworth, Tuminaro (2003,2008)

Now use AMG type methods on sub-problems.

Momentum transient convection-diffusion: $F\Delta\mathbf{u} = \mathbf{r_u}$

Pressure – Poisson type: $-\hat{S}\Delta p = \mathbf{r}_p$

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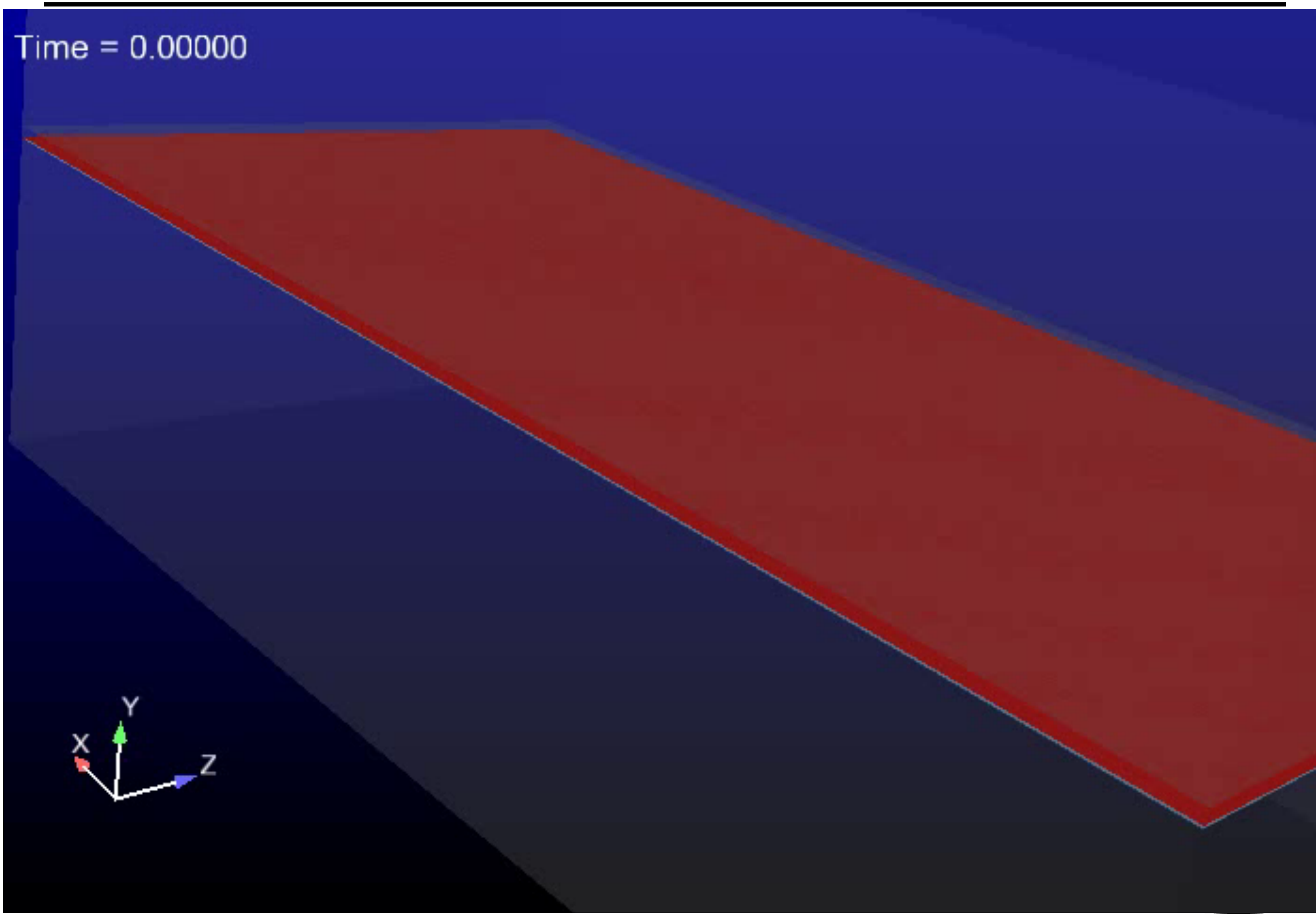
Transient Kelvin-Helmholtz: Re = 10^6



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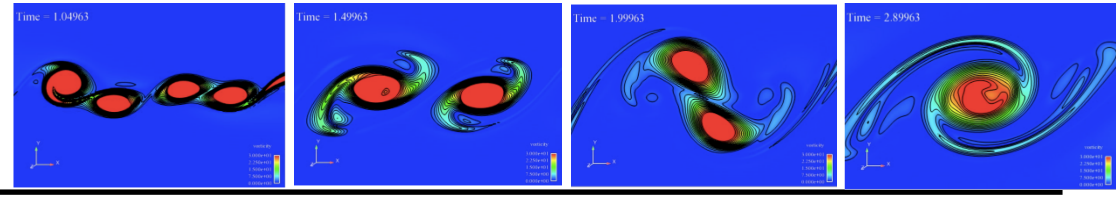
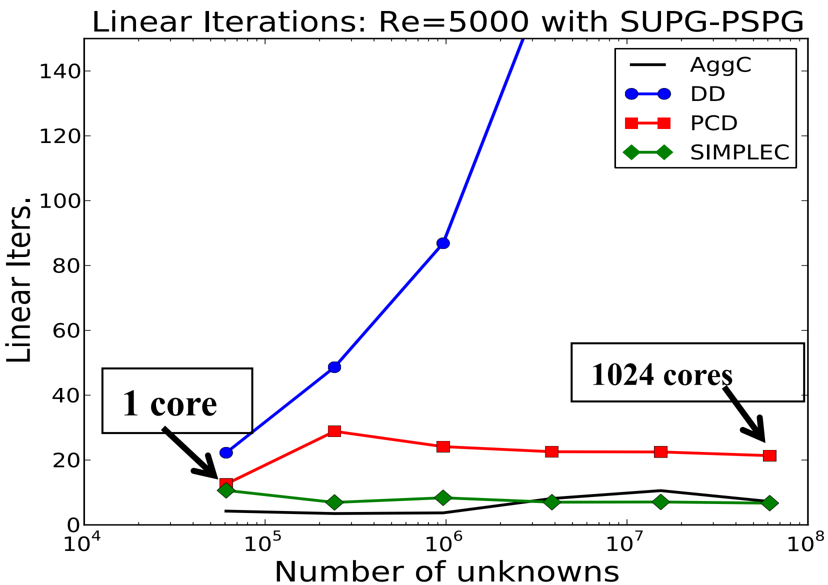
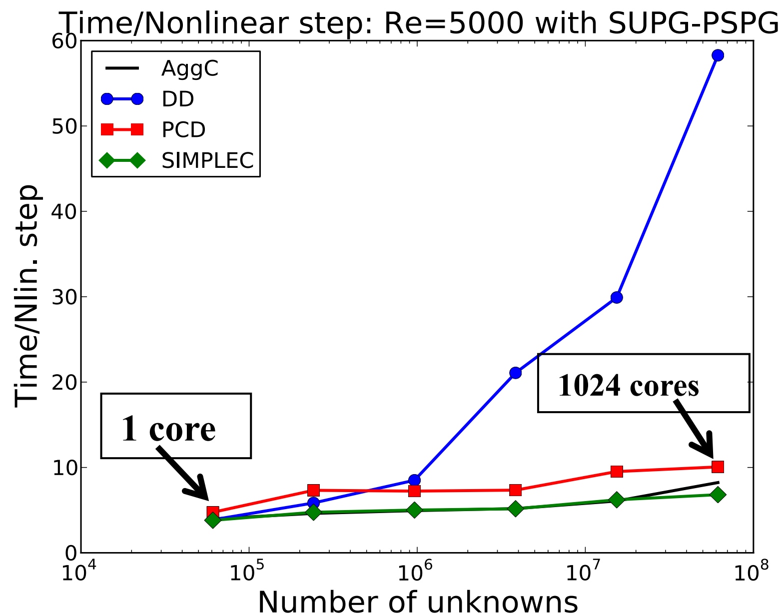
Transient Kelvin-Helmholtz







Kelvin Helmholtz: Re=5000, Weak scaling at CFL=2.5

- Run on 1 to 1024 cores
- Pressure - PSPG, Velocity - SUPG(residual and Jacobian)

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Incompressible MHD: 2D Vector Potential Formulation

Magnetohydrodynamics (MHD) equations couple fluid flow to Maxwell's equations

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

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

$$\frac{\partial A_z}{\partial t} + \mathbf{u} \cdot \nabla A_z - \frac{\eta}{\mu_0} \nabla^2 A_z = -E_z^0$$

$$\text{where } \mathbf{B} = \nabla \times \mathbf{A}, \ \mathbf{A} = (0, 0, A_z)$$

Incompressible flow: Primitive variable
Magnetics: Vector potential in 2D
Discretized using a stabilized finite element formulation

Incompressible MHD: Discrete Formulation

Stabilized finite element method in residual form

Momentum	$\mathbf{F}_{m,i} = \int_{\Omega} \Phi \mathbf{R}_{m,i} d\Omega + \sum_e \int_{\Omega_e} \hat{\tau}_m (\mathbf{v} \cdot \nabla \Phi) \mathbf{R}_{m,i} d\Omega$
Total Mass	$F_P = \int_{\Omega} \Phi R_P d\Omega + \sum_e \int_{\Omega_e} \hat{\tau}_m \nabla \Phi \cdot \mathbf{R}_m d\Omega$
Z-Vector Potential	$F_{A_z} = \int_{\Omega} \Phi R_{A_z} d\Omega + \sum_e \int_{\Omega_e} \hat{\tau}_{A_z} (\mathbf{v} \cdot \nabla \Phi) R_{A_z} d\Omega$

Structure of discretized Incompressible MHD system is

$$\mathcal{J}\mathbf{x} = \begin{bmatrix} F & B^T & Z \\ B & C & 0 \\ Y & 0 & D \end{bmatrix} \begin{bmatrix} u \\ p \\ A \end{bmatrix} = \begin{bmatrix} f \\ 0 \\ e \end{bmatrix}$$

Matrices F and D are transient convection operators, C is stabilization matrix

Nested Schur Complements

Block LU factorization gives

$$\begin{bmatrix} F & B^T & Z \\ B & C & 0 \\ Y & 0 & D \end{bmatrix} = \begin{bmatrix} I & & \\ BF^{-1} & I & \\ YF^{-1} & -YF^{-1}B^TS^{-1} & I \end{bmatrix} \begin{bmatrix} F & B^T & Z \\ & S & -BF^{-1}Z \\ & & P \end{bmatrix}$$

where

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

$$P = D - YF^{-1}(I + B^TS^{-1}BF^{-1})Z$$

- 3x3 system leads to nested Schur complements
- Nesting is independent of ordering (C^{-1} doesn't exist!)
- How is P approximated?
- Chacon & Knoll explored compressible flow and incompressible flow using stream-function vorticity

Try 3x3 System: SIMPLE Motivated Preconditioner
Quite Drastic Approximation

$$\mathcal{M} = \begin{bmatrix} F & B^T & Z \\ & S_{Neu} & -BF^{-1}Z \\ & & P_{Neu} \end{bmatrix}$$

where

$$\begin{aligned} F_{Neu} &= \textbf{AbsRowSum}(F) \\ S_{Neu} &= C - BF_{Neu}^{-1}B^T \\ P_{Neu} &= D - YF_{Neu}^{-1}\,\textbf{AbsRowSum}(I \\ &\qquad + B^T\textbf{AbsRowSum}(S_{Neu})^{-1}BF_{Neu}^{-1})Z \end{aligned}$$

Issues

- SIMPLEC Approximation has issues with large CFL
- Not scalable for fixed timesteps

Two Split Preconditioners for MHD: Use a defect-correction approach

$\hat{x} = \textbf{SplitPrec-NS}(\mathcal{J}, b)$:

$$x^* = \begin{bmatrix} F & & Z \\ & I & \\ Y & & D \end{bmatrix}^{-1} b,$$

$$r^* = b - \mathcal{J}x^*,$$

$$e = \begin{bmatrix} F & B^T & \\ B & C & \\ & & I \end{bmatrix}^{-1} r^*,$$

$$\hat{x} = x^* + e$$

$\hat{x} = \textbf{SplitPrec-MV}(\mathcal{J}, b)$:

$$x^* = \begin{bmatrix} F & B^T & \\ B & C & \\ & & I \end{bmatrix}^{-1} b,$$

$$r^* = b - \mathcal{J}x^*,$$

$$e = \begin{bmatrix} F & & Z \\ & I & \\ Y & & D \end{bmatrix}^{-1} r^*,$$

$$\hat{x} = x^* + e$$

1. Avoids nested Schur complement
2. Split Magnetics-Velocity (MV) from Navier-Stokes (NS)
3. Corresponds to a "split-factorization"

Splitting for MHD

Algorithm corresponds to an Approximate Block Factorization

$$\mathcal{J} \approx \mathcal{M} = \begin{bmatrix} F & & Z \\ & I & \\ Y & & D \end{bmatrix} \begin{bmatrix} F^{-1} & & \\ & I & \\ & & I \end{bmatrix} \begin{bmatrix} F & B^T & \\ B & C & \\ & & I \end{bmatrix}$$

- Need to compute $\mathcal{M}^{-1}$
- Requires two 2x2 solves
- Navier-Stokes operator well studied
- How to invert Magnetics-Velocity operator

Question: Do we think it will work?

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Splitting for MHD

Does splitting make a good preconditioner?

$$\mathcal{M} = \begin{bmatrix} F & & Z \\ & I & \\ Y & & D \end{bmatrix} \begin{bmatrix} F^{-1} & & \\ & I & \\ & & I \end{bmatrix} \begin{bmatrix} F & B^T & \\ B & C & \\ & & I \end{bmatrix}$$

1. Structurally small perturbation

$$\mathcal{M} = \begin{bmatrix} F & B^T & Z \\ B & C & \\ Y & \boxed{YF^{-1}B^T} & D \end{bmatrix}$$

2. Favorable spectrum

$$\mathcal{J}\mathcal{M}^{-1} = \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ K_u & K_p & (I - YF^{-1}B^T S^{-1} BF^{-1} ZP^{-1}) \end{bmatrix}$$

Challenges of splitting: Requires action of two 2x2 inverses

1. Navier-Stokes system – Block preconditioners PCD, LSC, SIMPLEC
2. Magnetics-Velocity system

Approximating Velocity/Magnetics Coupling: P_A An Approximate Commutator Approach

$$\begin{bmatrix} F & Z \\ Y & D \end{bmatrix} = \begin{bmatrix} I & \\ YF^{-1} & I \end{bmatrix} \begin{bmatrix} F & Z \\ & P \end{bmatrix}$$

where $P = D - YF^{-1}Z$

Strong form commuting assumption (e.g. motivated as in PCD)

$$\nabla A_z \cdot \left(\frac{\partial}{\partial t} + \mathbf{w} \cdot \nabla - \nu_F \nabla^2 \right) \approx \left(\frac{\partial}{\partial t} + \mathbf{w} \cdot \nabla - \nu_M \nabla^2 \right) \nabla A_z \cdot$$

$$\frac{\mu}{\rho} = \frac{\eta}{\mu_0}$$

$$\nabla A_z \approx const.$$

Also motivates a discrete commuting condition

$$Y Q_u^{-1} F \approx D Q_a^{-1} Y$$

which gives an approximate Schur complement

$$\hat{P}_A = D - YF^{-1}Z \approx D - (Q_a D^{-1} Y Q_u^{-1}) Z$$

$$= Q_a D^{-1} \left(D Q_a^{-1} D - Y Q_u^{-1} Z \right).$$

Requires approximate inverse!

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Approximating Velocity/Magnetics Coupling: P_B
A stiff wave analysis* of the 2x2 MV coupling

$$\begin{bmatrix} F & Z \\ Y & D \end{bmatrix} = \begin{bmatrix} I & \\ YF^{-1} & I \end{bmatrix} \begin{bmatrix} F & Z \\ & P \end{bmatrix}$$

$$\text{where} \quad P = D - YF^{-1}Z$$

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

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{u} \times \mathbf{B}) + \nabla \times \frac{\eta}{\mu_0} \nabla \times \mathbf{B} = 0$$

$$\mathbf{u} = \mathbf{u}_0 + \mathbf{u}_1$$

$$\mathbf{B} = \mathbf{B}_0 + \mathbf{B}_1.$$

$$Where \quad \mathbf{u}_0 = 0;$$

$$\mathbf{B}_0 = const.$$

$$\eta = \mu = 0$$

Linearization

$$\frac{\partial \mathbf{u}_1}{\partial t} - \frac{1}{\mu_0} (\nabla \times \mathbf{B}_1) \times \mathbf{B}_0 = 0$$

$$\frac{\partial \mathbf{B}_1}{\partial t} + \nabla \times (\mathbf{u}_1 \times \mathbf{B}_0) = 0.$$

$$\frac{\partial^2 \mathbf{B}_1}{\partial t^2} + \frac{1}{\mu_0} \nabla \times ([(\nabla \times \mathbf{B}_1) \times \mathbf{B}_0] \times \mathbf{B}_0) = 0.$$

$$\mathbf{B}_1 = \nabla \times \mathbf{A}_1$$

$$\frac{\partial^2 A_{z1}}{\partial t^2} - \frac{\|\mathbf{B}_0\|^2}{\rho \mu_0} \nabla \cdot \nabla A_{z1} = 0.$$

*Classical wave analysis texts; Knoll and Chacon et. al Stiff Wave paper (JCP 2004)

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Approximating Velocity/Magnetics Coupling: P_C A simple Approximation for F in P

$$\begin{bmatrix} F & Z \\ Y & D \end{bmatrix} = \begin{bmatrix} I & \\ YF^{-1} & I \end{bmatrix} \begin{bmatrix} F & Z \\ & P \end{bmatrix}$$

$$\text{where} \;\; P = D - YF^{-1}Z$$

1st term Neumann Series (or Pressure Proj.) approximation for F;

$$F \approx \frac{1}{\Delta t} Q_u. \longrightarrow \hat{P}_C = D - \Delta t Y Q_u^{-1} Z.$$

Brief Structure of ABF Iterative solves

- Outer solve: non-restarted GMRES
- ABF Preconditioning
  - SIMPLEC [3x3]: Use SIMPLEC diagonal matrix approximation in both S, P
  - Split I: [2x2] Velocity-Pressure (PCD); [2x2] Magnetics-Velocity (P_I); I = A, B, C
- Sub-block solves ML AMG V(1,1)
  - Velocity-Pressure
    - Momentum- Fully-coupled AMG NSA: ILU(2)
    - Pressure Schur Complement- SA: GS
  - Magnetics-Velocity
    - Momentum- Same as above
    - Magnetics Schur Complement- NSA: ILU(2)

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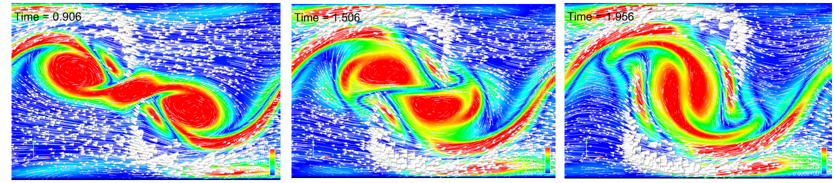
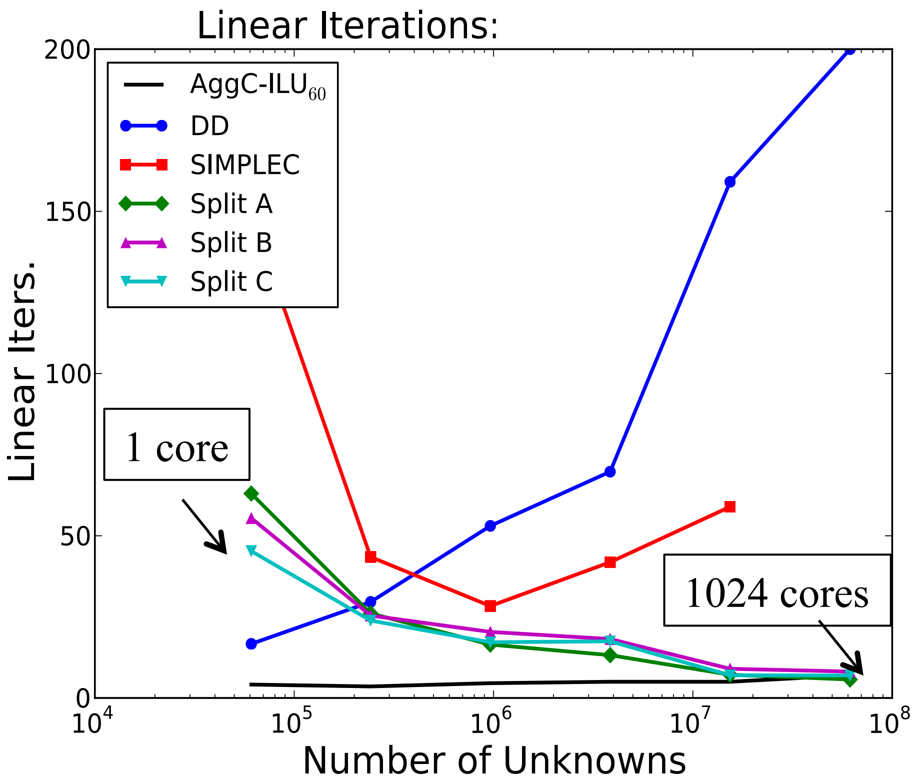
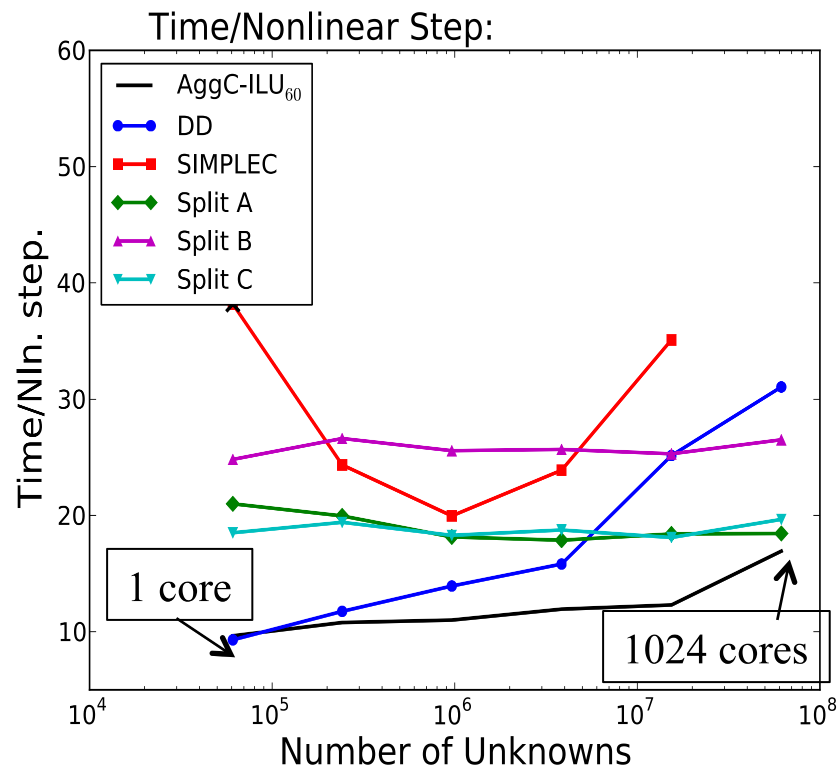
Hydromagnetic Kelvin-Helmholtz

Re = 10^3, S= 10^3; M_A = 1.5; CFL ~5







Take home: Split preconditioner scales algorithmically, more relevant for mixed discretizations; Need optimization of CPU time; Fully-coupled ML AMG does well.

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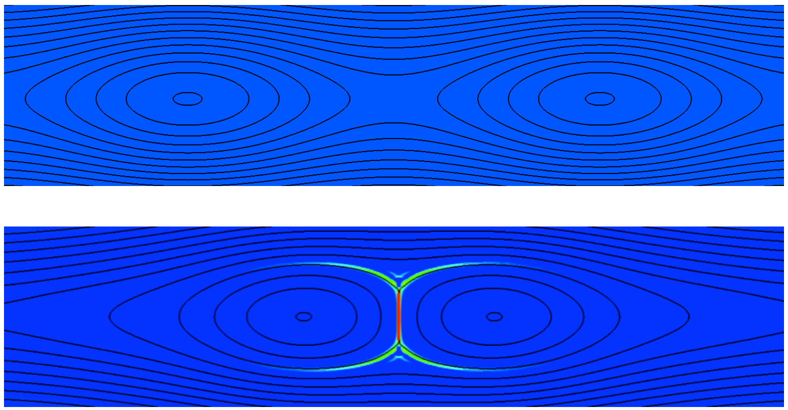
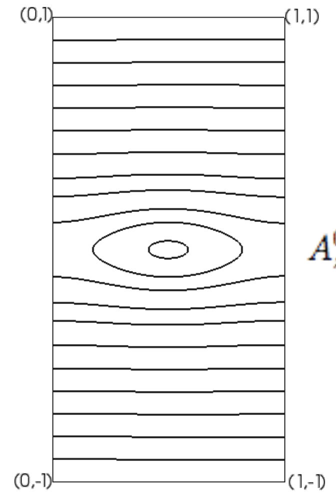
Results: Island Coalescence





Simulation on half domain

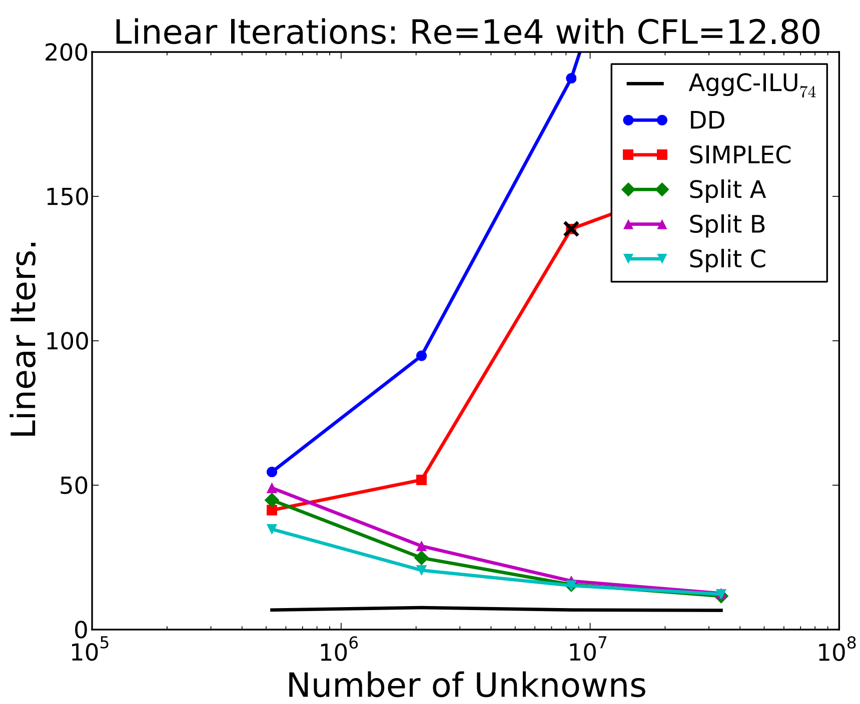
- Symmetry BC
- Perturbed Harris-Sheet

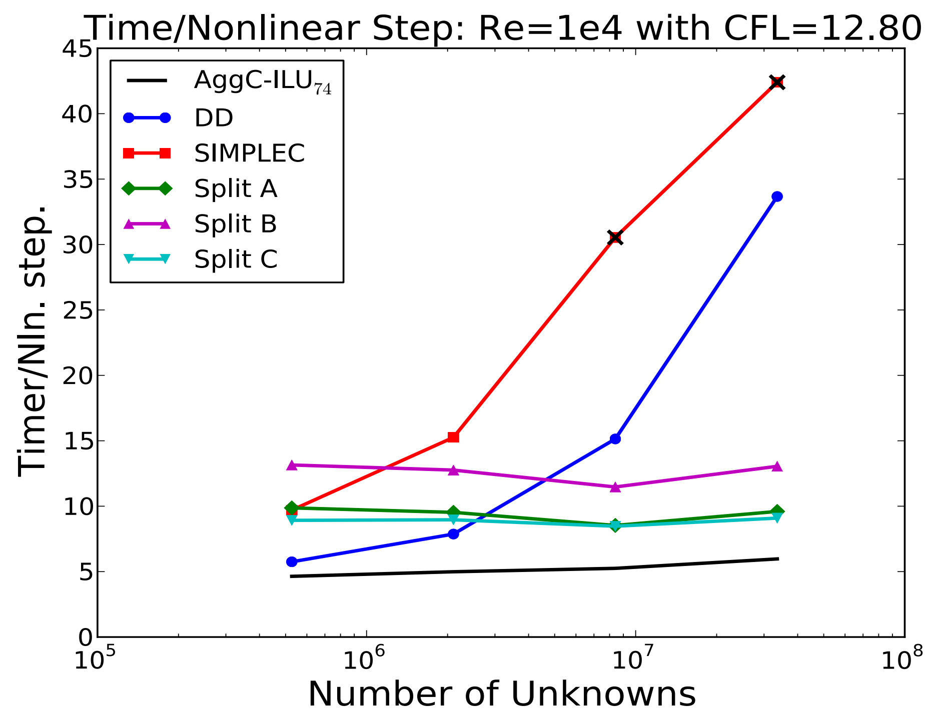
$$A_z^0(x,y,0) = \delta\ ln\left[\cosh\left(\frac{y}{\delta}\right) + \epsilon\ \cos\left(\frac{x}{\delta}\right)\right]$$

Results details

- Lundquist number: 10^4
- Starting time right before reconnection event
  Results averaged over 45 uniform timesteps
- Run on 1, 4, 16, 64, 256, and 1024 processors (33,000 unks/core)

MHD Weak Scaling: Transient Island Coalescence at S= 10^4
Fixed Alfven CFL

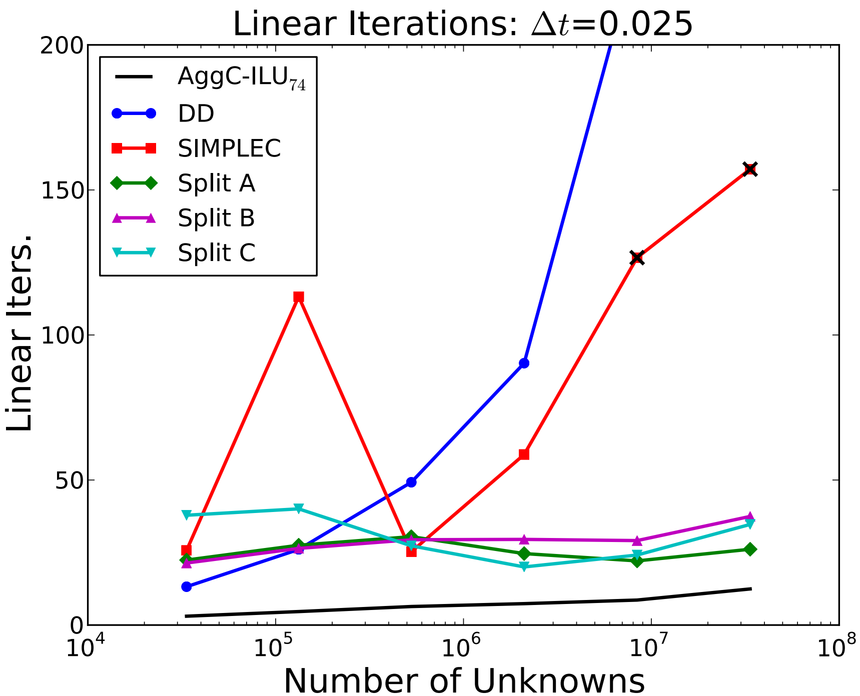


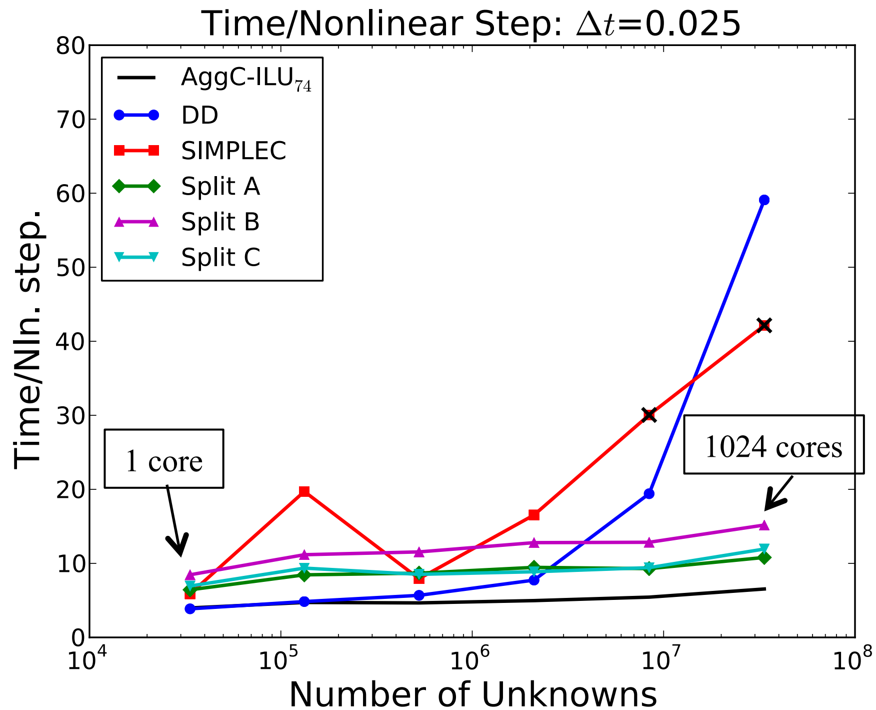


Take home: Split preconditioner scales algorithmically, more relevant for mixed discretizations; Need optimization of CPU time; Fully-coupled ML AMG does well.

MHD Weak Scaling: Transient Island Coalescence at S= 10^4

Fixed Time Step (Alfven CFL_{max} ~ 100)





Take home: Split preconditioners scale reasonably, more relevant for mixed discretizations; Need optimization of split preconditioners; Fully-coupled ML AMG does well.

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Conclusions

- Demonstrated ABF preconditioners for primitive variable incompressible MHD
- 3x3 block system has nested Schur complement structure
- ABF performance not optimized, however results are encouraging
- Uses operator splitting approach
    - Separates fluid and magnetics couplings
    - Preconditioner is (structurally) small perturbation of original operator
    - Requires approximating inverse action of two 2x2 operators
    - Weak scaling for fixed CFL, time-step (reasonable)
    - Can be used for mixed and physics compatible discretizations
- Explored usage of SIMPLEC preconditioner
    - Strong dependence on CFL number, some strange behavior in scaling at large time steps (fixed CFL – coarse mesh)

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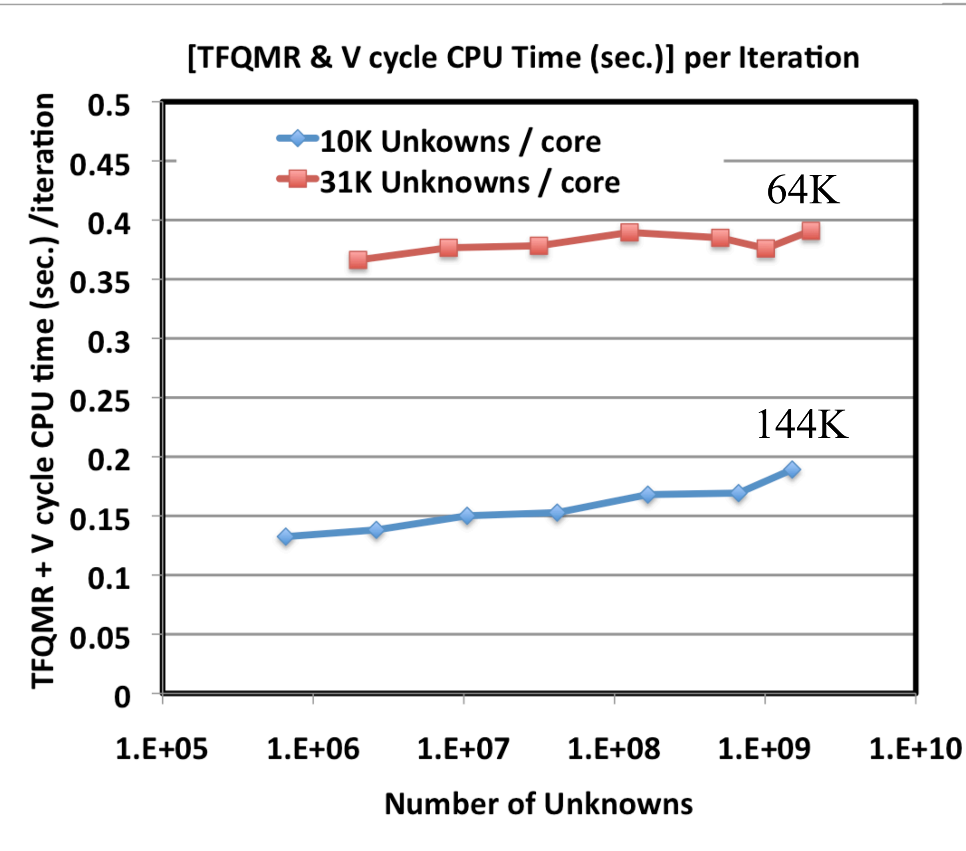
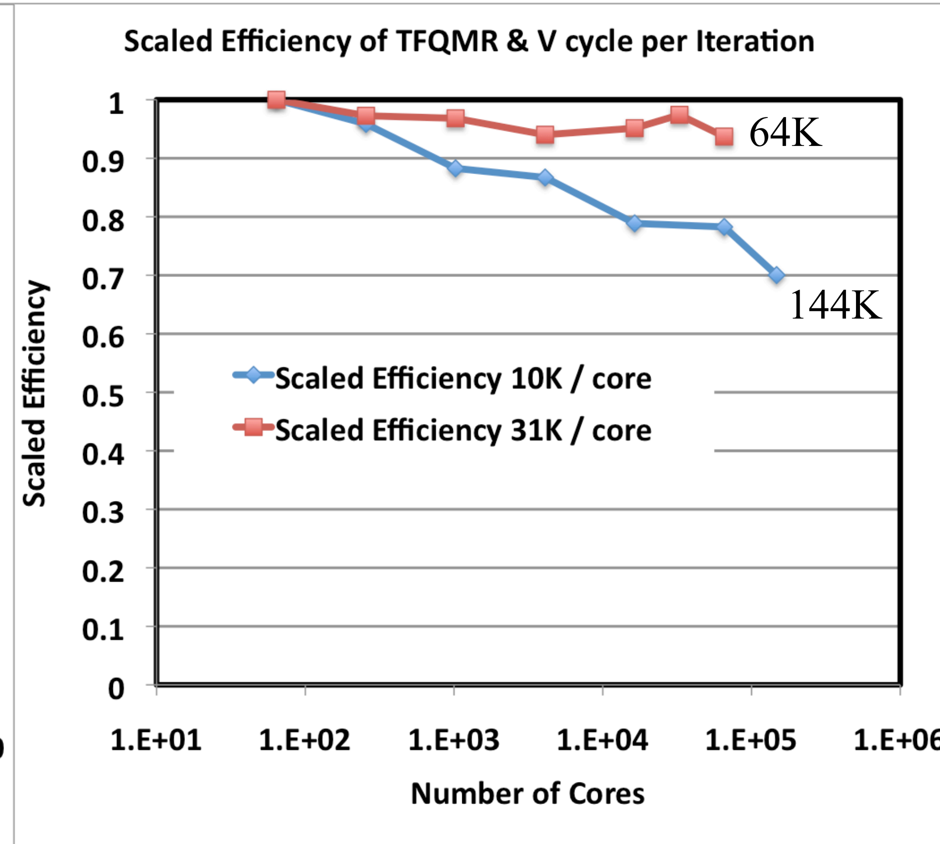
Weak Scaling Uncoupled Aggregation Scheme: Time/iteration on BlueGene/P (Drift – Diffusion BJT: P. Lin)





- TFQMR: used to look at time/iteration of multilevel preconditioners.
- W-cyc time/iteration not doing well due to significant increase in work on coarse levels (not shown)
- Good scaled efficiency for large-scale problems on larger core counts for 31K Unknowns / core

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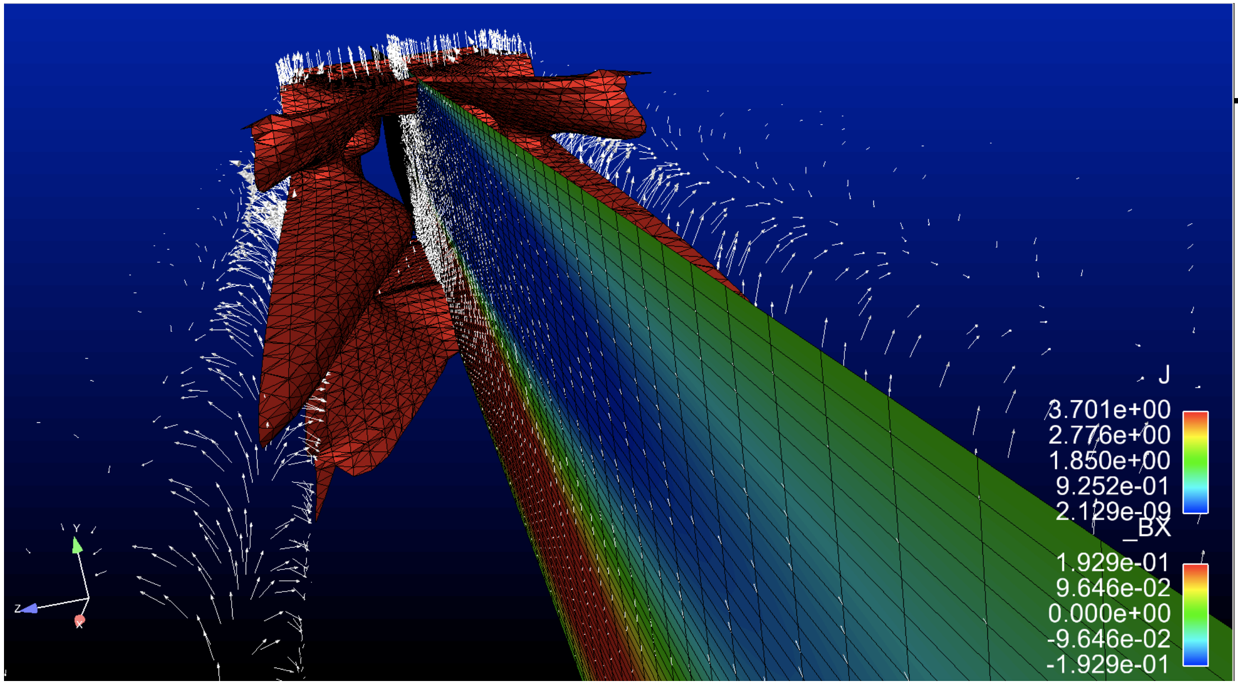
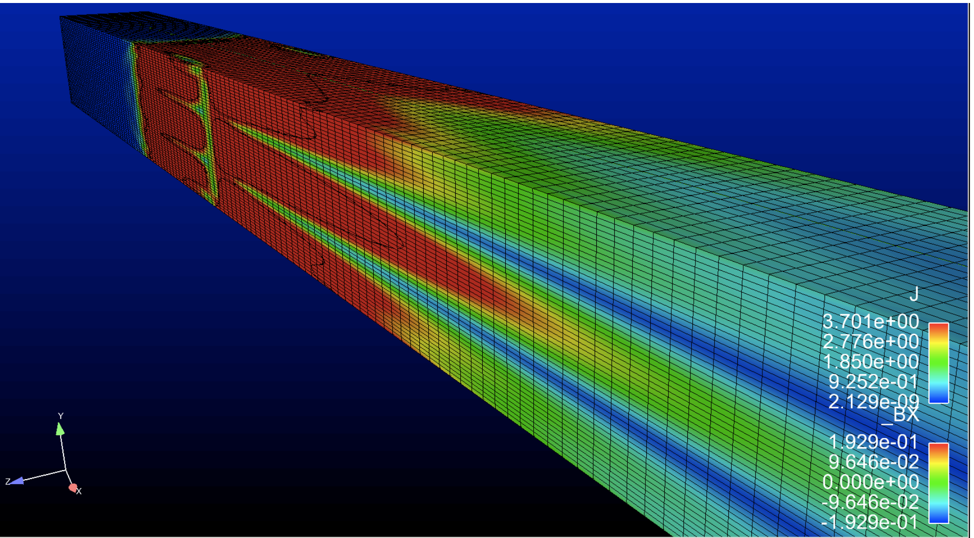
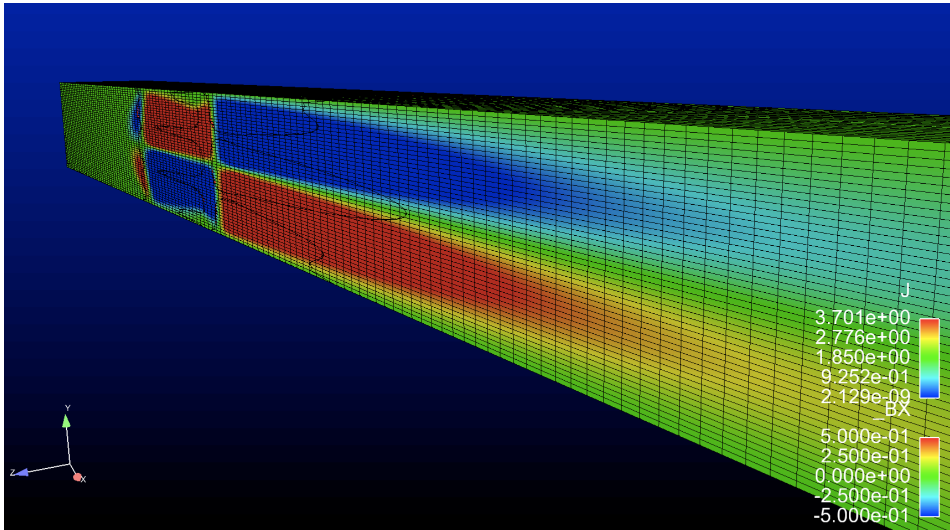
3D B-Field Lagrange Multiplier Formulation (Divergence form)



Initial Prototype MHD Generator





Plasma Physics Studies: Plasmoid formation in magnetic reconnection

Magnetic reconnection: fundamental process whereby magnetic field topology is altered resulting in a rapid conversion of magnetic field energy into plasma energy and significant plasma transport. Mechanisms and time scales have been an open issue for last 50 years.

Critical process in astrophysical and laboratory plasmas.