

Approximate Block Factorization Preconditioners for Scalable Solution of Multiphysics MHD Systems.

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Outline

- **General Scientific and Mathematical/Computational Motivation**
- **Motivation for Fully Implicit Newton – Krylov Solution Methods**
- **Brief Overview of 3D Resistive MHD Equations and Numerical Approximation**
- **Motivation for Approximate Block Factorization (ABF) Preconditioners**
 - **indicate Scaling of Fully-coupled AMG for Systems (Stabilized FE MHD)**
 - **Scaling of ABF Preconditioners (Stabilized FE MHD)**
 - **Scaling of ABF for Mixed Integration and Edge-element Formulations**
- **Conclusions**

Motivation: Science/Technology and Mathematical / Computational

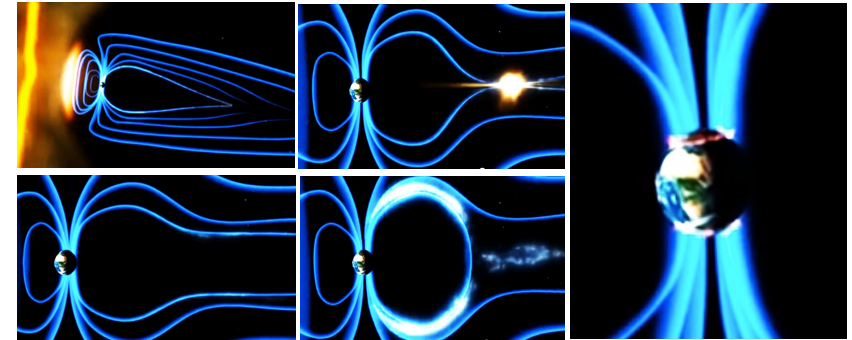
Science / Technology Motivation:

Resistive and extended MHD models are used to study important plasma physics systems

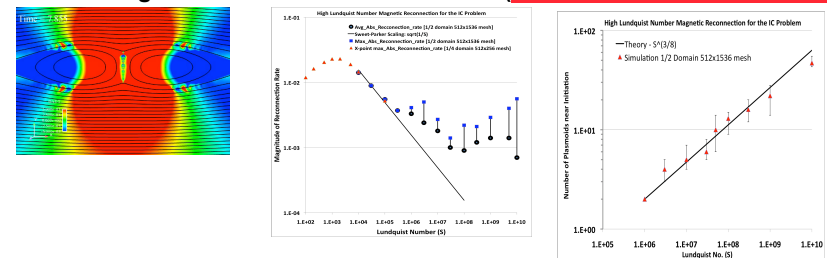
- **Astrophysics:** Magnetic reconnection, solar flares, ..
- **Planetary-physics:** Earth's magnetospheric substorms, Aurora, geo-dynamo, planetary-dynamos
- **Fusion:** Magnetic Confinement [MCF] (e.g. ITER), Inertial Conf. [ICF] (e.g. NIF, Z-pinch)

Mathematical/Computational Motivation:

Achieving Scalable Predictive Simulations of Complex Highly Nonlinear Multiphysics Systems to Enable Scientific Discovery and Engineering Design/Optimization



NASA Magnetic Reconnection Animation (https://www.youtube.com/watch?v=i_x3s80DaKg)



Magnetic Reconnection: $S = 1e+9$ (left), Reconn. Rate vs. SP theory (right)

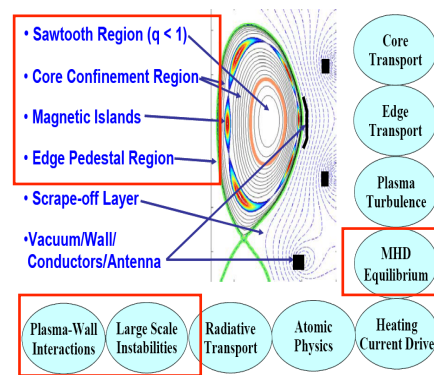
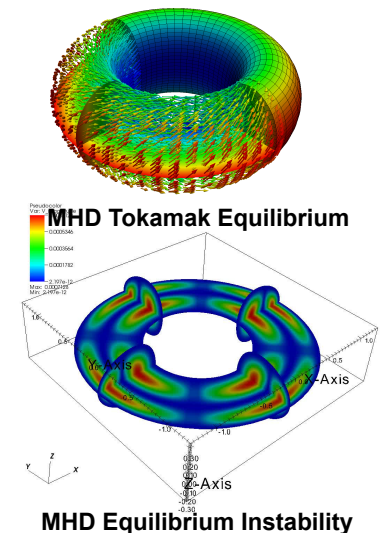


Fig. 2: Illustration of the interacting physical processes within a tokamak discharge.



What are multi-physics systems? (A multiple-time-scale perspective)

These systems are characterized by a myriad of complex, interacting, nonlinear multiple time- and length-scale physical mechanisms.

These mechanisms:

- can be dominated by one, or a few processes, that drive a short dynamical time-scale consistent with these dominating modes,
- consist of a set of widely separated time-scales that produce a stiff system response,
- nearly balance to evolve a solution on a dynamical time-scale that is long relative to the component time scales,
- or balance to produce steady-state behavior.

Mathematical Approach - develop:

- Stable & higher-order accurate fully-implicit / IMEX formulations allowing resolution of dynamical time-scale of interest
- Stable and accurate spatial discretizations for complex geom.,
Options enforcing key mathematical properties (e.g. positivity), and structure-preserving-forms (e.g. $\text{div } \mathbf{B} = 0$)
- Robust and efficient fully-coupled nonlinear/linear iterative solution methods based on Newton-Krylov (NK) methods
- Scalable and efficient preconditioners utilizing multi-level (AMG) methods (Fully-coupled AMG, physics-based, approx. block factorization)
=> Also enables beyond forward simulation & integrated UQ

3D Resistive MHD Equations: Lagrange-Multiplier Formulation and VMS

Resistive MHD Model in Residual Notation

$$\mathbf{R}_{\mathbf{v}} = \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot [\rho \mathbf{v} \otimes \mathbf{v} - (\mathbf{T} + \mathbf{T}_M)] + 2\rho \Omega \times \mathbf{v} - \rho \mathbf{g} = \mathbf{0}$$

$$\mathbf{T} = -[P - \frac{2}{3}\mu(\nabla \cdot \mathbf{v})]\mathbf{I} + \mu[\nabla \mathbf{v} + \nabla \mathbf{v}^T]$$

$$\mathbf{T}_M = \frac{1}{\mu_0} \mathbf{B} \otimes \mathbf{B} - \frac{1}{2\mu_0} \|\mathbf{B}\|^2 \mathbf{I}$$

$$R_P = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$R_e = \frac{\partial(\rho e)}{\partial t} + \nabla \cdot [\rho \mathbf{v} e + \mathbf{q}] - \mathbf{T} : \nabla \mathbf{v} - \eta \left\| \frac{1}{\mu_0} \nabla \times \mathbf{B} \right\|^2 = 0$$

$$\mathbf{R}_{\mathbf{B}} = \frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot \left[\mathbf{B} \otimes \mathbf{v} - \mathbf{v} \otimes \mathbf{B} - \frac{\eta}{\mu_0} (\nabla \mathbf{B} - (\nabla \mathbf{B})^T) + \psi \mathbf{I} \right] = \mathbf{0}$$

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

$$\mathcal{R}(\mathbf{u}) = \mathcal{L}(\mathbf{u}) - \mathbf{f} = \mathbf{0}$$

- Divergence free involution enforced as elliptic constraint with a Lagrange multiplier.
(Dedner et. al. 2002; Codina et. al. 2006, 2011)
 - Only weakly divergence free in FE implementation (stabilization of B - ψ coupling)
- Can show relationship with projection (e.g. Brackbill and Barnes 1980) when 1st order-splitting is used.
- Issue for using C^0 FE for domains with re-entrant corners / soln singularities
(Costabel et. al. 2000, 2002, Codina, 2011, see Badia et. al. 2013 for stabilized FE that is unconditionally stable on appropriate meshes)

Multiple-time-scale systems: E.g. 2D Tearing Mode
 Low Mach number compressible; $M \sim 10^{-4}$; Fully-implicit (BDF2), IMEX (SSP3)

Time = 0.000

Approx. Computational Time Scales:

- Divergence Constraint ($\nabla \cdot \mathbf{B} = 0$): $1/\infty = 0$
- Fast Magnetosonic Wave (c_f): 10^{-4} to 10^{-2}
- Alfvén Wave (c_a): 10^{-4} to 10^{-2}
- Slow Magnetosonic Wave (c_s): 10^{-2} to 10^{-1}
- Sound Wave (c): 10^{-2}
- Advection (c_v): ∞ to 10^1
- Diffusion: 10^{-4} to 10^{-2}
- Macroscopic Tearing Mode: 10^2

Wave speeds

$$\|\mathbf{u}\|, \|\mathbf{u}\| \pm c_s, \|\mathbf{u}\| \pm c_a, \|\mathbf{u}\| \pm c_f, \pm c_h$$

Fully-implicit (BDF2) / IMEX SSP3
 Max CFL:

$$\begin{aligned} \text{CFL}_{\text{div}} &= \infty \\ \text{CFL}_{\text{cf}} &\sim 10^5 \text{ to } 10^4 \\ \text{CFL}_{\text{ca}} &\sim 10^5 \text{ to } 10^4 \\ \text{CFL}_{\text{cs}} &\sim 10^3 \text{ to } 10^2 \\ \text{CFL}_c &\sim 10^3 \text{ to } 10^2 \\ \text{CFL}_{\text{cv}} &\sim 1 \text{ to } 0.25 \end{aligned}$$

Summary of Structure of Linear Systems Generated in Newton's Method

$$\mathcal{J} \Delta \mathbf{x} = -\mathcal{F}$$

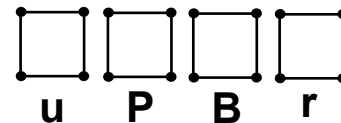
VMS Stabilize produces SUPG like terms, stabilizing terms for inf-sup condition (all Q1 interpolants), physics cross-coupling terms and discontinuity Capturing type operators

$$\mathcal{J} = \begin{bmatrix} F & B_p^T & Z & \\ B_p & C_u & & \\ Y & & D & B_r^T \\ & & B_r & C_B \end{bmatrix} \quad \mathbf{x} = [\mathbf{v}, P, \mathbf{B}, r]^T$$

$$\mathcal{F} = [\mathbf{F}_v, F_P, \mathbf{F}_B, F_r]^T$$

$$C_u = \sum_e \int_{\Omega^e} \rho \tau_m \nabla \Phi \cdot \nabla \Phi \, d\Omega$$

$$C_B = \sum_e \int_{\Omega^e} \tau_B \nabla \Phi \cdot \nabla \Phi \, d\Omega$$

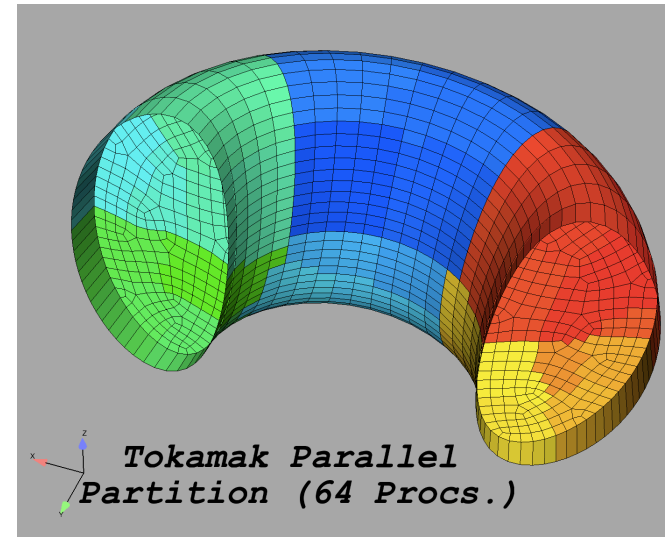


Preconditioning

Three variants 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 eff., non-optimal algorithmic scalability



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

Fully-coupled Algebraic Multilevel methods

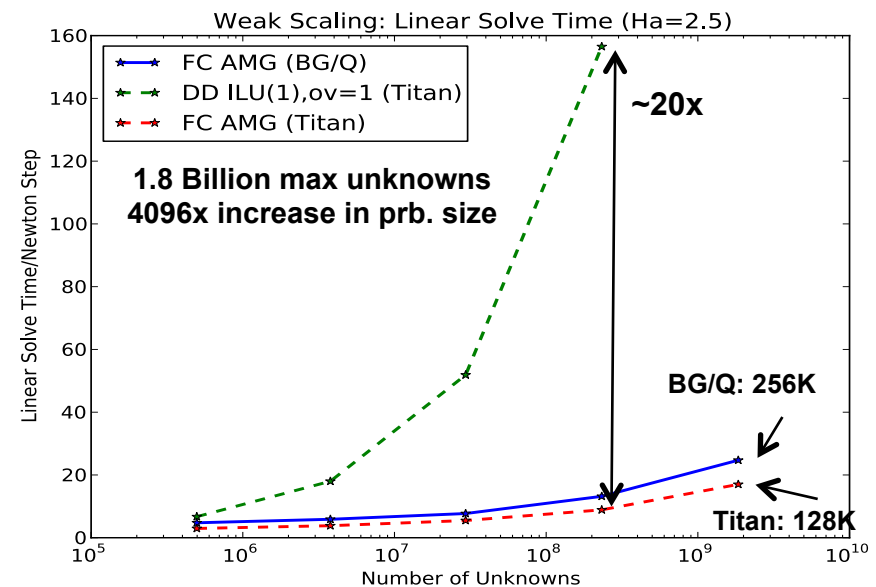
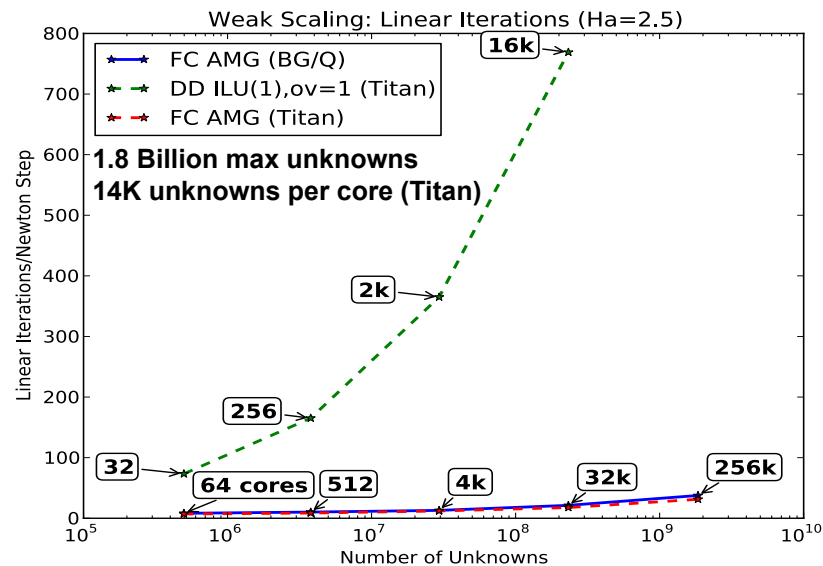
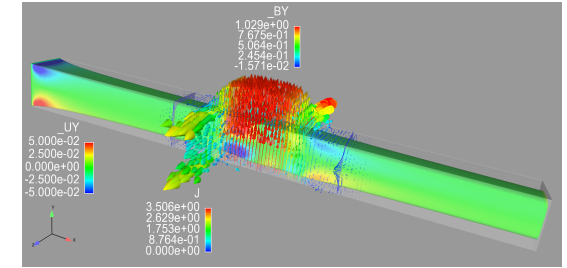
- Consistent set of DOF-ordered blocks at each node (e.g. Stabilized FE)
- Uses block non-zero structure of Jacobian
- Aggregation techniques and rates can be chosen
- Jacobi, GS, ILU(k) as smoothers
- Can provide optimal algorithmic scalability

(See Paul Lin Talk)

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

- **Applies to mixed interpolation (FE), staggered (FV), physics compatible discretization approaches using segregated unknown blocking**
- **Applies to systems where coupled AMG is difficult or might fail**
- **Enables specialized AMG, e.g. $H(\text{grad})$, $H(\text{curl})$ to be applied to distinct discretizations.**
- Can provide optimal algorithmic scalability for coupled systems

SFE Initial Scaling Studies for Cray XK7 AND BG/Q. 3D MHD Generator [$Re = 500$, $Re_m = 1$, $Ha = 2.5$]



Details: See Paul Lin's Talk Afternoon Session

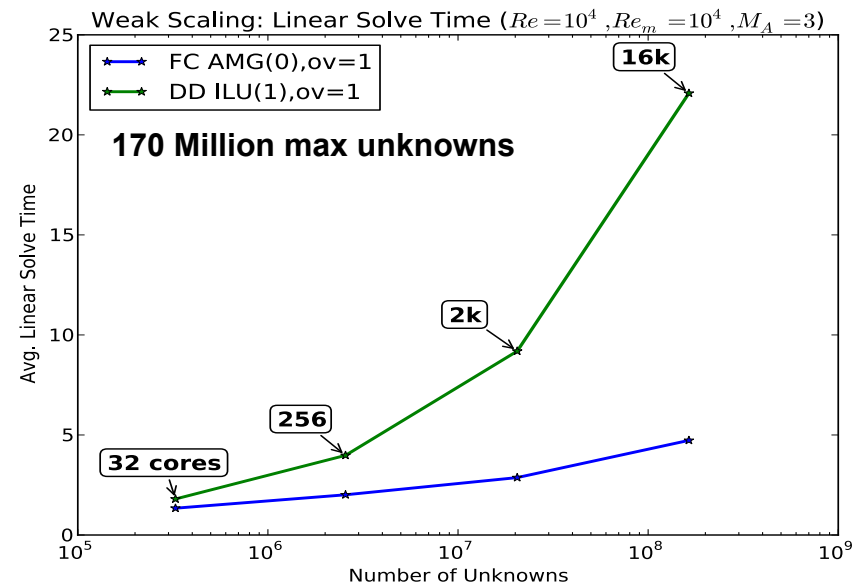
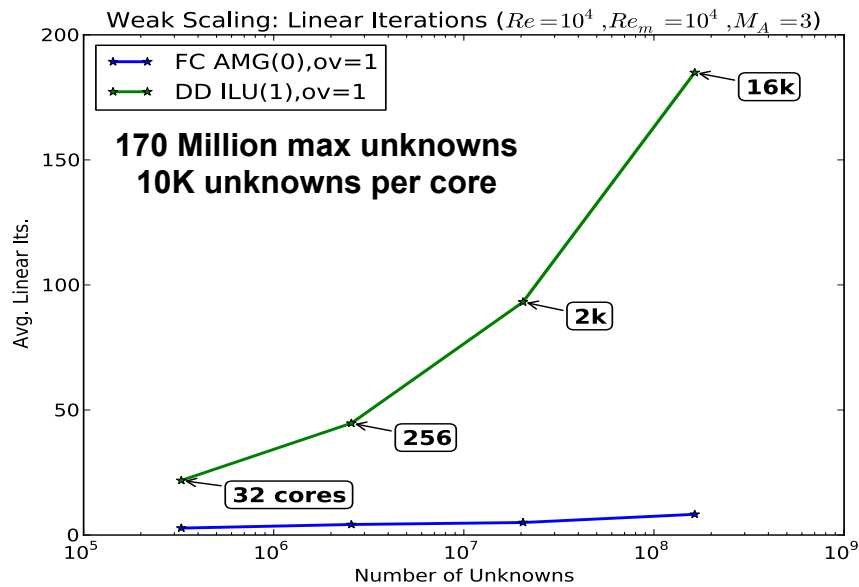
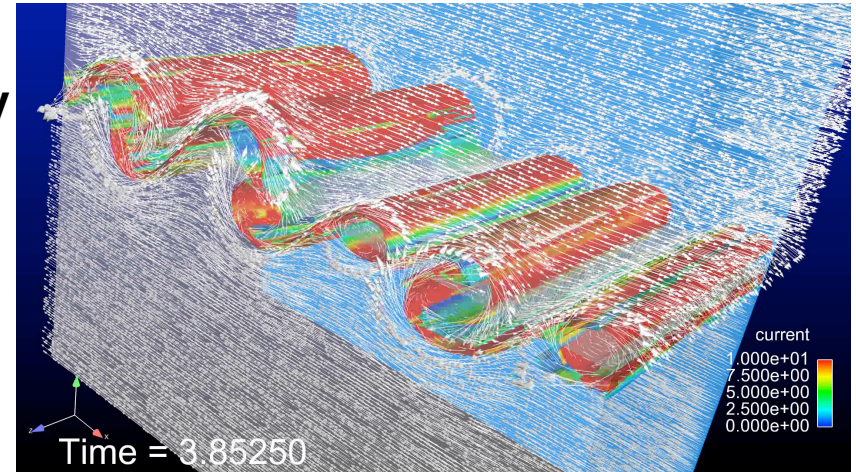
(DOE/ORNL Titan Cray XK7: Joule Metric)



Initial Scaling Study for Cray XK7.

3D Hydromagnetic Kelvin-Helmholtz Instability

[$Re = 10^4$, $Re_m = 10^4$, $M_A = 3$; $CFL_{max} \sim 5$]



Physics-based and Approximate Block Factorizations: Coercing **Strongly Coupled Off-Diagonal Physics** / Disparate Discretizations and Scalable Multigrid to play well together

Physics-based (Parabolization):

$$\partial_t u = \partial_x v, \quad \partial_t v = \partial_x u.$$

$$u^{n+1} = u^n + \Delta t \partial_x v^{n+1}, \quad v^{n+1} = v^n + \Delta t \partial_x u^{n+1}.$$

$$(I - \Delta t^2 \partial_{xx}) u^{n+1} = u^n + \Delta t \partial_x v^n$$

Schur Complement, (Approximate) Block Factorization:

$$\begin{bmatrix} I & -\Delta t C_x \\ -\Delta t C_x & I \end{bmatrix} \begin{bmatrix} u^{n+1} \\ v^{n+1} \end{bmatrix} = \begin{bmatrix} u^n - \Delta t C_x v^n \\ v^n - \Delta t C_x u^n \end{bmatrix}$$

$$\begin{bmatrix} D_1 & U \\ L & D_2 \end{bmatrix} = \begin{bmatrix} I & U D_2^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} D_1 - U D_2^{-1} L & 0 \\ 0 & D_2 \end{bmatrix} \begin{bmatrix} I & 0 \\ D_2^{-1} L & I \end{bmatrix}$$

The Schur complement is then

$$D_1 - U D_2^{-1} L = (I - \Delta t^2 C_x C_x) = (I - \Delta t^2 \partial_{xx})$$

Result:

- 1) Stiff (large-magnitude) off-diagonal hyperbolic type operators (blocks) are now combined onto diagonal parabolic type operator (block).
- 2) Coupled physics is segregated into partitioned sub-systems to which specialized solvers can be applied (optimal AMG methods e.g. H(grad), H(curl))
- 3) Effective Schur complement approximations need to preserve strong cross-coupling physics and time scales.

Knoll, Chacon et. al. JFNK Methods for accurate time integration of stiff-wave systems, *Journal of Scientific Computing*, 2005

L. Chacon, "An optimal, parallel, fully implicit Newton-Krylov solver for three-dimensional visco-resistive magnetohydrodynamics," *Phys. Plasmas*, 2008

Elman, Howle, Shadid, and Tuminaro, "A Parallel Block Multi-level Preconditioner for the Three-Dimensional Incompressible Navier-Stokes", *JCP*, 2003

Elman, Howle, Shadid, Shuttlesworth, Tuminaro, "A Taxonomy of Parallel Multi-level Block Preconditioners for the Incompressible Navier-Stokes", *JCP*, 2008

Cyr, Shadid, Tuminaro, Pawlowski, Chacon, "A new approximate block factorization preconditioner for 2D incompressible (reduced) resistive MHD," *SISC*, 2012



Incompressible Resistive MHD a Nested Schur Complement Approach

Block LU factorization gives

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

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

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

- 3x3 system leads to embedded Schur complements
- Embedding is independent of ordering (**C⁻¹ doesn't need to exist!**)
- How is P approximated?
- Chacon & Knoll (2004,..) explored compressible flow
($\frac{\partial \rho}{\partial t}$ included in C) and incompressible flow using
stream-function vorticity to simplify factors (i.e, eliminate
 $\nabla \cdot \mathbf{v} = 0$ elliptic constraint).
- Can we simplify nested structure? E.g. Operator split prec.

Operator split / Residual-based Defect-Correction ABF Preconditioner

- 1) Residual defect-correction factorization procedure strongly couples operators producing the pressure wave (infinite speed) and Alfven wave (finite speed) and reduces to two 2x2 blocks for the ABF:

$$\begin{bmatrix} F & B^T & Z \\ B & C & 0 \\ Y & 0 & D \end{bmatrix} \approx \begin{bmatrix} F & I & Z \\ Y & & D \end{bmatrix} \begin{bmatrix} F^{-1} & & \\ & I & \\ & & I \end{bmatrix} \begin{bmatrix} F & B^T \\ B & C \\ & I \end{bmatrix} = \begin{bmatrix} F & B^T & Z \\ B & C & \\ Y & \boxed{YF^{-1}B^T} & D \end{bmatrix}$$

- 2) 3x3 -> two 2x2 sub-systems that contain dominate coupling (pressure wave, Alfven wave)

$$\mathcal{S} = C_u - B\hat{F}^{-1}B^T$$

$$\mathcal{P} = D - Y\hat{F}^{-1}Z$$

Relation to pressure wave (elliptic constraint)

Formally assume

- Stable mixed integration
- Transient with small time-step-size

$$\hat{\mathbf{S}} = -\mathbf{B}[\Delta t \mathbf{Q}_L^{-1}] \mathbf{B}^T \approx -\Delta t \tilde{\mathbf{L}}_p$$

Relation to Alfven wave

Formally assume a stiff wave linearized analysis (with $\mathbf{u}_0 = 0$ & $\mathbf{B}_0 = \text{const.}$)

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

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

Consider NS Schur complement methods (e.g. Pressure Proj., SIMPLEC), Press-Conv-Diff (PCD) and Least Squares comutator (LSC) type approaches)

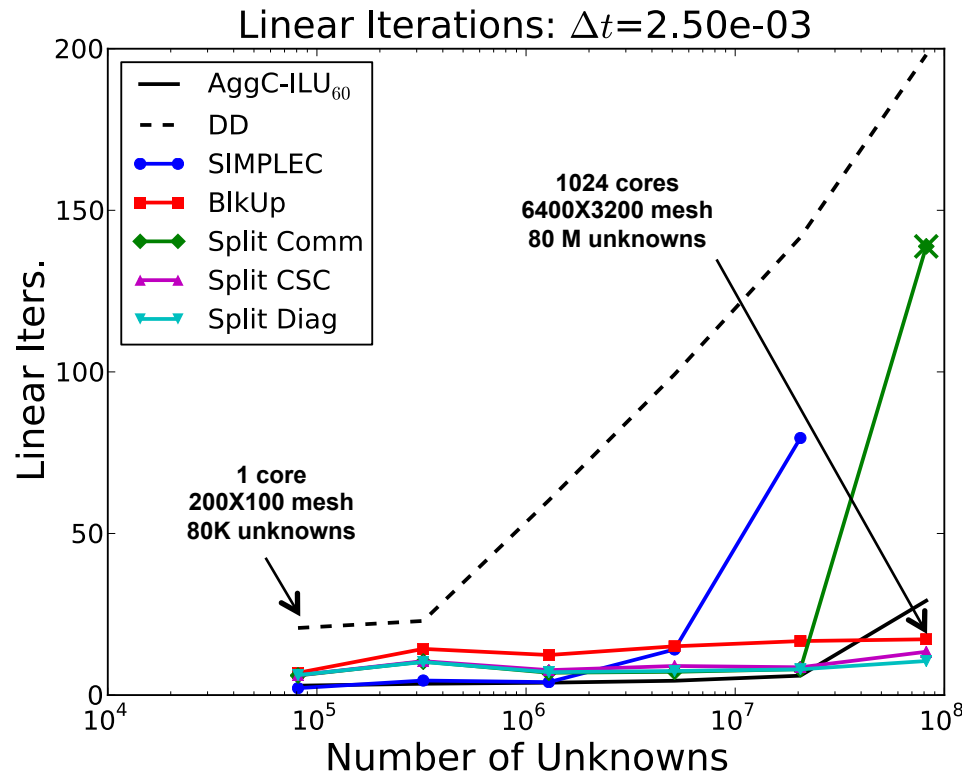
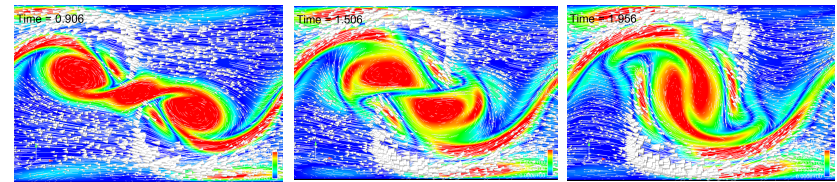
See e.g. Elman, Howle, S., Shuttleworth, Tuminaro, "A Taxonomy of Parallel Multilevel Block Preconditioners for the Incompressible Navier-Stokes Equations", JCP, v. 227, 3, pp 1790 - 1808, 2008

Cyr, S., Tuminaro, Pawlowski, and Chacon, "A new approximate block factorization preconditioner for 2D incompressible (reduced) resistive MHD," SIAM Journal on Scientific Computing, 35:B701-B730, 2013

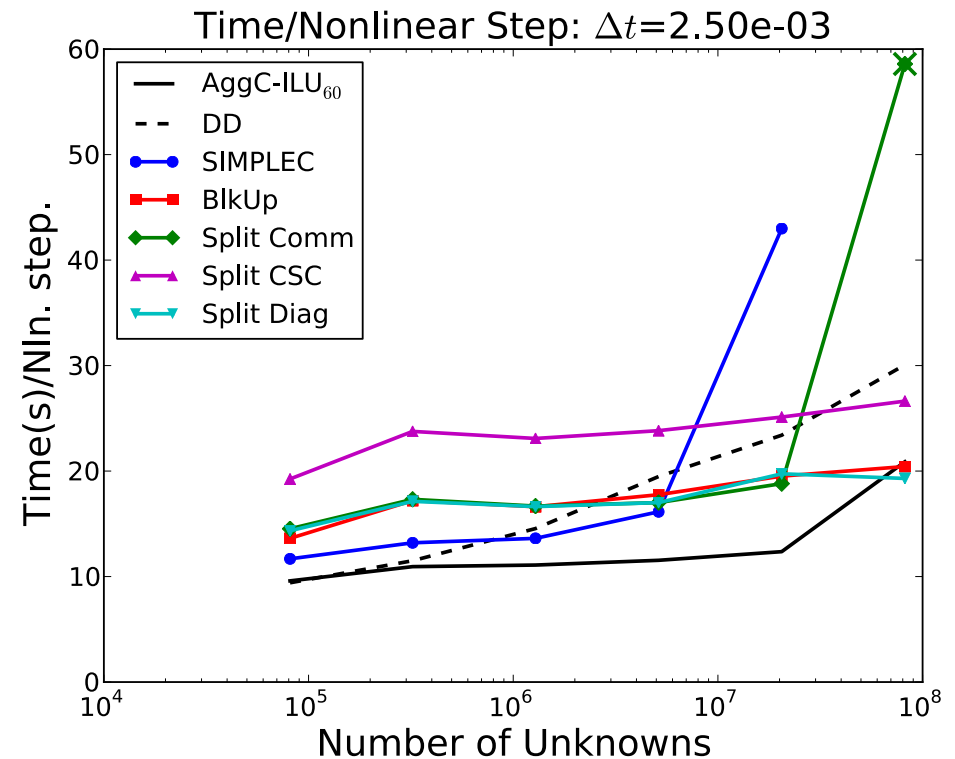


Transient 2D Hydromagnetic Kelvin-Helmholtz Problem, SFE

$Re = 5e+3$, $S = 1e+3$; $M_A = 1.5$; $CFL_{max} \sim 10$



Comm – comutator; CSC – continuous Schur comp.;
Diag. – diagonal approx of inverse in Schur comp.



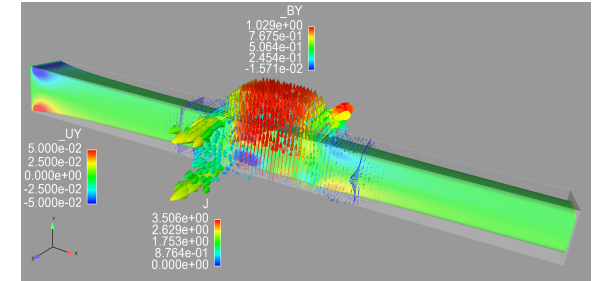
Quad-core Nehalems with Infini-band SNL Red Sky

Cyr, S., Tuminaro, Pawlowski, and Chacon, "A new approximate block factorization preconditioner for 2D incompressible (reduced) resistive mhd," *SIAM Journal on Scientific Computing*, 35:B701-B730, 2013

Cyr, S., and Tuminaro, "Teko an abstract block preconditioning capability with concrete example applications to Navier-Stokes and resistive MHD," Submitted to *SISC*.

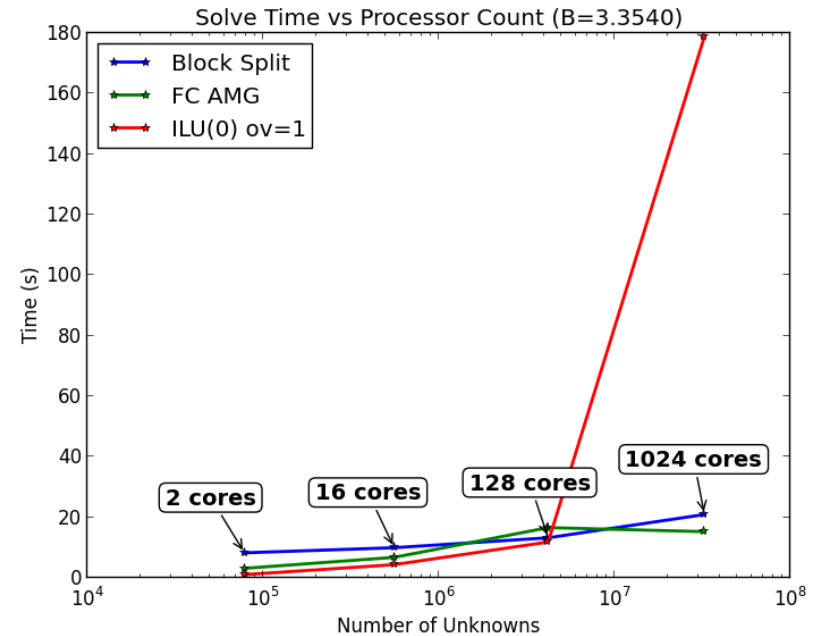
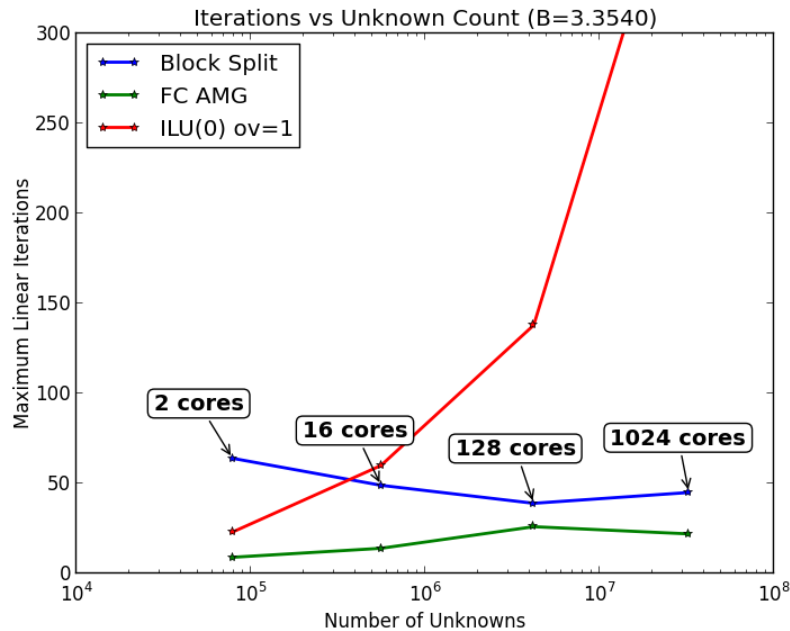


Extensions to 3D: Initial Approximate Block Preconditioning 3D MHD Generator [Re = 500, Re_m = 1, Ha = 2.5], SFE



$$\mathcal{J} = \begin{bmatrix} F & B_p^T & Z \\ B_p & C_u & \\ Y & & D & B_r^T \\ & & B_r & C_B \end{bmatrix} \Rightarrow \begin{bmatrix} F & B_p^T & \hat{Z} \\ B_p & C_u & \\ \hat{Y} & & \hat{D} \end{bmatrix}$$

$$\mathcal{J} \approx \mathcal{M}_{Split} = \begin{bmatrix} F & & Z \\ & I & \\ Y & & \hat{D} \end{bmatrix} \begin{bmatrix} F^{-1} & & \\ & I & \\ & & I \end{bmatrix} \begin{bmatrix} F & B^T \\ B & C \\ & & I \end{bmatrix} \quad \begin{aligned} S &= C - BF^{-1}B^T \\ \hat{P} &= \hat{D} - YF^{-1}Z \end{aligned}$$



Weak scaling of FC-AMG and block preconditioners reasonable to 1024 cores
Both suffer some performance degradation on this capacity machine (Redsky)

New residual defect-correction ABF strongly couples Alfven wave operators and reduces to three 2x2 blocks

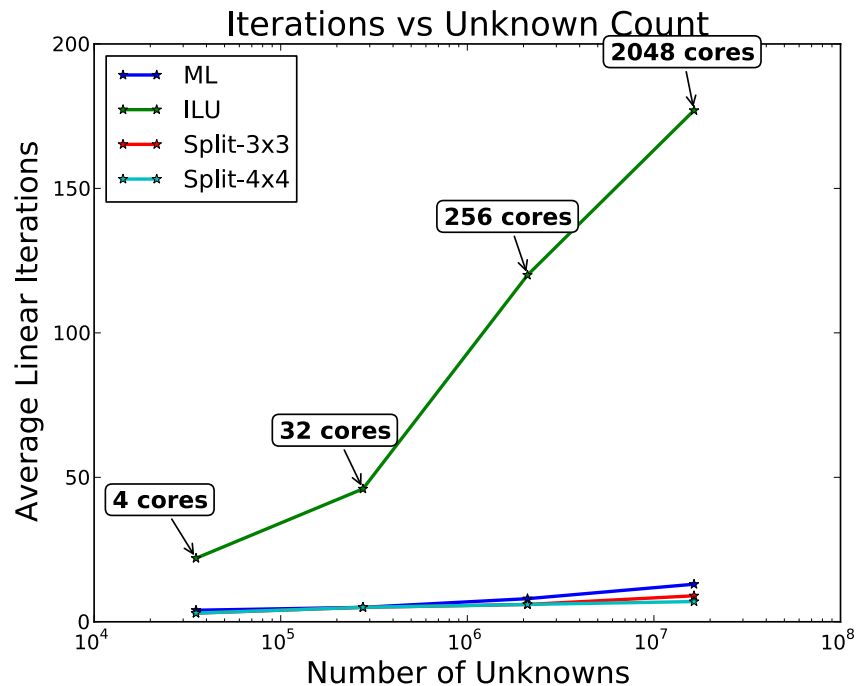
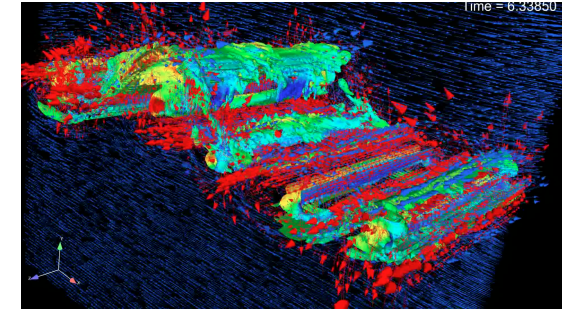
$M_1 \tilde{x} = b$; $M_2(\hat{x} - \tilde{x}) = (b - \mathcal{J}\tilde{x})$; leads to this ABF $\hat{x} = M_2^{-1}(M_1 + M_2 - \mathcal{J})M_1^{-1}b$

$$\begin{bmatrix} F_m & B^T & Z & 0 \\ B & C_P & 0 & 0 \\ Y & 0 & F_B & B^T \\ 0 & 0 & B & C_\psi \end{bmatrix} \approx \begin{bmatrix} F_m & 0 & Z & 0 \\ 0 & I & 0 & 0 \\ Y & 0 & F_B & I \\ 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} F_m^{-1} & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & F_B^{-1} & 0 \\ 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} F_m & B^T & 0 & 0 \\ B & C_P & 0 & 0 \\ 0 & 0 & F_B & B^T \\ 0 & 0 & B & C_\psi \end{bmatrix}$$

$$= \begin{bmatrix} F_m & B^T & Z & ZF_B^{-1}B^T \\ B & C_P & 0 & 0 \\ Y & YF_m^{-1}B^T & F_B & B^T \\ 0 & 0 & B & C_\psi \end{bmatrix}$$

- **Order-of-magnitude analysis of structural error terms for ABF and previous work on 2D and 3x3 systems suggests diagonal, and comutator approaches should be workable in appropriate parameter regimes.**
- **Reduction to 2 problem types that are similar to what we have studied and developed Schur complement approaches for**
 - **Saddle point systems** $S_m = C_P - B\hat{F}_m^{-1}B^T$; $S_B = C_\psi - B\hat{F}_B^{-1}B^T$
 - **Momentum-magnetics coupling** $P = F_B - Y\hat{F}_m^{-1}Z$

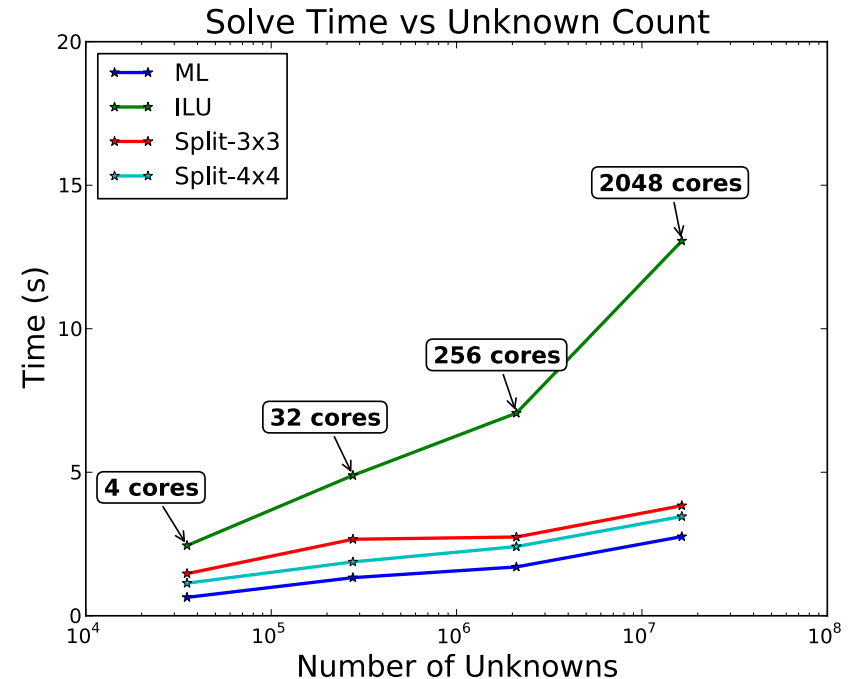
Extensions to 3D: Initial Approximate Block Preconditioning
3D HMKH [Re =10⁴, Rem=10⁴, M_A = 3; CFL ~0.125], SFE
FC-AMG – ILU(0), V(3,3); 3x3, 4x4 SIMPLEC and Gauss-Seidel



Fully coupled Algebraic

ML: Uncoupled AMG with repartitioning

DD: Additive Schwarz Domain Decomposition



Block Preconditioners

Split-3x3: 3x3 (SIMPLEC everywhere)

Preliminary Split-4x4: 4x4

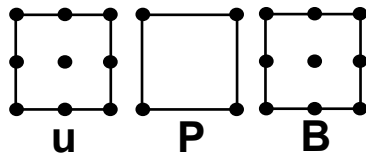
ABF preconditioners scale algorithmically, more relevant for mixed and physics-compatible discretizations

General Structure of Newton System: $\mathcal{J} \Delta \mathbf{x} = -\mathcal{F}$

$$\mathcal{J} = \begin{bmatrix} F & B_p^T & Z \\ B_p & 0 & 0 \\ Y & 0 & D \end{bmatrix} \quad \begin{array}{l} \mathbf{x} = [\mathbf{v}, P, \mathbf{B}]^T \\ \mathcal{F} = [\mathbf{F}_v, F_P, \mathbf{F}_B]^T \end{array}$$

Exact Penalty Formulation: (Q2/Q1 Navier-Stokes, Q2 B field; see e.g. Gunzburger et. al. 1991, Phillips et. al. 2014)

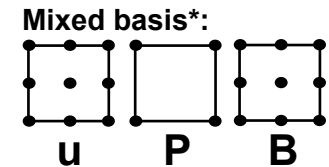
Mixed basis*:



Weak correspondence to parabolic divergence cleaning method for $\nabla \cdot \mathbf{B}$ errors (see e.g. Dedner 2002).

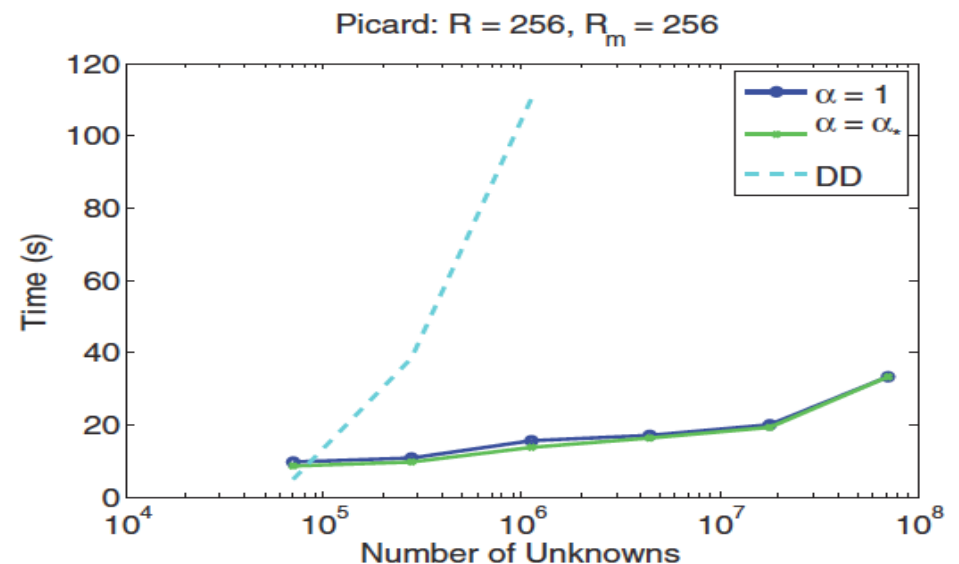
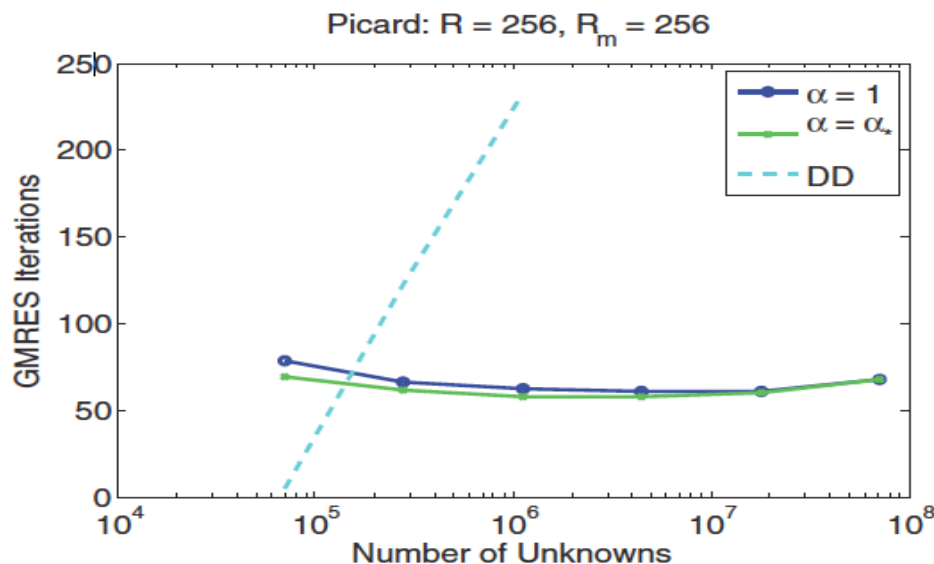
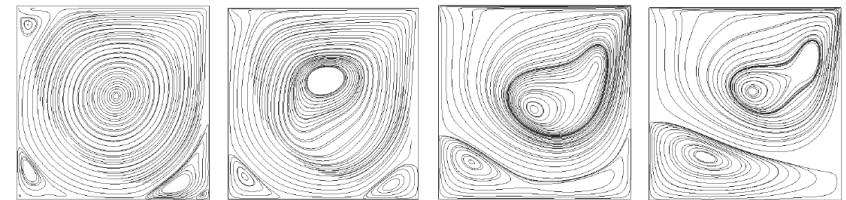
Physics-based and Approximate Block Factorizations: Coercing Strongly Coupled Off-Diagonal Physics / Disparate Discretizations and Scalable Multigrid to play well together
(w/ H. Elman, UMD)

Exact Penalty Formulation: (Q2/Q1 Navier-Stokes, Q2 B field; see e.g. Gunzburger)



$$\mathcal{A}_P = \begin{pmatrix} F & B^t & Z \\ B & 0 & 0 \\ -Z^t & 0 & A \end{pmatrix}, \quad \mathcal{P}_{P,\alpha} = \begin{pmatrix} \hat{A} & -Z^t & 0 \\ 0 & \hat{X} & B^t \\ 0 & 0 & \hat{Y}_\alpha \end{pmatrix} \quad \begin{aligned} X &= F + ZA^{-1}Z^t, \\ Y &= -BX^{-1}B^t. \end{aligned}$$

$$\mathbf{x} = [\mathbf{u}, P, \mathbf{B}]^T \quad \mathbf{x} = [\mathbf{B}, \mathbf{u}, P]^T$$

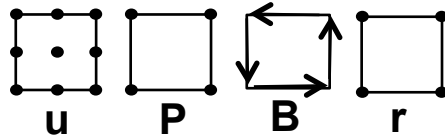


General Structure of Newton System: $\mathcal{J} \Delta \mathbf{x} = -\mathcal{F}$

$$\mathcal{J} = \begin{bmatrix} F & B_n^T & Z & \\ B_p & 0 & & \\ Y & & D & B_r^T \\ & & B_r & 0 \end{bmatrix} \quad \begin{aligned} \mathbf{x} &= [\mathbf{v}, P, \mathbf{B}, r]^T \\ \mathcal{F} &= [\mathbf{F}_v, F_P, \mathbf{F}_B, F_r]^T \end{aligned}$$

Shotzau Formulation: (Q2/Q1 Navier-Stokes, B -edge, Q1 Lagrange Multiplier, see e.g. Shotzau 2004)

Mixed basis*:



$$\nabla \cdot \mathbf{J} = 0 \quad \text{to machine precision.}$$

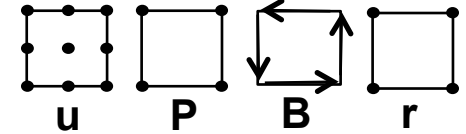
Drekar – Element types implemented with
*Intrepid (PI-Bochev, Ridzal, Peterson)



Shotzau Formulation: (Q2/Q1 Navier-Stokes, B -edge, Q1 Lagrange Multiplier)

Structure of preconditioner and Maxwell ABF (w/ H. Elman, UMD)

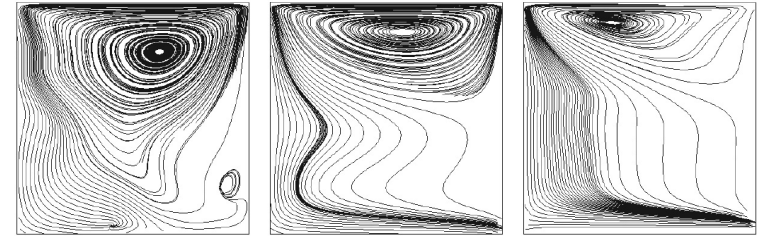
Mixed basis*:



$$\mathcal{A}_P = \begin{pmatrix} A & D^t & -Z^t & 0 \\ D & 0 & 0 & 0 \\ Z & 0 & F & B^t \\ 0 & 0 & B & 0 \end{pmatrix} \quad \mathcal{P}_P = \begin{pmatrix} \hat{\mathcal{M}}_P & -Z^t & 0 \\ 0 & \hat{X} & B^t \\ 0 & 0 & \hat{Y} \end{pmatrix}$$

$$\hat{\mathcal{M}}_{P,2} = \begin{pmatrix} A + tD^t\bar{Q}_r^{-1}D & 0 \\ 0 & \frac{1}{t}\bar{Q}_r \end{pmatrix}$$

$$\hat{X} \approx F + Z\hat{\mathcal{M}}_P^{-1}Z^t, \quad Y = -B\hat{X}^{-1}B^t$$



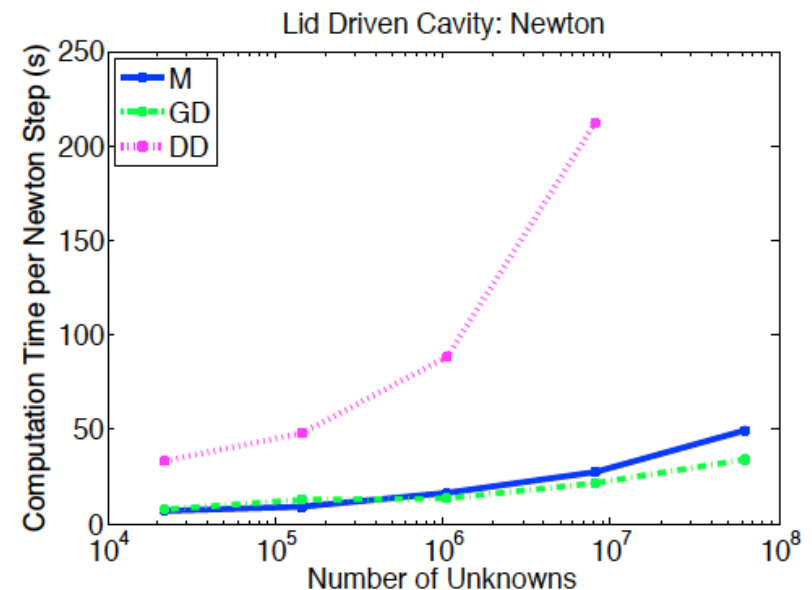
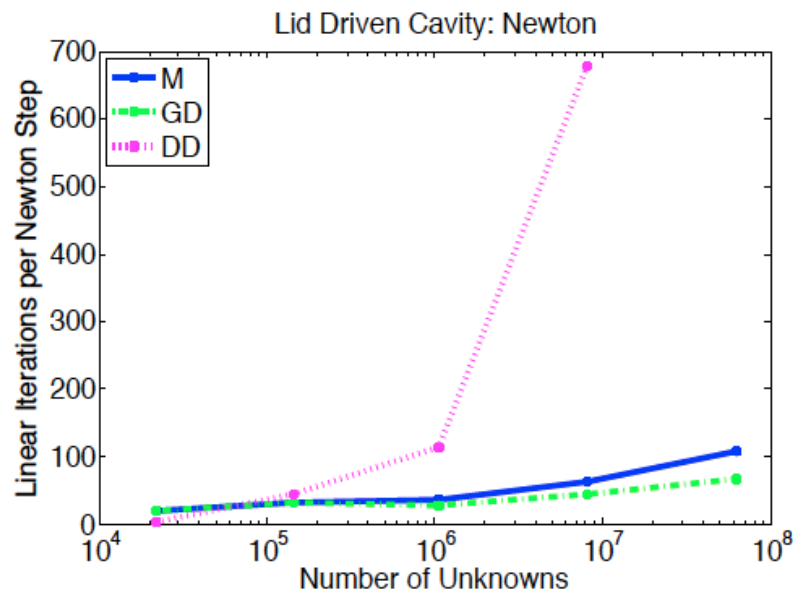
$Re_m = 1$

$Re_m = 10$

$Re_m = 100$

Segregation into

- H(grad) system AMG for velocity,
- Scalar H(grad) AMG for pressure,
- H(curl) AMG for magnetic field



- Number of processors: 1, 8, 64, 512, 4096, $h = \frac{1}{8}, \frac{1}{16}, \frac{1}{32}, \frac{1}{64}, \frac{1}{128}$
- $Re = 100, Re_m = 10, S = 1$

Drekar – Element types implemented with
*Intrepid (Bochev, Ridzal, Peterson)

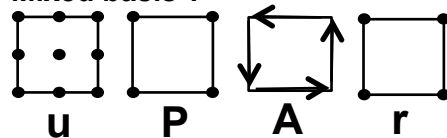


General Structure of Newton System: $\mathcal{J} \Delta \mathbf{x} = -\mathcal{F}$

$$\mathcal{J} = \begin{bmatrix} F & B_p^T & Z & \\ B_p & 0 & D & B_r^T \\ Y & & B_r & C_A \end{bmatrix} \quad \begin{aligned} \mathbf{x} &= [\mathbf{v}, P, \mathbf{A}, r]^T \\ \mathcal{F} &= [\mathbf{F}_v, F_P, \mathbf{F}_A, F_r]^T \end{aligned}$$

Magnetic Vector Potential Formulation: (Q2/Q1 Navier-Stokes, A -edge, Q1 Scalar Potential)

Mixed basis*:



$\nabla \cdot \mathbf{B} = 0$ to machine precision.

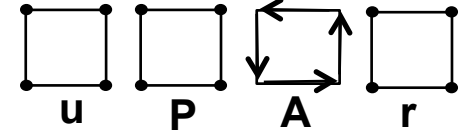
Magentic Vector-Potential Formulation: (Q1 Navier-Stokes, A-edge, Q1 Lagrange Multiplier)

Structure of preconditioner and Maxwell ABF

$$\begin{pmatrix} F & B^t & Z \\ B & C & 0 \\ Y & 0 & G \end{pmatrix} \approx \begin{pmatrix} F & 0 & Z \\ 0 & I & 0 \\ Y & 0 & G \end{pmatrix} \begin{pmatrix} F^{-1} & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix} \begin{pmatrix} F & B^t & 0 \\ B & C & 0 \\ 0 & 0 & I \end{pmatrix}$$

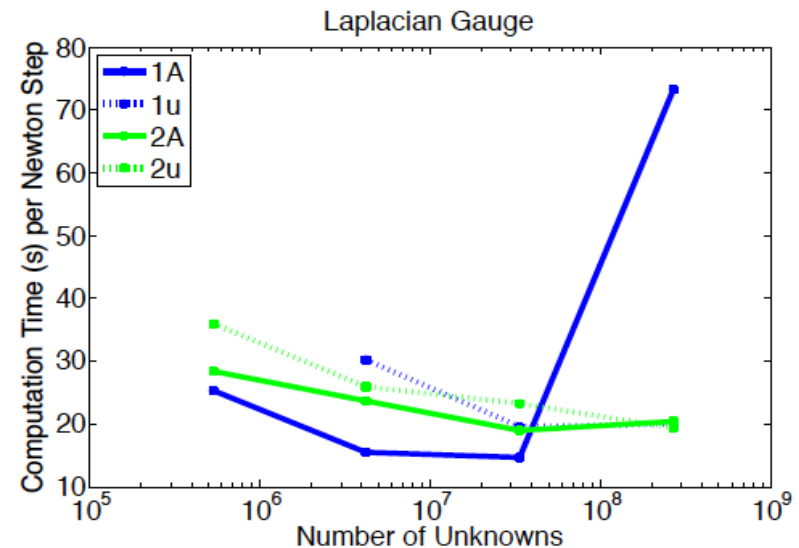
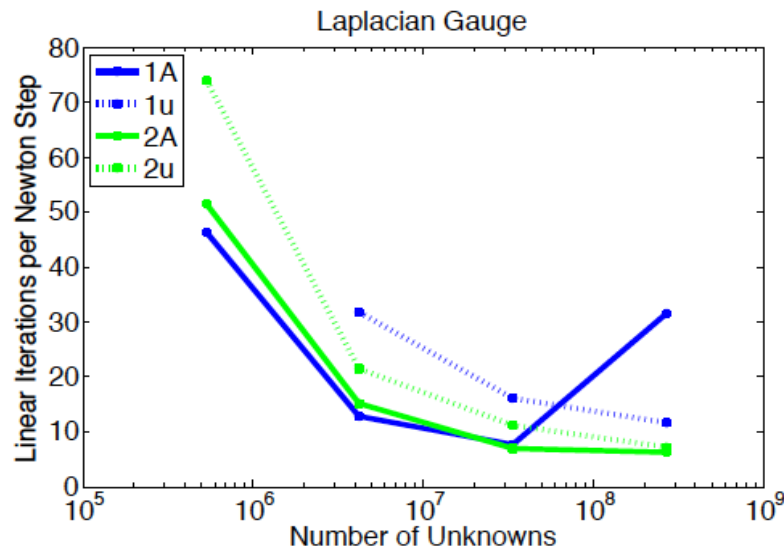
$$\text{or} \begin{pmatrix} F & B^t & 0 \\ B & C & 0 \\ 0 & 0 & I \end{pmatrix} \begin{pmatrix} F^{-1} & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix} \begin{pmatrix} F & 0 & Z \\ 0 & I & 0 \\ Y & 0 & G \end{pmatrix}$$

Mixed basis*:



Segregation into

- H(grad) system AMG for velocity,
- Scalar H(grad) AMG for pressure, Lagrange multiplier
- H(curl) AMG for magnetic vector potential



Conclusions

- Initial results for 3D Stabilized/VMS FE Lagrange multiplier and structure preserving discretizations for low-flow Mach number resistive MHD system is very encouraging.
- Robustness, efficiency and scalability of parallel Newton-Krylov solvers is very good.

Preconditioning critical:

- FC-AMG (ML) scales well for stabilized / VMS 3D resistive MHD systems
- ABF methods must have effective approximation of dominate off-diagonal coupling and time-scale represented.
 - ABF & AMG $H(\text{grad})$ results are encouraging for VMS Lagrange multiplier formulations.
 - Initial ABF & AMG [$H(\text{grad}) + H(\text{curl})$] results for structure preserving formulations is promising
- Fully-implicit Newton-Krylov solvers have enabled initial adjoint based UQ capabilities
 - a posteriori error-estimation
 - Integrated sensitivity analysis
 - efficient surrogate model construction for UQ