SAND2015-3270C

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

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Outline

- **General Scientific and Mathematical/Computational Motivation**
- **Brief Overview of 3D Resistive MHD Equations and Numerical Approximation**
- **Motivation for Fully Implicit Newton – Krylov Solution Methods**
- **Motivation for Approximate Block Factorization Preconditioners**
  - **Scaling of Block Preconditioners for Stabilized FE MHD**
  - **Scaling for Mixed Integration (u,P) and Edge-element Formulations**
- **Scaling of Fully-coupled AMG preconditioner**
- **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 sub-storms, Aurora, geo-dynamo, planetary-dynamos
- Fusion: Magnetic Confinement [MCF] (e.g. ITER), Inertial Conf. [ICF] (e.g. NIF, Z-pinch)

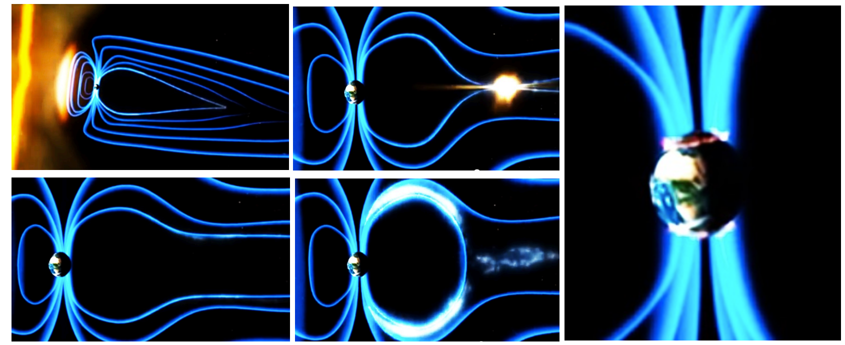
Mathematical/Computational Motivation:

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

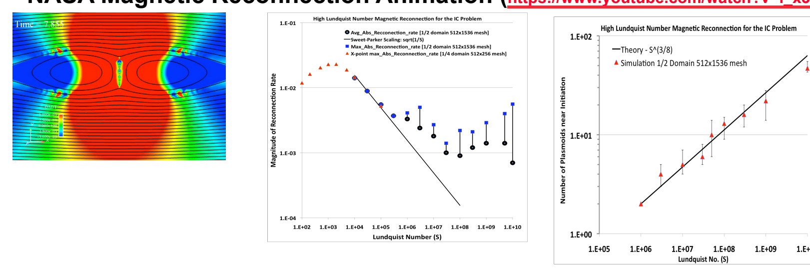
Mathematical Approach - develop:

- Stable and higher-order accurate fully-implicit formulations
- Stable and accurate spatial discretizations for complex geom., Options enforcing key mathematical properties (e.g. positivity, div 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



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



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

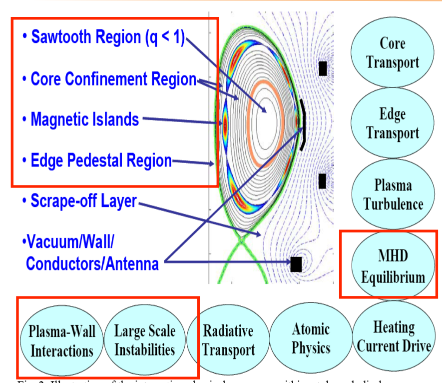
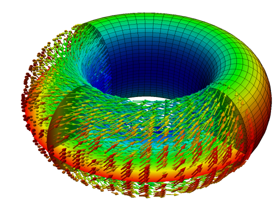
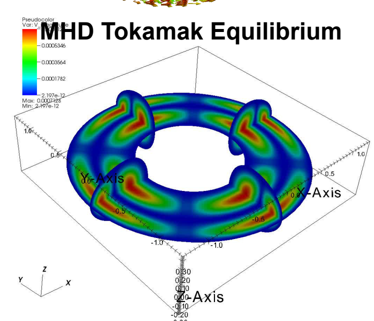


Fig. 2: Illustration of the interacting physical processes within a tokamak discharge.



MHD Tokamak Equilibrium



MHD Equilibrium Instability

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.**

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Why Newton-Krylov Methods?

Newton-Krylov

→ **Direct-to-steady-state**

→ **Fully-implicit / IMEX transient**

Robustness, Convergence and Flexibility

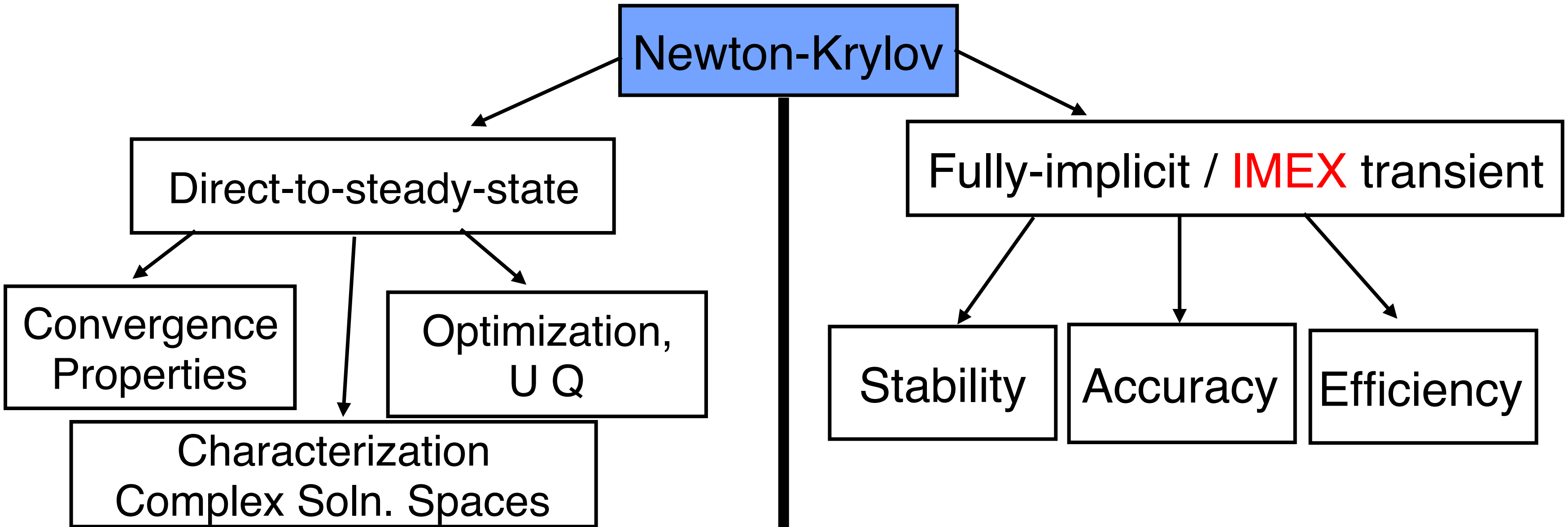
- **Strongly coupled multi-physics often requires a strongly coupled nonlinear solver**
- **Quadratic convergence near solutions**
- **Enables continuation, bifurcation, stability analysis, etc.**

Stability, Accuracy and Efficiency

- **Stable (stiff systems)**
- **High order methods**
- **Variable order techniques with error-control**
- **Can be stable, accurate and efficient run at the dynamical time-scale of interest in multiple-time-scale systems**

(See e.g. Knoll et. al., Brown & Woodward., Chacon and Knoll, S. and Ober, S. and Ropp)

Why Newton-Krylov Methods?



Very Large Problems -> Parallel Iterative Solution of Sub-problems

Krylov Methods - Robust, Scalable and Efficient Parallel Preconditioners

- Approximate Block Factorizations
- Physics-based Preconditioners
- Multi-level solvers for systems and scalar equations

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One Fluid Resistive MHD Equations

Resistive MHD Model in Residual Notation

$$\mathbf{R_u} = \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot [\rho \mathbf{u} \otimes \mathbf{u} - (\mathbf{T} + \mathbf{T}_M)] + 2\rho\Omega \times \mathbf{u} - \rho \mathbf{g} = \mathbf{0}; \quad \mathbf{T} = -\left(P + \frac{2}{3}\mu(\nabla \bullet \mathbf{u})\right)\mathbf{I} + \mu[\nabla \mathbf{u} + \nabla \mathbf{u}^T]$$

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

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

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

Reduced From of Maxwell's Equations

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

$$\mathbf{J} = \frac{1}{\mu_0}\nabla \times \mathbf{B};$$

$$\mathbf{E} = -\underbrace{\mathbf{u} \times \mathbf{B}}_{\text{Ideal}} + \underbrace{\eta \mathbf{J}}_{\text{Resistive}} + \underbrace{\frac{d_i}{n}(\mathbf{J} \times \mathbf{B} - \nabla P_e)}_{\text{Hall}} + \underbrace{\frac{d_e^2}{n}\frac{d\mathbf{J}}{dt}}_{\text{e inertia}}$$

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Resistive MHD Equations

Resistive MHD Model in Residual Notation

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

$$\mathbf{T} = -\left(P + \frac{2}{3}\mu(\nabla \bullet \mathbf{u})\right)\mathbf{I} + \mu[\nabla \mathbf{u} + \nabla \mathbf{u}^T]$$

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

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

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

$$\mathbf{R_B} = \frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{u} \times \mathbf{B}) + \nabla \times (\frac{\eta}{\mu_0} \nabla \times \mathbf{B}) = \mathbf{0}. \qquad \nabla \cdot \mathbf{B} = 0$$

Complex coupled multiphysics system

- Highly nonlinear
- multiple-time and -length scales
- Elliptic, parabolic and hyperbolic character in different parameter ranges
- Involution on magnetic induction. If $\nabla \cdot \mathbf{B}|_{t=0} = 0$ then $\nabla \cdot \mathbf{B} = 0 \;\; \forall t > 0$

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3D Resistive MHD Equations

Resistive MHD Model in Residual Notation

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

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

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

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

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

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

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

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

- 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, Badia et. al. 2013)

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Approaches to Deal with Evolution Equation for B and Involution $\nabla \cdot \mathbf{B} = 0$

- Transform to Potential Form (e.g. $\mathbf{B} = \nabla \times \mathbf{A}$)
  - See e.g. Evans, Hawley 1988; Jardin et. al. 2010; Rossmanith et. al. 2006; *Chacon et. al 2002*; *Robinson et. al. 2008*; *S. et. al. 2010, 2014; ……*

- Projection / Divergence Cleaning
  - See e,g. Brackbill and Barnes 1980, Powell et. al. 1994, Dai and Woodward 1998; Toth et. al. 2000; Munz et. al 2000, Dedner et. al. 2002, Balsara and Kim 2004; ….

- Regularization / Augmentation of Saddle Point System
  - Exact- / Weighted Exact- Penalty: See e.g. Gunzburger et. al. 1991; Costable 2000;
  - Lagrange Multiplier/Stabilized Methods: See e.g. Salah et. al. 1999; Dedner 2002; Schotzau 2004; Codina et. al. 2006,2011; Badia et. al. 2013; *S. and Cyr et. al. 2014; Phillips et. al. 2014;*….

- Structure Preserving / Physics Compatible
  - Constrained Transport and Staggered Grids
    - See e.g. Yee for Maxwell1966, Evans and Hawley 1988; Dai and Woodward 1988; Toth et. al. 2000; Balsara and Kim 2004; Chacon 2004, 2008*; ….*
  - De Rham Sequence
    - See e.g. Nedelec 1980; Bossavit 1998; *Bochev et. al.* 2003; Xu et. al. 2014; *S. et. al. 2015;*

- Other ………

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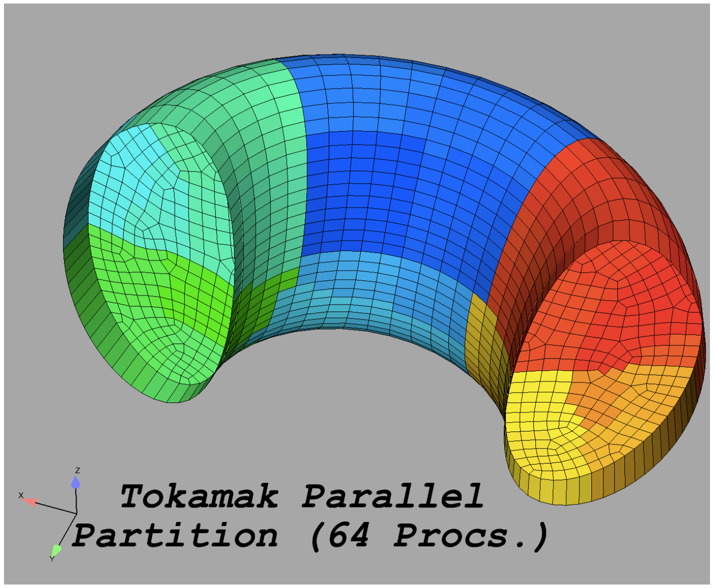
Preconditioning



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 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-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

3. Approximate Block Factorization / Physics-based (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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Summary of Structure of Linear Systems Generated in Newton's Method

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

Stabilized Q1/Q1 V-P elements, SUPG like terms, stabilizing terms for inf-sup condition, cross-coupling terms and discontinuity Capturing type operators

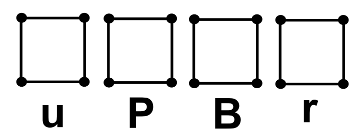
$$\mathcal{J} = \begin{bmatrix} F & B_p^T & Z & \\ B_p & C_u & & \\ Y & & D & B_r^T \\ & & B_r & C_B \end{bmatrix}$$

$$\mathbf{x} = [\mathbf{v}, P, \mathbf{B}, r]^T$$

$$\mathcal{F} = [\mathbf{F}_{\mathbf{v}}, F_P, \mathbf{F}_{\mathbf{B}}, F_r]^T$$

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

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



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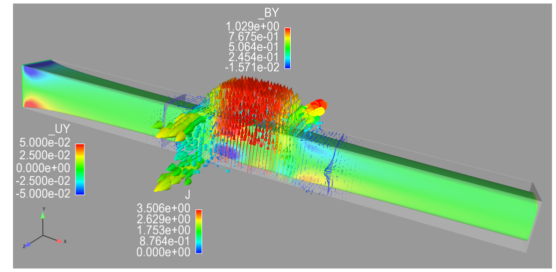
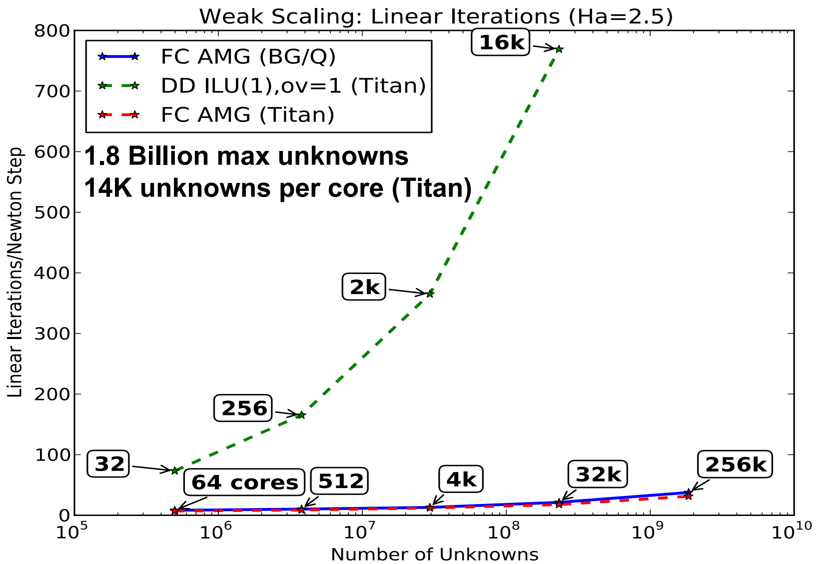
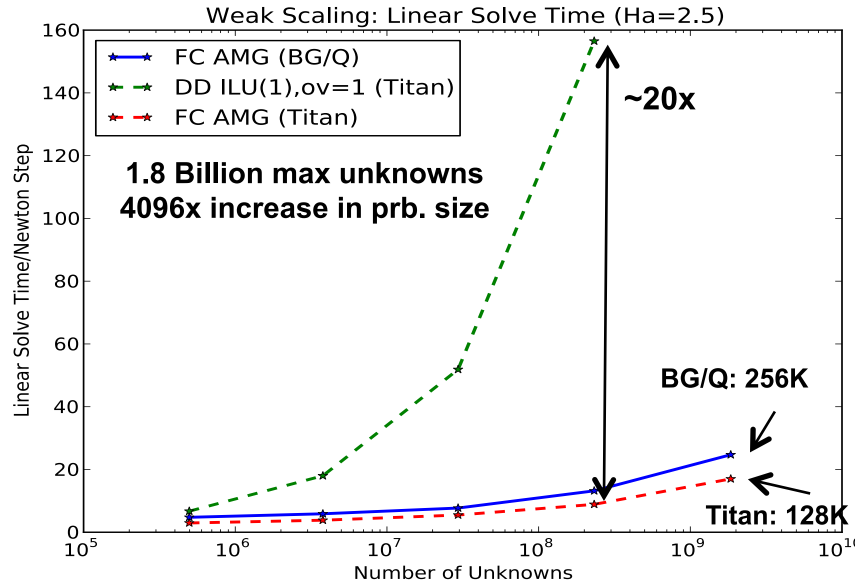
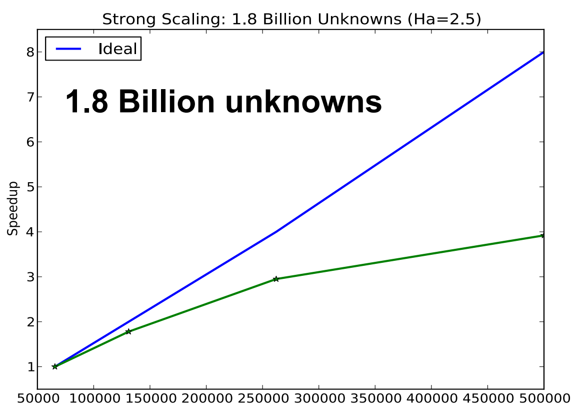
SFE Initial Scaling Studies for Cray XK7 AND BG/Q. 3D MHD Generator [Re = 500, Re_m = 1, Ha = 2.5]







MHD Recently run on ½ M cores of BG/Q



Largest fully-coupled solves demonstrated to date:

- **MHD (steady): 10B DoF, 1.25B elem, on 128K cores**
- **CFD (Transient): 40B DoF, 10B elem, on 128K cores**

[Preliminary strong scaling of Krylov linear solver + preconditioner (ML: FC – AMG), Tuminaro, Hu, Siefert et. al.]

(DOE/ORNL Titan Cray XK7: Joule Metric)

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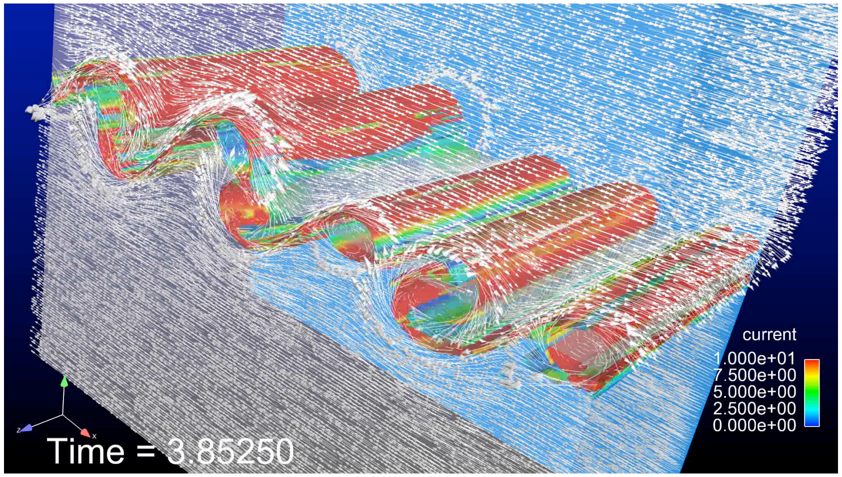
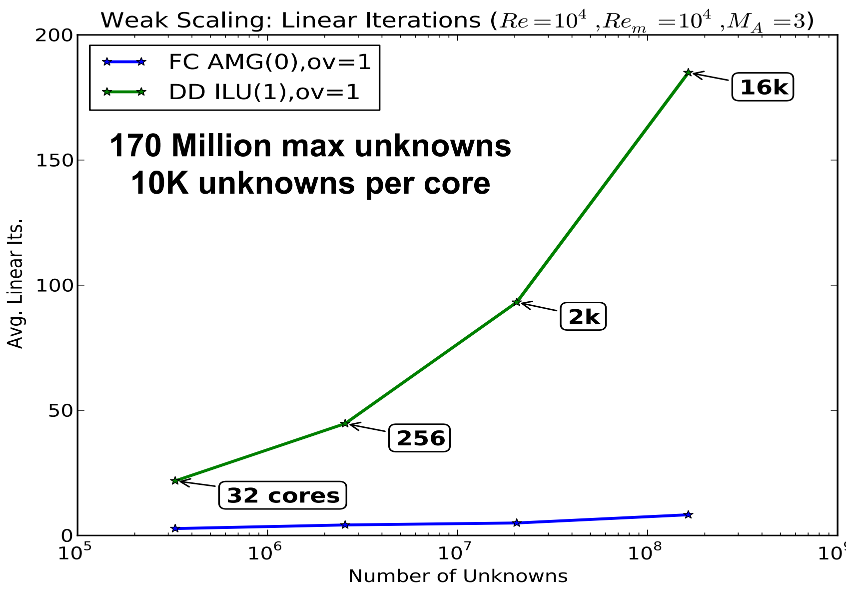
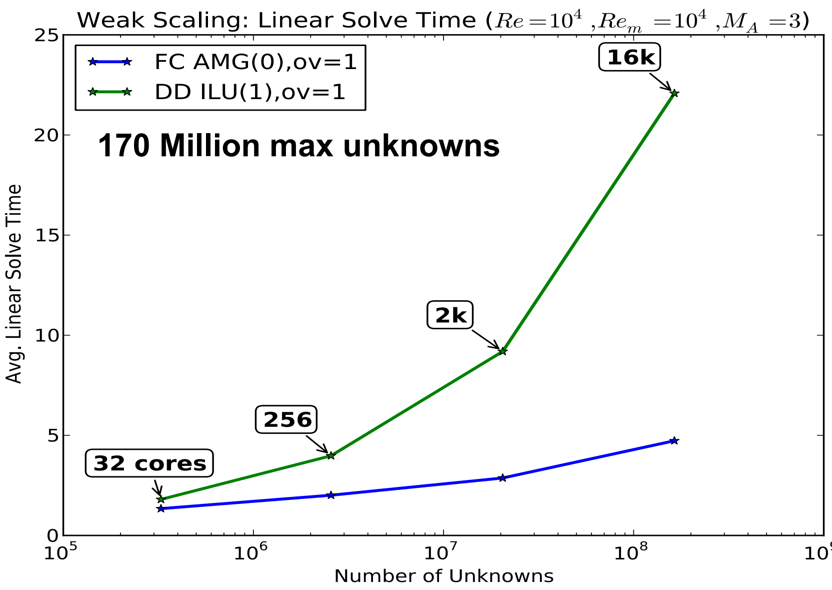
Initial Scaling Study for Cray XK7.
3D Hydromagnetic Kelvin-Helmholtz Instability
[$Re = 10^4$, $Re_m = 10^4$, $M_A = 3$; CFL_{max} ~5]







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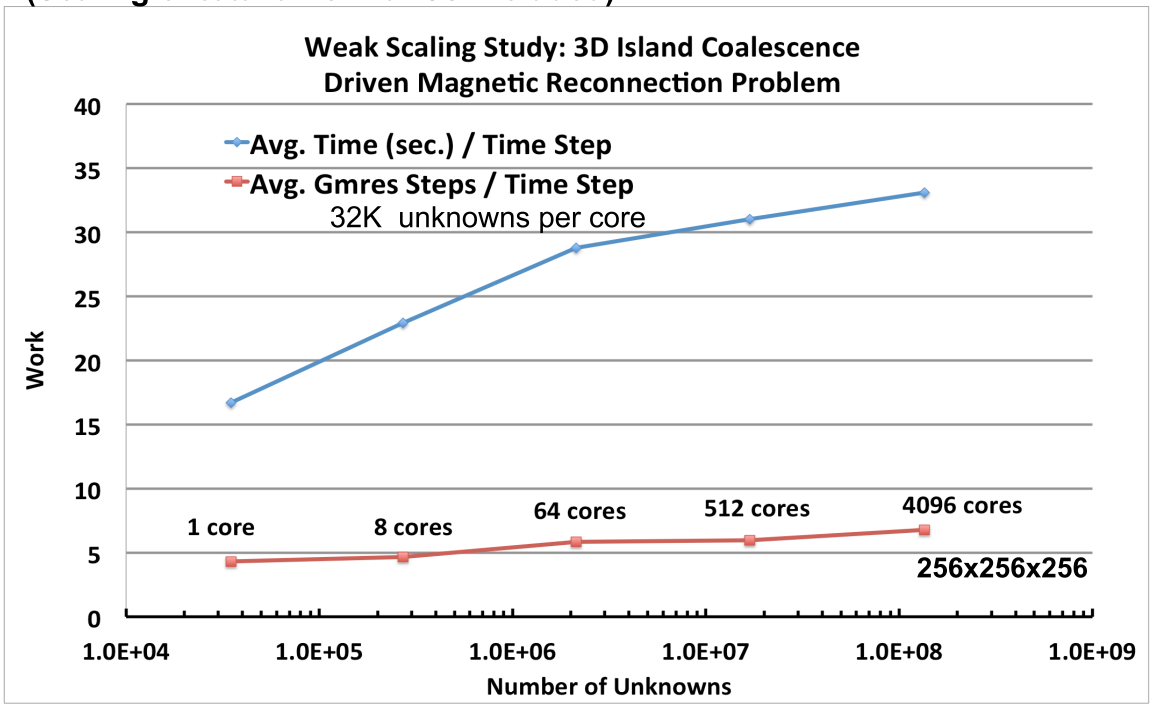
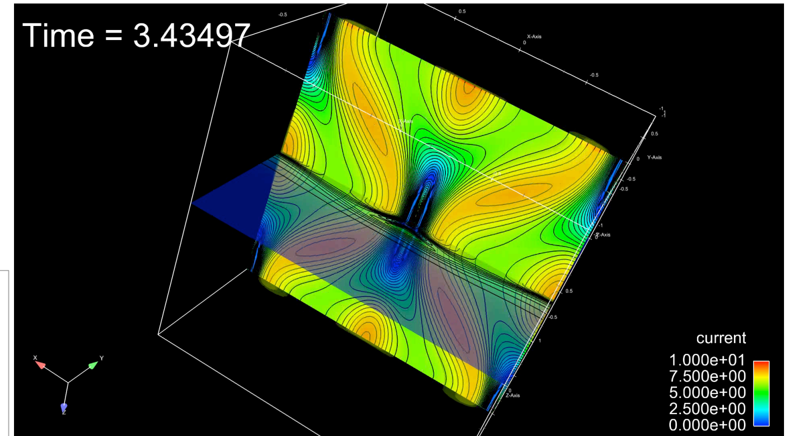
Scaling for Lagrange Multiplier Formulation. 3D Island Coalescence [S = 10^3, dt = 0.1], SFE

(Scaling of total time with I/O included)





Scaling with Lundquist No.

Lundquist No. S	Newt. Steps / dt	Gmres Steps / dt
1.0E+03	1.36	5.2
5.0E+03	1.43	5.7
1.0E+04	1.51	6
5.0E+04	2	9.8
1.0E+05	2	12
5.0E+05	2	8.4
1.0E+06	2	8.4

BDF2 NK FC-AMG ILU(fill=0,ov=1), V(3,3)

SNL Capacity Cluster: Chama

Mesh: 128x128x128, dt = 0.0333.

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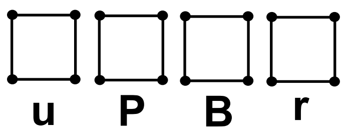
General Structure of Newton System:

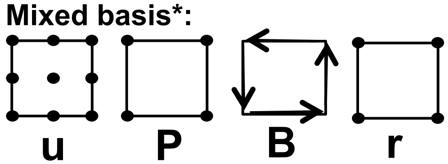
$$\mathcal{J}\Delta\mathbf{x} = -\mathcal{F} \qquad \mathcal{J} = \begin{bmatrix} F & B_p^T & Z & \\ B_p & 0 & 0 & \\ Y & 0 & \Gamma & \\ & & & 0 \end{bmatrix}$$

Stabilized FE Methods , Q1 interpolation; C_u and C_B weighted Laplacian matrix;



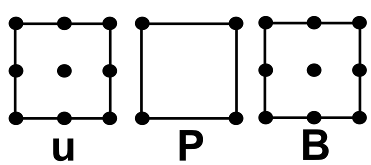
Shotzau Formulation: (Q2/Q1 Navier-Stokes, B -edge, Q1 Lagrange Multiplier, see e.g. Shotzau 2004)

Mixed basis*:



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

Mixed basis*:



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

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

Physics-based (Parabolization):

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

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

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

Schur Complement, (Approximate) Block Factorization:

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

$$\begin{bmatrix} D_1 & U \\ L & D_2 \end{bmatrix} = \begin{bmatrix} I & UD_2^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} D_1 - UD_2^{-1}L & 0 \\ 0 & D_2 \end{bmatrix} \begin{bmatrix} I & 0 \\ D_2^{-1}L & I \end{bmatrix}$$

The Schur complement is then

$$D_1 - UD_2^{-1}L = (I - \Delta t^2 C_x C_x) = (I - \Delta t^2 \partial_{xx})$$

Result: Stiff (large-magnitude) off-diagonal hyperbolic type operators (blocks) are now combined onto diagonal parabolic operator (block).

Scalar equation multigrid can now be used effectively on this operator

Our General Approach:

ABF: Understand stiff physics, consider spectral properties of operators, develop approximate block factorization(s) to simplified system(s) while approximating critical operators to maintain stiff coupling in approximate Schur complement(s)

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, Shuttleworth, Tuminaro,"A Taxonomy of Parallel Mulit-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, 2013

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Step back to CFD for a moment to

Introduce block approximate factorization (physics-based) preconditioners

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	$\mathbf{F}^{-1}$	$(\Delta t \mathbf{I})^{-1}$	$\mathbf{C} + \Delta t \hat{\mathbf{B}} \mathbf{B}^{\mathbf{T}}$	Chorin(1967);Temam (1969); Perot (1993): Quateroni et. al. (2000) as solvers.
SIMPLEC	$\mathbf{F}^{-1}$	$(\mathrm{diag}(\sum \lvert \mathbf{F} \rvert))^{-1}$	$\mathbf{C} + \hat{\mathbf{B}}(\mathrm{diag}(\sum \lvert \mathbf{F} \rvert))^{-1} \mathbf{B}^{\mathbf{T}}$	Patankar et. al. (1980) as solvers; Pernice and Tocci (2001) as smothers/MG
Pressure Convection / Diffusion	0	$\mathbf{F}^{-1}$	$\mathbf{F}_p^{-1} \mathbf{A}_p$	Kay, Loghin, Wathan, Silvester, Elman (1999 - 2006); Elman, Howle, Shadid, 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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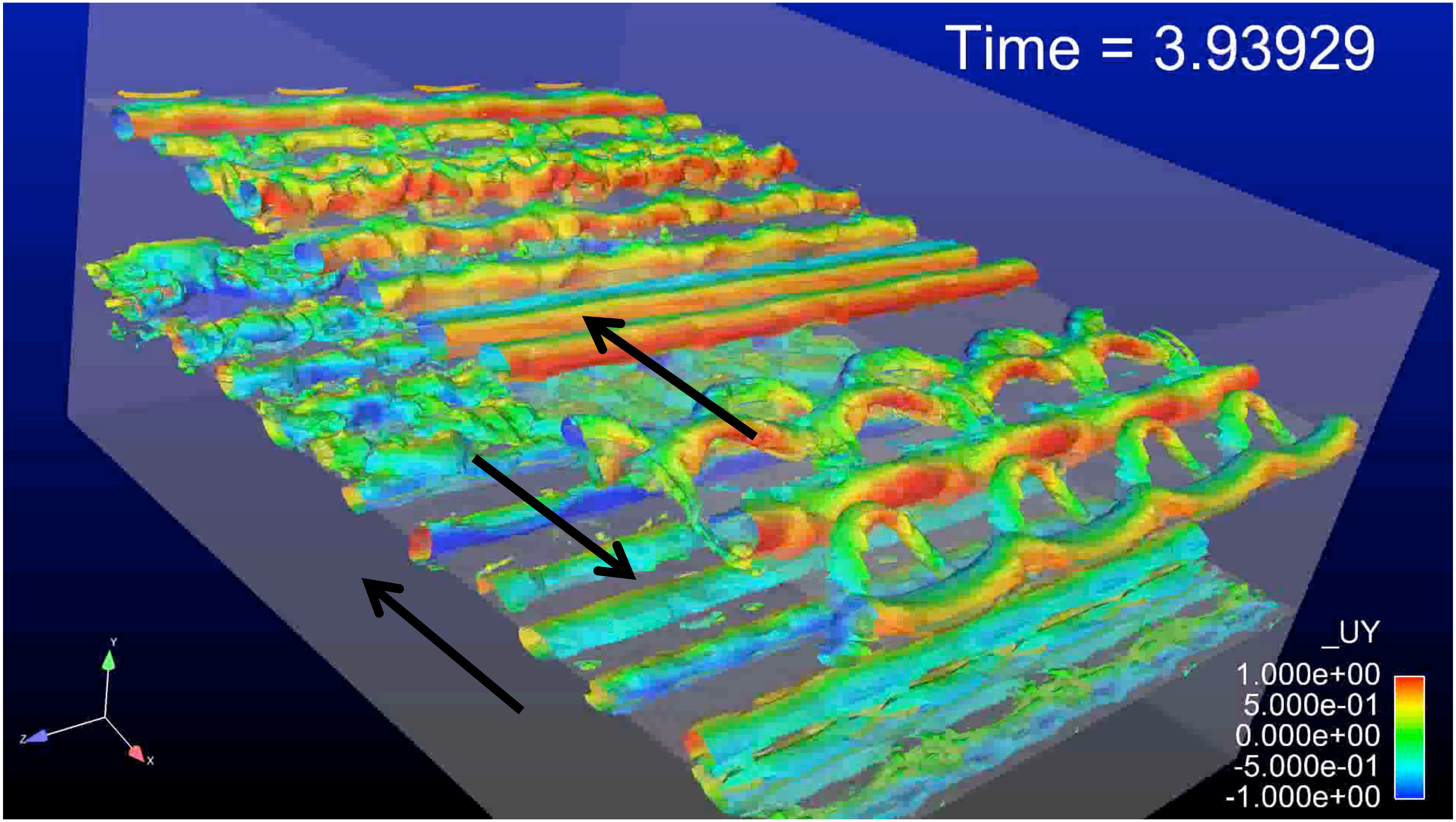
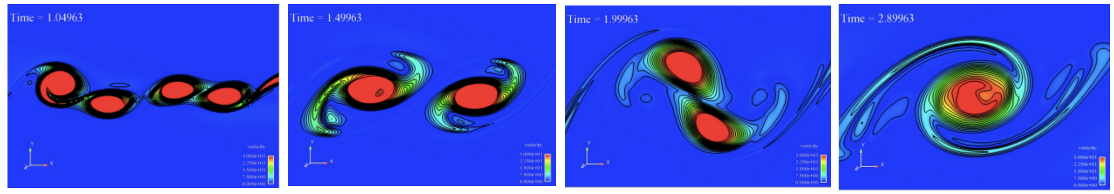
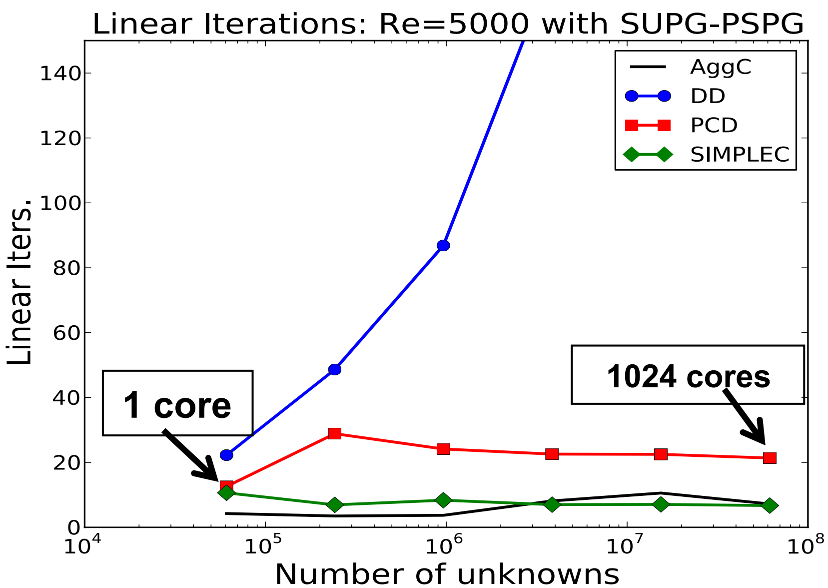
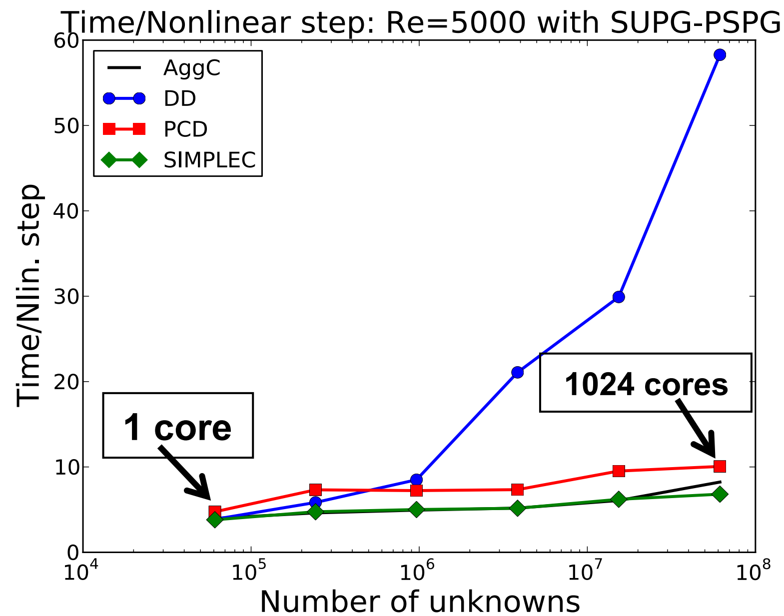
3D Plane Jet; Kelvin-Helmholtz Unstable with Secondary Cross-stream Instability; VMS LES Model; Re = 10^8



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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Now Return to MHD

Block approximate factorization (physics-based) preconditioners

Incompressible Resistive MHD a New Nested Schur Complement Approach

Block LU factorization gives

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

where

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

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

- **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.**

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Operator split / Residual-based Defect-Correction ABF Preconditioner

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

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

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

2) **3x3 -> two 2x2 sub-systems**

$$\mathcal{S} = C_u - B\hat{F}^{-1}B^T \qquad \mathcal{P} = D - Y\hat{F}^{-1}Z$$

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

Spectrum of preconditioned system for defect-correction MHD Preconditioner.

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

See e.g. Elman, Howle, S., Shuttleworth, Tuminaro,"A Taxonomy of Parallel Mulit-level 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

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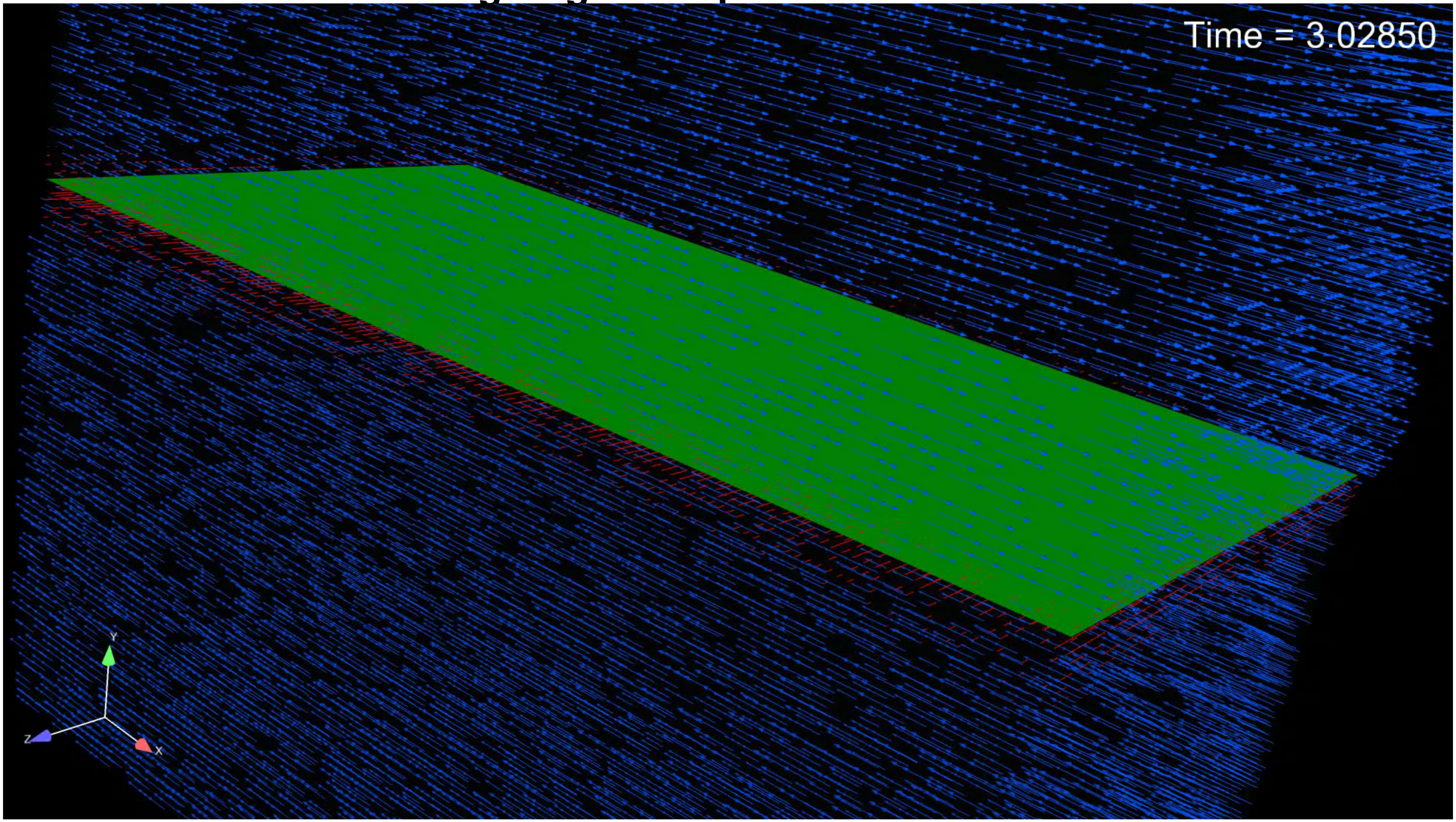
3D Hydromagnetic Kelvin-Helmholtz Instability. Re = Re_m = 10^4, Ma_A = 3.0
Lagrange Multiplier Formulation



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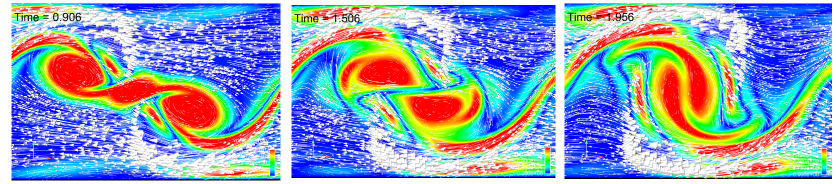
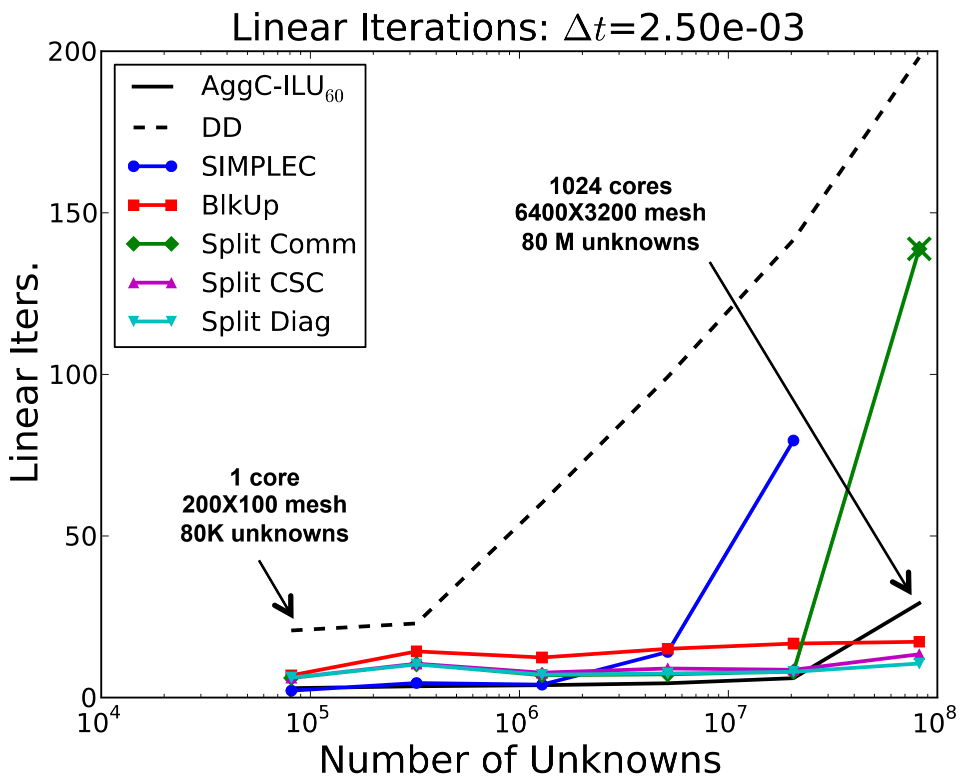
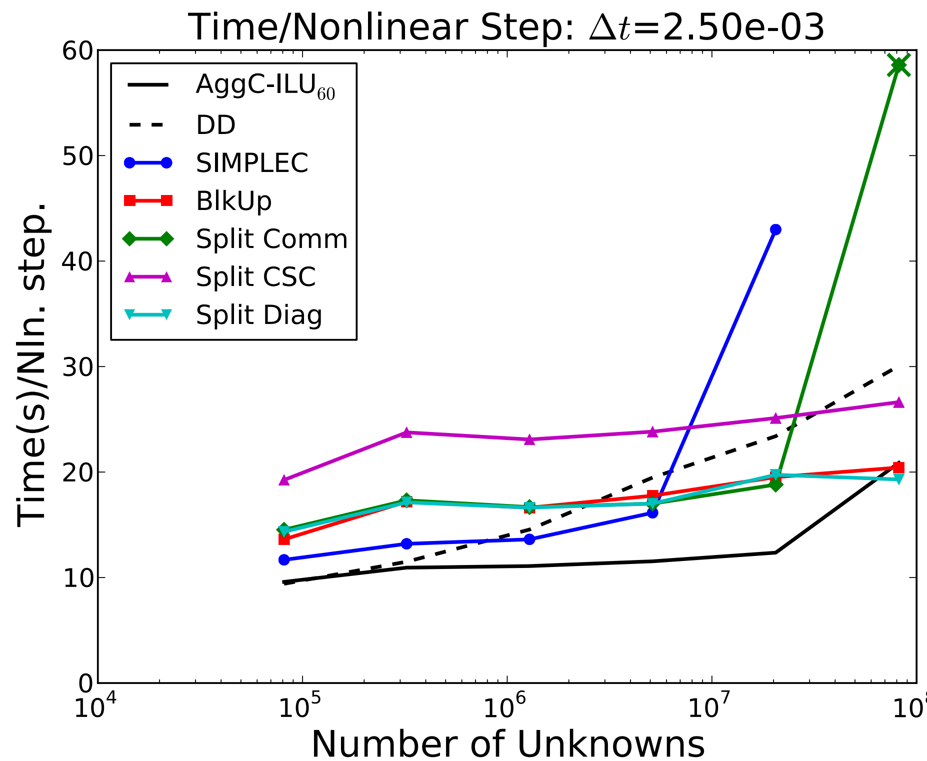
Transient 2D Hydromagnetic Kelvin-Helmholtz Problem, SFE
Re = 5e+3, S = 1e+3; M_A = 1.5; CFL_{max} ~ 10







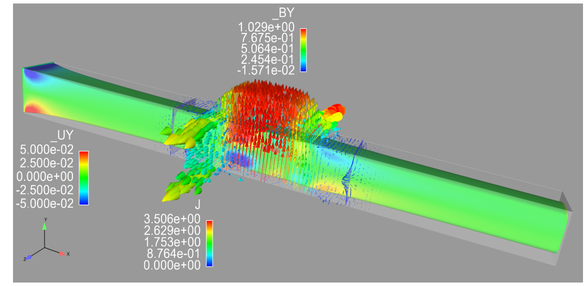
Comm – comutator; CSC – continuous Schur comp.; Diag. – diagonal approx of inverse in Schur comp.

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," in preparation , 2014.

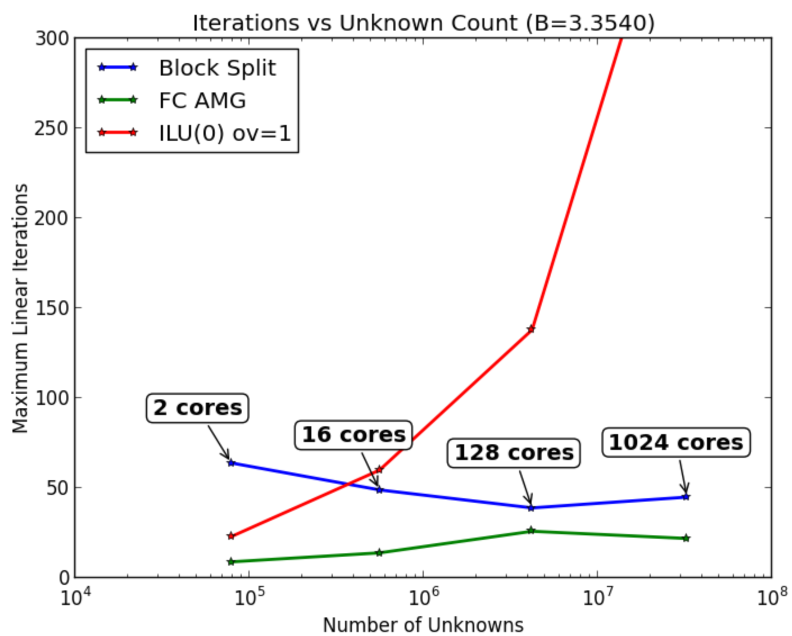
Extensions to 3D: Initial Approximate Block Preconditioning
3D MHD Generator [Re = 500, Re_m = 1, Ha = 2.5], SFE

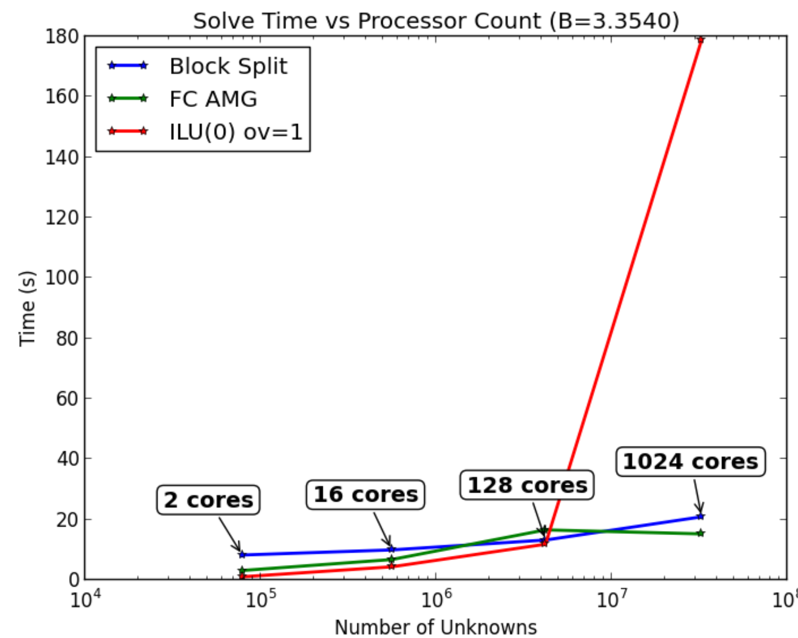


$$\mathcal{J} = \begin{bmatrix} F & B_p^T & Z & \\ B_p & C_u & & \\ Y & & D & B_r^T \\ & & B_r & C_B \end{bmatrix} \overset{\Rightarrow}{=} \begin{bmatrix} F & B_p^T & \hat{Z} \\ B_p & C_u & \\ \hat{Y} & & \hat{D} \end{bmatrix}$$

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

$$S = C - BF^{-1}B^T$$
$$\hat{P} = \hat{D} - YF^{-1}Z$$





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

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

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

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

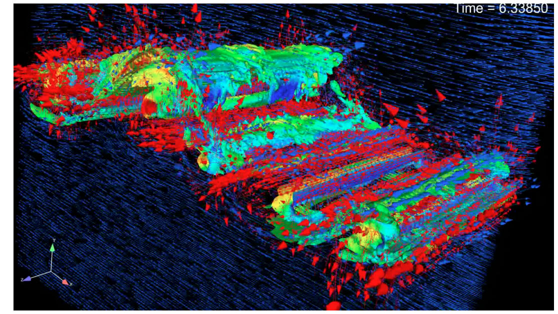
$$= \begin{bmatrix} F_m & B^T & Z & \boxed{ZF_B^{-1}B^T} \\ B & C_P & 0 & 0 \\ Y & \boxed{YF_m^{-1}B^T} & F_B & B^T \\ 0 & 0 & B & C_\psi \end{bmatrix}$$

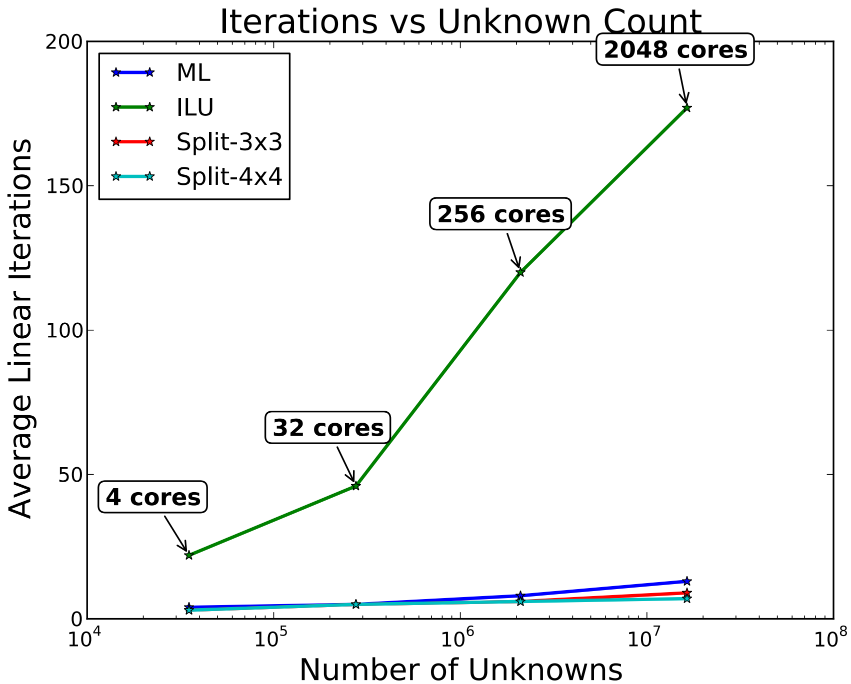
- **Order-of-magnitude analysis of structural error terms for ABF and previous work on 2D and 3x3 systems suggests diagonal, and comutator approaches should be workable in appropriate parameter regimes.**

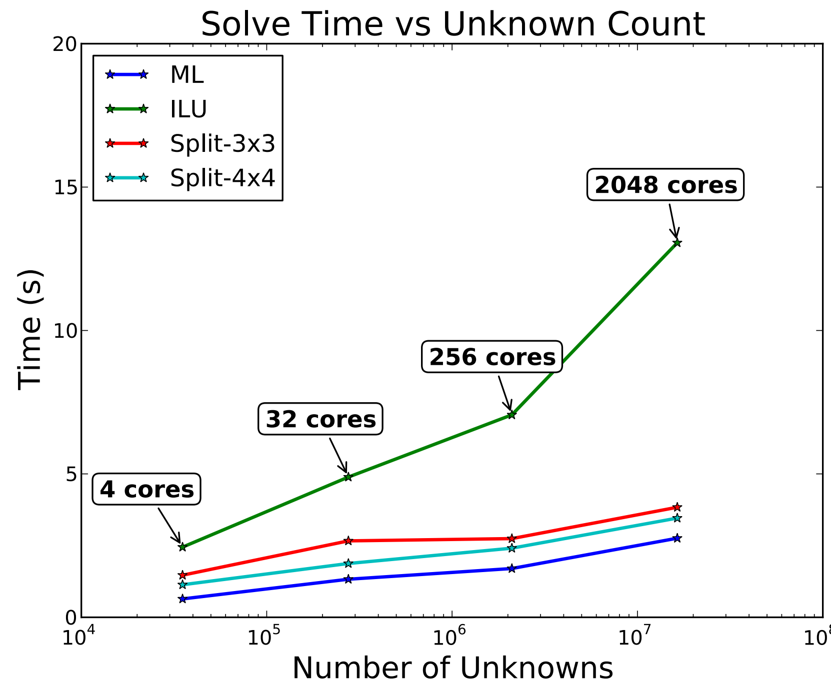
- **Reduction to 2 problem types that are similar to what we have studied and developed Schur complement approaches for**
  - **Saddle point systems** $S_m = C_P - B\hat{F}_m^{-1}B^T\ ; \quad S_B = C_\psi - B\hat{F}_B^{-1}B^T$
  - **Momentum-magnetics coupling** $P = F_B - Y\hat{F}_m^{-1}Z$

Extensions to 3D: Initial Approximate Block Preconditioning
3D HMKH [Re $=10^4$, Rem$=10^4$, $M_A = 3$; CFL ~0.125], SFE

FC-AMG – ILU(0), V(3,3); 3x3, 4x4 SIMPLEC and Gauss-Seidel







<u>Fully coupled Algebraic</u>
ML: Uncoupled AMG with repartitioning
DD: Additive Schwarz Domain Decomposition

<u>Block Preconditioners</u>
<u>Split-3x3</u>: 3x3 (SIMPLEC everywhere)
<u>Preliminary Split-4x4</u>: 4x4

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

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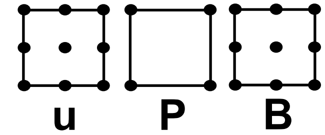
Physics-based and Approximate Block Factorizations: Coercing Strongly Coupled Off-Diagonal Physics / Disparate Discretizations and Scalable Multigrid to play well together

(w/ H. Elman, UMD)

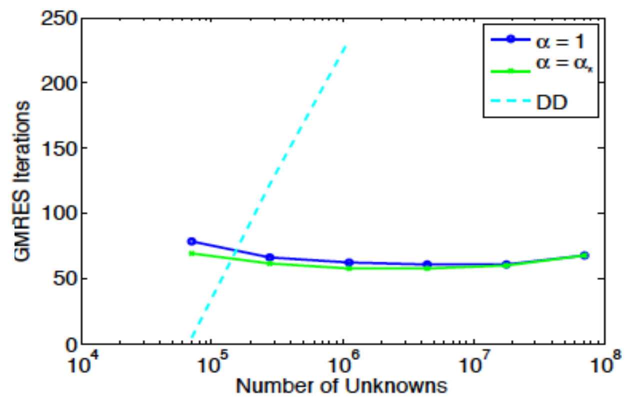
Mixed basis*:



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

$$\mathcal{A}_P = \begin{pmatrix} F & B^t & Z \\ B & 0 & 0 \\ -Z^t & 0 & A \end{pmatrix}$$

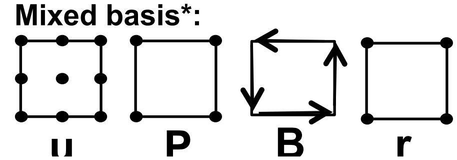
$$\mathcal{P}_{P,\alpha} = \begin{pmatrix} \hat{A} & -Z^t & 0 \\ 0 & \hat{X} & B^t \\ 0 & 0 & \hat{Y}_\alpha \end{pmatrix} \quad X = F + ZA^{-1}Z^t, \quad Y = -BX^{-1}B^t.$$



Phillips, Elman, Cyr, S., Pawlowski, A Block Preconditioner for an Exact Penalty Formulation for Stationary MHD, Accepted in SISC

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

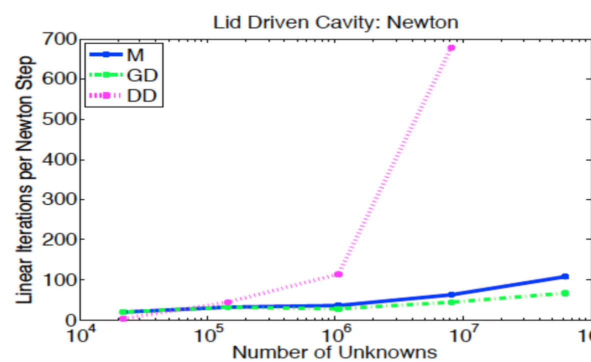
Mixed basis*:



Structure of preconditioner and Maxwell ABF

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

$$\hat{\mathcal{M}}_{P,2} = \begin{pmatrix} A + tD^t\bar{Q}_r^{-1}D & 0 \\ 0 & \frac{1}{t}\bar{Q}_r \end{pmatrix} \quad \hat{X} \approx F + \mathcal{Z}\hat{\mathcal{M}}_P^{-1}\mathcal{Z}^t, \quad Y = -B\hat{X}^{-1}B^t$$



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

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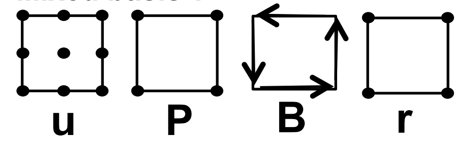
Shotzau Formulation: (Q2/Q1 Navier-Stokes, B -edge, Q1 Lagrange Multiplier)

Structure of preconditioner and Maxwell ABF

Mixed basis*:



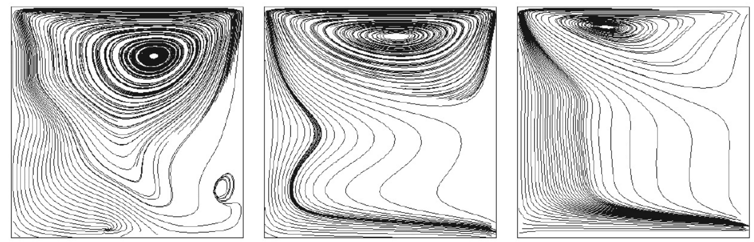
(w/ H. Elman, UMD)

$$\mathcal{A}_P = \begin{pmatrix} A & D^t & -Z^t & 0 \\ D & 0 & 0 & 0 \\ Z & 0 & F & B^t \\ 0 & 0 & B & 0 \end{pmatrix}$$

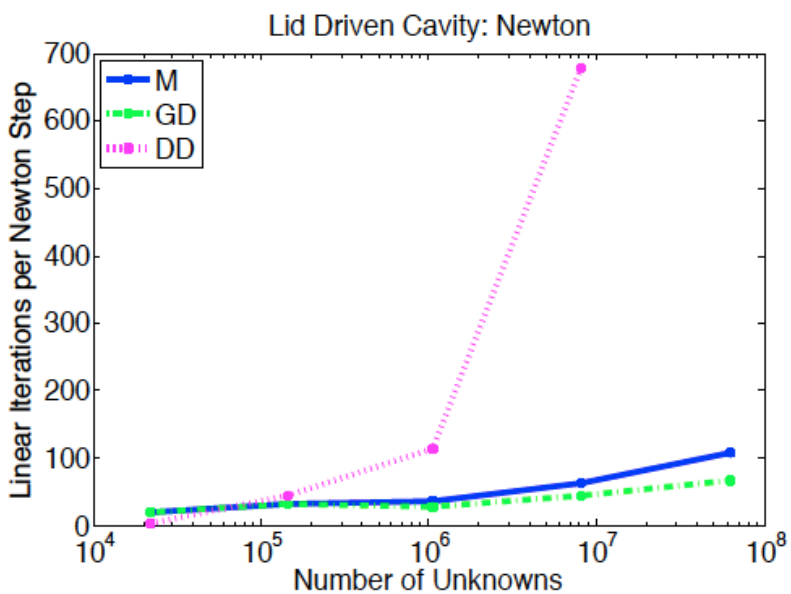
$$\mathcal{P}_P = \begin{pmatrix} \hat{\mathcal{M}}_P & -\mathcal{Z}^t & 0 \\ 0 & \hat{X} & B^t \\ 0 & 0 & \hat{Y} \end{pmatrix}$$

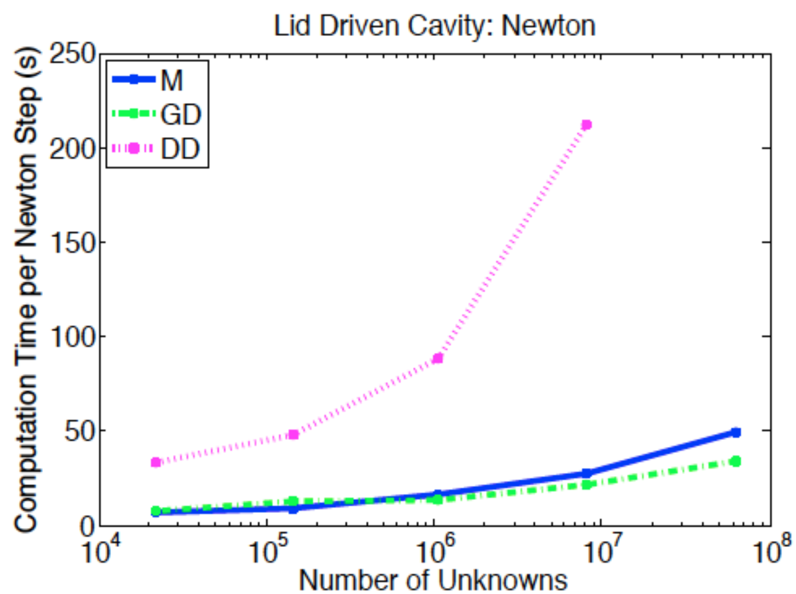
$$\hat{\mathcal{M}}_{P,2} = \begin{pmatrix} A + tD^t \bar{Q}_r^{-1} D & 0 \\ 0 & \frac{1}{t}\bar{Q}_r \end{pmatrix}$$

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



$Re_m = 1$ $Re_m = 10$ $Re_m = 100$





- 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)**

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Conclusions

- **Initial results for 3D Stabilized/VMS FE Lagrange multiplier formulation for low-flow Mach number resistive MHD system is very** encouraging (e.g. MHD generator, HMKH, geo-dynamo physics, isotropic decay of MHD turbulence, soon a tokamak model..)

- **Robustness, efficiency and scalability of parallel Newton-Krylov solvers is very good. Preconditioning critical:**
  - **FC-AMG (ML) for new 3D MHD systems continues to work very well (stabilized FE)**
  - **Approx. block factorization results are encouraging for Lagrange multiplier system. Applies to more general discretizations (mixed interp., [edge, face, ..])**
  - **Initial scaling of NK/FC-AMG linear solver to near extreme-scale (256K, ½ Million cores) is encouraging, still more work for preconditioner setup.**

- **Preliminary results for integrated adjoint based error-estimation and sensitivity capabilities for resistive MHD is very encouraging.**
  - Next consider complex systems (e.g. tokamak, geo-dynamo, plasmoids)
  - Explore application for laboratory experiments for dynamo studies.

- **MHD turbulence modeling with full VMS 3D resistive MHD formulation appears very promising.** Need to apply to more challenging plasma physics (e.g. planetary-dynamos)

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