

Scalable Implicit Resistive MHD with Stabilized Finite Element Methods and Fully-coupled Newton-Krylov-AMG Solution Methods

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Outline

- **General Scientific and Mathematical/Computational Motivation**
- **Brief Overview of 3D Resistive MHD Equations and VMS/Stabilized FE formulation**
- **Motivation for Fully Implicit Newton – Krylov Solution Methods**
 - **General comments**
 - **Facilitating adjoint methods for error-estimation and sensitivity analysis**
- **Scaling of Fully-coupled AMG preconditioner (block prec. Discussed earlier)**
- **Results for Preliminary Simulations for Geodynamo Relevant Flow Mechanisms**
 - **Rotating thermal convection in spherical geometry**
 - **High Rayleigh number thermal convection (validation w/lab experiments)**
- **VMS MHD Turbulence modeling: Initial results Taylor-Green MHD Vortex Decay**
- **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)

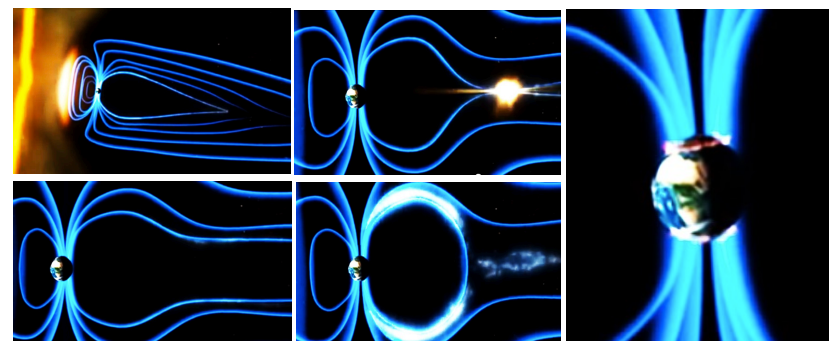
Mathematical/Computational Motivation:

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

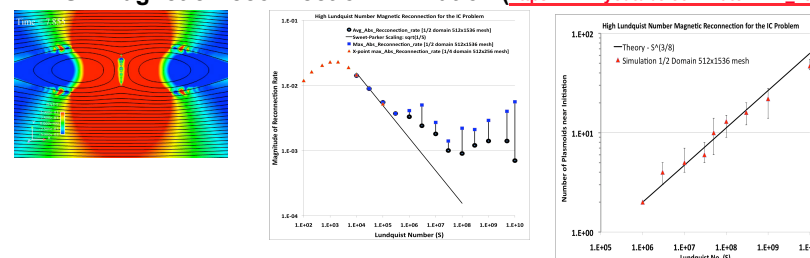
Mathematical Approach - develop:

- Stable and higher-order accurate fully-implicit formulations
- Stable and accurate spatial discretizations for complex geom., Options enforcing key mathematical properties (e.g. positivity, $\text{div } \mathbf{B} = 0$)
- 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)

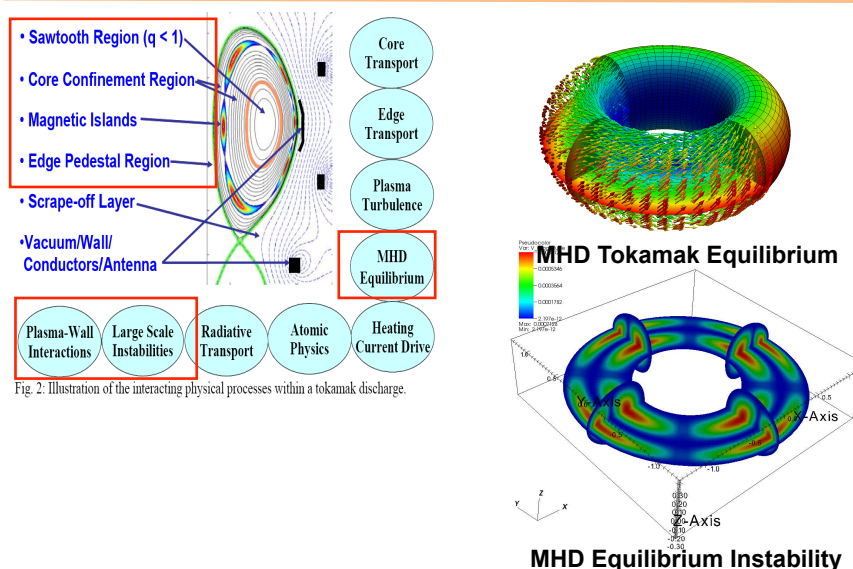
=> Also enables beyond forward simulation & integrated UQ



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



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



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

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.

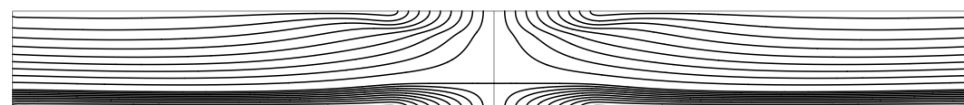
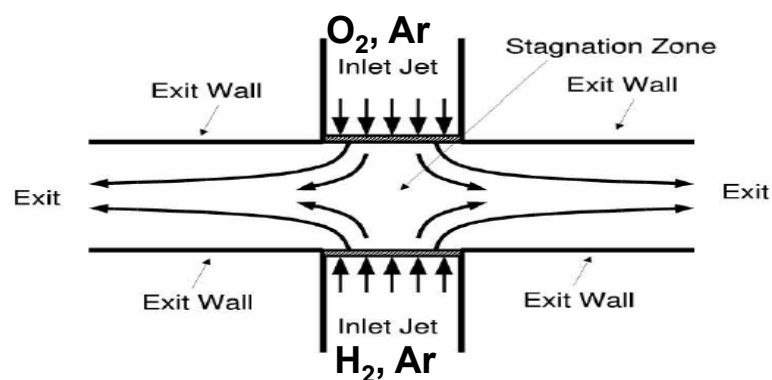
These mechanisms:

- 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.

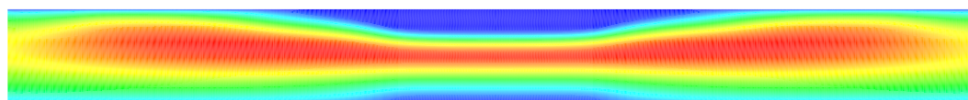
Our goal is to develop:

- Stable and higher-order accurate fully-implicit formulations,
- Robust fully-coupled nonlinear/linear iterative solution methods,
- Scalable and efficient parallel preconditioners,
- Integrated sensitivity and error-estimation to enable UQ capabilities.

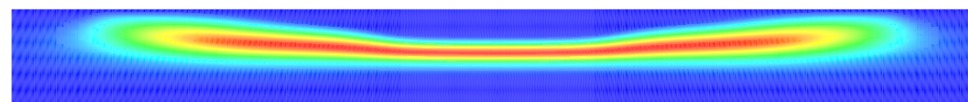
Multiple-time-scale systems: Bifurcation Analysis of a Steady Reacting H_2 , O_2 , Ar, Opposed Flow Jet Reactor (10 species, 19 reactions)



Streamlines

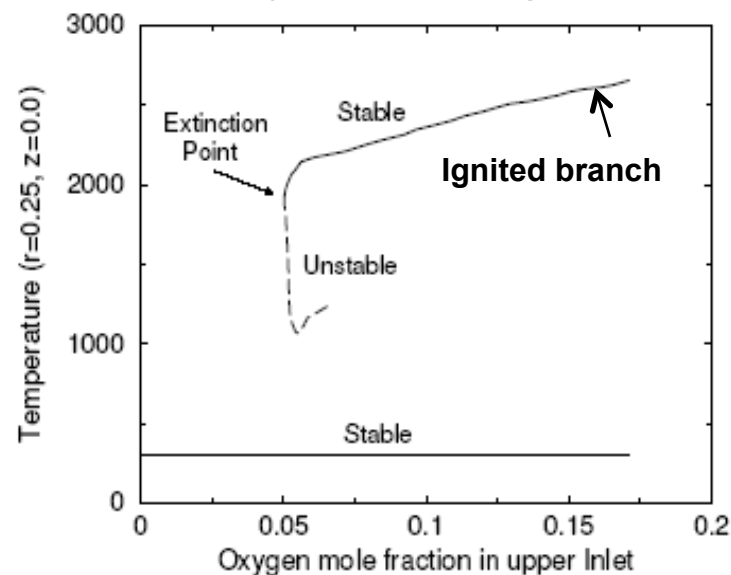


Temperature (Min. 300°K, Max 2727°K)



OH (Min. 0.0, Max 0.177)

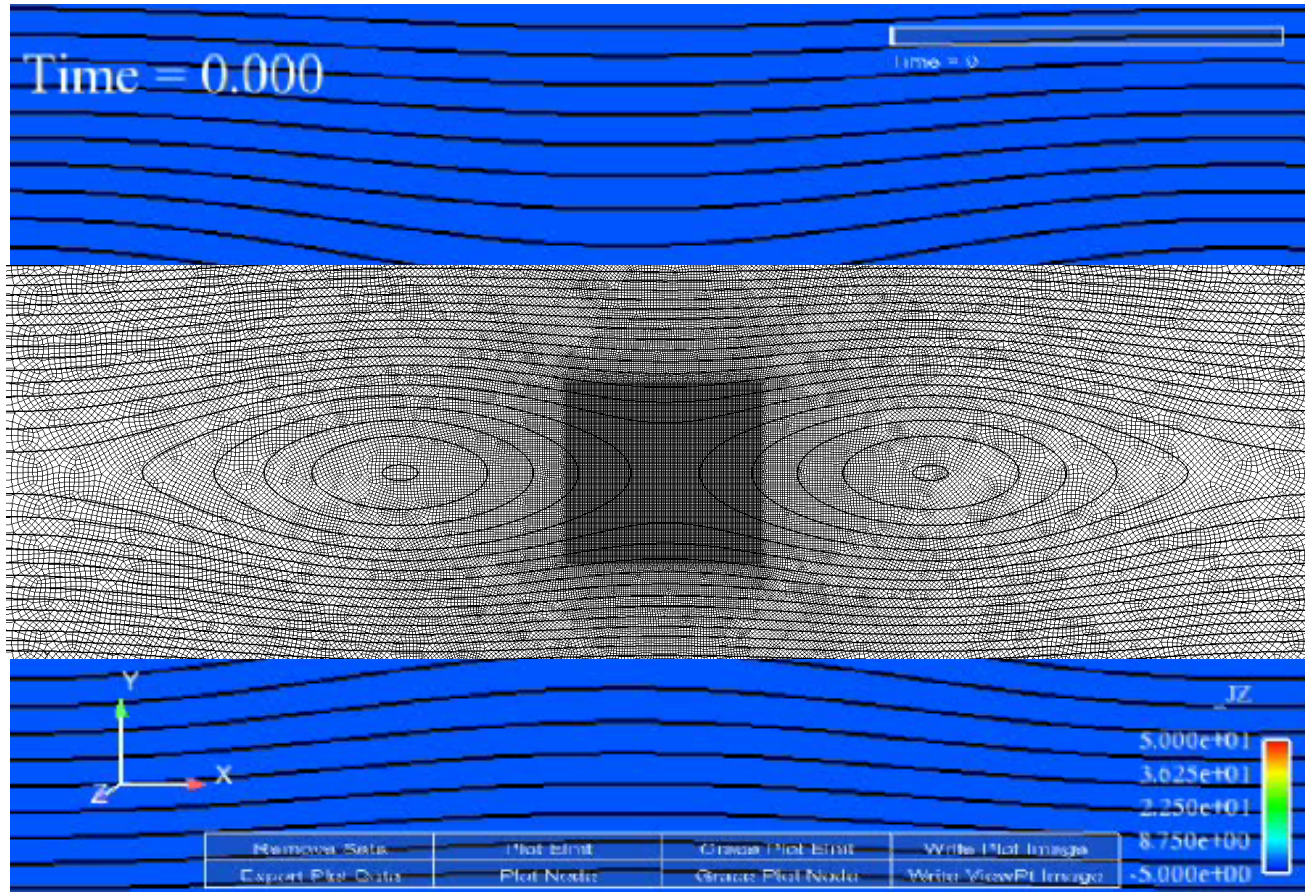
70 steady state reacting flow solves



Approx. Physical Time scales (sec.):

- Chemical kinetics: 10^{-12} to 10^{-4}
- Momentum diffusion: 10^{-6}
- Heat conduction: 10^{-6}
- Mass diffusion: 10^{-5} to 10^{-4}
- Convection: 10^{-5} to 10^{-4}
- Diffusion flame dynamics: ∞ (steady)

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

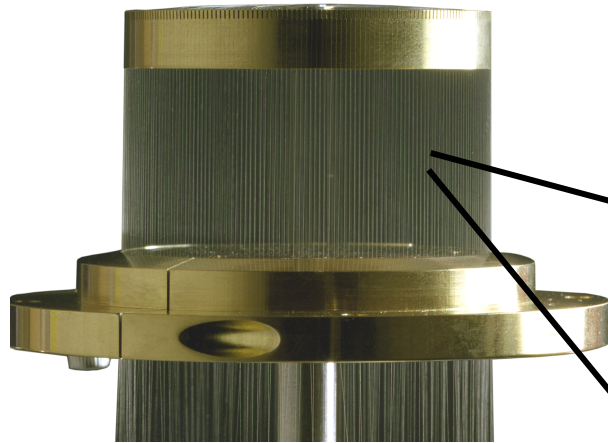


Approx. Computational Time Scales:

- Ion Momentum Diffusion: 10^{-7} to 10^{-3}
- Magnetic Flux Diffusion: 10^{-7} to 10^{-3}
- Ion Momentum Advection: 10^{-4} to 10^{-2}
- Alfvén Wave $\left(\tau_A = \frac{h \sqrt{\rho \mu_0}}{B_0}\right)$: 10^{-4} to 10^{-2}
- 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

[Finn and Kaw 1977; Chacon and Knoll Phys. 2006]

Z-pinch Double Hohlraum Schematic (ICF concept)



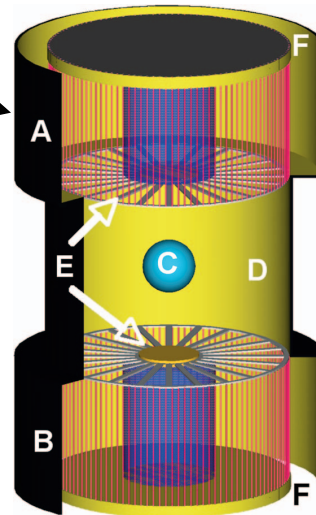
Z Machine (Approximate Ranges)

22 MJ stored energy

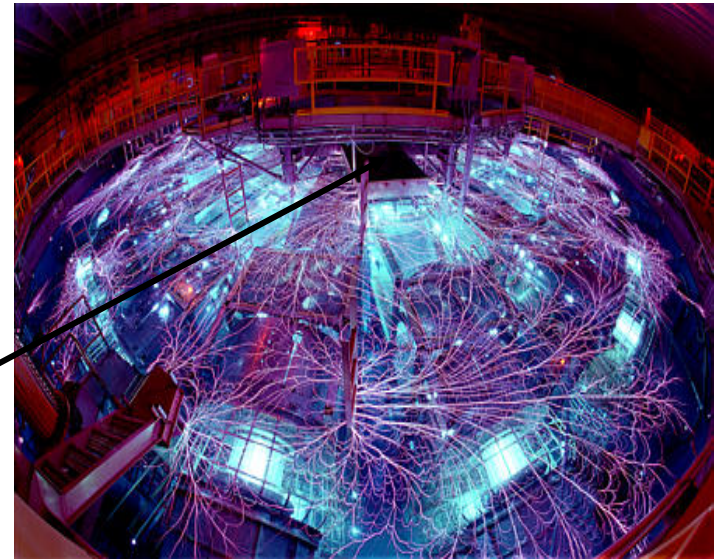
**100ns current rise time for
26 MA peak electrical current**

**250 ns plasma shell collapse
and stagnation**

**10-30 ns X-ray power pulse
~350 TW peak power**



*Double hohlraum
PoP Figure



Computational Stability Constraints:

Hyperbolic Operators: $\Delta t < \Delta x / c$

- Alfvén waves
- Magneto-sonic waves
- Material transport
- **Radiation transport**

Parabolic Operators: $\Delta t < (\Delta x)^2 / D$

- **Magnetic Diffusion**
- **Heat Conduction**

Hall Physics: Whistler waves

$$\rightarrow \Delta t < (\Delta x)^2 / (V_A d_i)$$

A Recent Physics Review: K. Matzen, et. al., PoP 12, 055503 (2005)

*Double z-pinch: Vessy, et. al., PoP 14, 056302 (2007)

Simulations: C. J. Garasi et. al., Physics of Plasmas, 11 (5), May 2004, pp. 2729-2737

Alegra: A. C. Robinson, W. J. Rider et. al., AIAA, 2008-1235

3D Resistive MHD Equations

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)

3D Resistive MHD Equations: VMS Formulation

Resistive MHD Model in Residual Notation

$$\mathbf{R}_v = \frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot [\mathcal{N}_v + P\mathbf{I} - \mathbf{\Pi}] - \rho \mathbf{g} = \mathbf{0}$$

$$\mathcal{N}_v = \rho \mathbf{v} \otimes \mathbf{v} - \frac{1}{\mu_0} \mathbf{B} \otimes \mathbf{B} + \frac{1}{2\mu_0} (\mathbf{B} \cdot \mathbf{B}) \mathbf{I}$$

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

$$\mathbf{\Pi} = \mu [\nabla \mathbf{u} + \nabla \mathbf{u}^T]$$

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

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

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

- Divergence free involution enforced as elliptic constraint with a Lagrange multiplier.
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(Costabel et. al. 2000, 2002, Codina, 2011)

Briefly Following Variational Multiscale Method (Hughes et. al.) Develop FE VMS MHD model

$$\text{Let } \mathbf{u} = \mathbf{u}^h + \mathbf{u}' \quad (\text{overlapping sum decomposition of solution})$$
$$\mathbf{w} = \mathbf{w}^h + \mathbf{w}' \quad (\text{weighting function})$$

Consider, $\mathbf{u}^h$ resolved/coarse scales, and $\mathbf{u}'$ unresolved/sub-grid scales

Following the VMS development the coarse and sub-grid scale equations become

$$\mathcal{A}(\mathbf{w}^h, \mathbf{u}^h) + (\mathcal{L}^* \mathbf{w}^h, \mathbf{u}')_{\Omega'} = (\mathbf{w}^h, \mathbf{f}) \quad \forall \mathbf{w}^h \in \mathbf{W}^h$$
$$(\mathbf{w}', \mathcal{L} \mathbf{u}') = -(\mathbf{w}', \mathcal{L}(\mathbf{u}^h) - \mathbf{f}) = -(\mathbf{w}', \mathcal{R}(\mathbf{u}^h)) \quad \forall \mathbf{w}' \in \mathbf{W}'$$

- Unresolved scales are driven by PDE residual of resolved scale solution.
- Formally the exact solution satisfies this representation
- Conceptually - resolved scale PDE residual “measures” unresolved or sub-grid scale effects (Contributes to both accuracy and stability. Hughes et. al. CMAME, 1998, Codina CMAME, 2000, Hughes et. al. Enc. Comp. Mech. 2007)

It is further assumed that the unresolved (sub-grid) scales are modeled by

$$\mathbf{u}' = -\tau[\mathcal{R}(\mathbf{u}^h)]$$

**Focus on Nonlinear contributions to flux terms:
VMS induced cross term fluxes (sub-grid to resolved scales)**

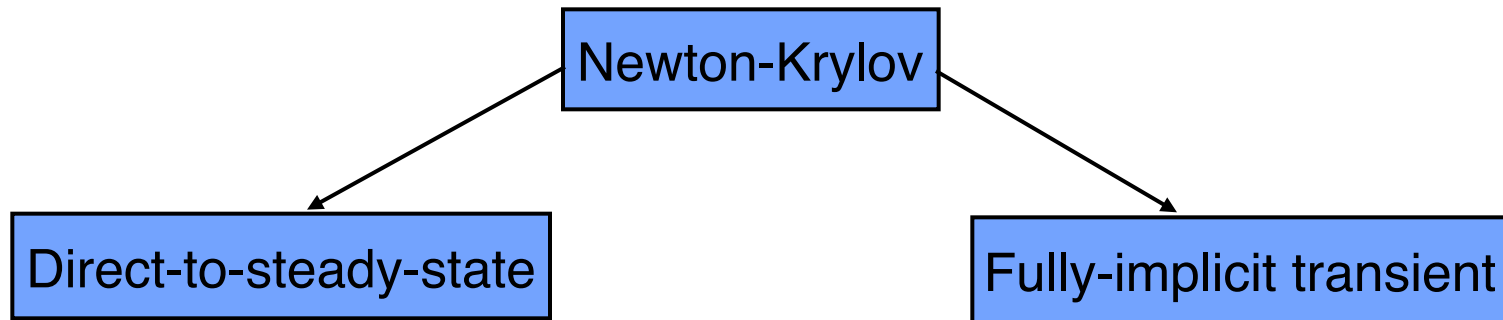
$$\mathcal{N}_{\mathbf{v}}^{(1)} = \rho \left(\mathbf{v}' \otimes \mathbf{v}^h \right)$$

$$\mathcal{N}_{\mathbf{B}}^{(1)} = \left(-\mathbf{v}^h \otimes \mathbf{B}' + \mathbf{B}' \otimes \mathbf{v}^h \right)$$

Summary of Initial VMS/Stabilized FE Weak form of Equations
for Low Flow Mach Number MHD System;

Governing Equation	Stabilized FE Residual (following Hughes et. al., Shakib - Navier-Stokes; Salah et. al. 99 & 01, Codina et. al. 2006 –Curl form magnetics)
Momentum	$F_{\mathbf{u}} = \int_{\Omega} \Phi \cdot \mathbf{R}_m d\Omega + \sum_e \int_{\Omega_e} \rho \tau_m \mathbf{R}_m \otimes \mathbf{u} : \nabla \Phi d\Omega + \sum_e \int_{\Omega_e} \hat{\tau}_P (\nabla \cdot \Phi) R_P d\Omega$
Total Mass	$F_P = \int_{\Omega} \Phi R_P d\Omega + \sum_e \int_{\Omega_e} \rho \tau_m \nabla \Phi \cdot \mathbf{R}_m d\Omega$ $\sum_e \int_{\Omega_e} \rho \tau_m \nabla \Phi \cdot \left[\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot [\rho \mathbf{v} \otimes \mathbf{v}] + \nabla P - \nabla \cdot \Pi - \mathbf{J} \times \mathbf{B} \right] d\Omega$
Thermal Energy	$F_T = \int_{\Omega} \Phi R_T d\Omega + \sum_e \int_{\Omega_e} \rho C_P \tau_T (\mathbf{u} \cdot \nabla \Phi) R_T d\Omega + \sum_e \int_{\Omega_e} \nu_T \nabla \Phi \cdot \mathbf{C}^c \nabla T d\Omega$
Magnetics: Induction	$F_B = \int_{\Omega} \Phi \cdot R_B d\Omega + \sum_e \int_{\Omega_e} \tau_B (\mathbf{R}_B \otimes \mathbf{u} - \mathbf{u} \otimes \mathbf{R}_B) : \nabla \Phi d\Omega + \sum_e \int_{\Omega_e} \tau_{\psi} (\nabla \cdot \Phi) (\nabla \cdot \mathbf{B}) d\Omega$
Divergence Constraint	$F_{\Psi} = \int_{\Omega} \Phi R_{\psi} d\Omega + \sum_e \int_{\Omega_e} \tau_B \nabla \Phi \cdot \mathbf{R}_B d\Omega$ $\sum_e \int_{\Omega_e} \tau_B \nabla \Phi \cdot \left[\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot [\mathbf{u} \otimes \mathbf{B} - \mathbf{B} \otimes \mathbf{u} - \frac{\eta}{\mu_0} (\nabla \mathbf{B} - (\nabla \mathbf{B})^T)] + \nabla \psi \right] d\Omega$

Why Newton-Krylov Methods?



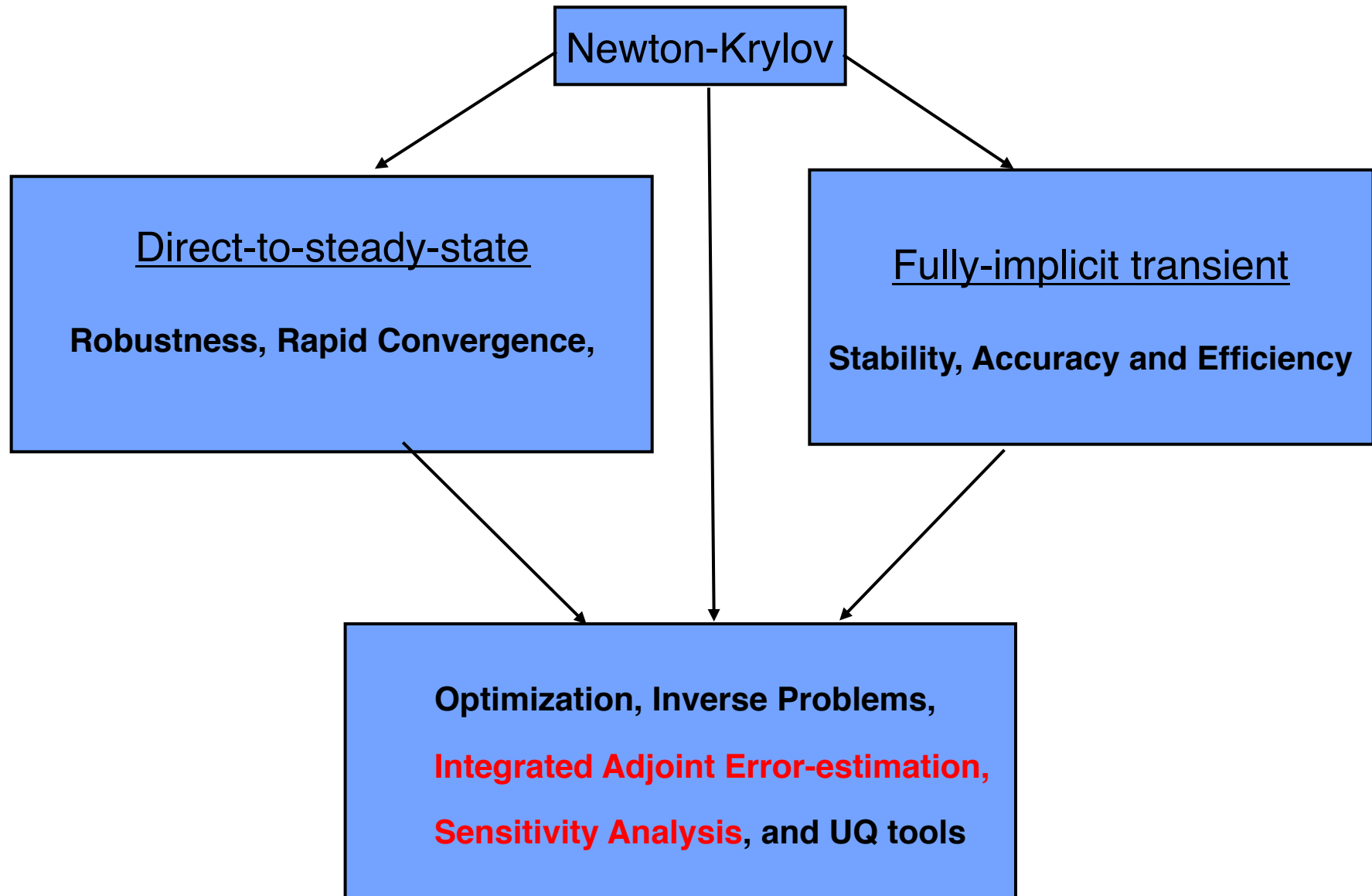
Robustness, Convergence and Flexibility

- 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?



Predictive computational analysis and uncertainty quantification (UQ) for multiphysics has many open challenges

Challenges Include:

- Uncertainties arise from: discretization errors, boundary and initial conditions, model parameters, physical parameters,
- Analysis and design often focus on a set of quantities of interest (Qol) rather than the entire state (e.g. partial differential equation (PDE) solution)
- The stability, error, uncertainty propagation and sensitivity characteristics for Qol can be significantly different from the PDE solution itself

We are addressing these challenges for studies of a **moderate number of Qols** dependent on **a large-number of parameters** using **adjoint-based methods** to accurately and efficiently compute numerical error estimates and to conduct sensitivity analysis for Qol

*Adjoint methods have been well studied and demonstrated for single-physics parabolic PDEs.
[e.g. Rannacher, Oden, C. Johnson, Estep, Bangerth, Barth, Suli, Braack,]*

Predictive computational analysis and uncertainty quantification (UQ) for multiphysics has many open challenges

Forward problem: $\mathcal{L}(u; \mathbf{p}) = f(\mathbf{p})$

Adjoint problem: $(\mathcal{L}'(u; \mathbf{p}))^* \psi = \partial_u g(u, \mathbf{p})$.

Adjoint Sensitivities: $\partial_p g(U; p) = (\psi, \partial_p \mathcal{R}(u; p))$; Error Estimate: $g(u; p) - g(U; p) \approx (\psi, \mathcal{R}(u; p))$

Adjoint methods for stabilized FE methods:

Context of adjoint methods in optimization

Collis, S., and Heinkenschloss, M. Technical Report TR02-01, Rice University 2002.

Error estimation for SUPG

Houston, P., Rannacher, R., and Suli, E. CMAME (2000)

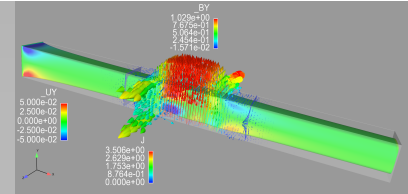
Rannacher, R. CMAME, 1998

Cyr, Shadid, Wildey, *Approaches for adjoint-based a posteriori analysis of stabilized finite element methods, to appear SISC*

*We have studied variational adjoints, **discrete adjoints** and alternate error representations for stabilized methods in transport and Navier-Stokes (**steady** and transients)*

Initial Adjoint Error Estimate Study for Resistive MHD:

Analytic Hartmann Flow



■ **Qol (1): Average Fluid velocity (Vx)**

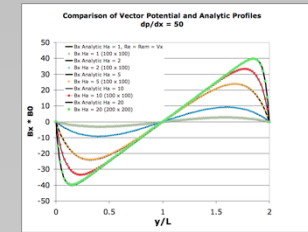
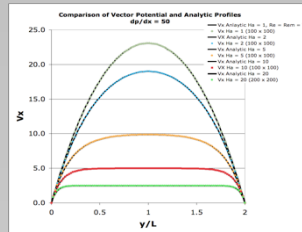
$$\bar{V} = \frac{1}{2} \int_{-1}^1 V_x dy$$

■ **Qol (2) Magnetics: Average of half-domain induced field in streamwise direction (Bx)**

$$\bar{B}_x = \int_0^1 B_x dy$$

$$u_x = -\frac{G_0 L^2}{\mu Ha \tanh[Ha]} \left(1 - \frac{\cosh[Ha y/L]}{\cosh[Ha]}\right)$$

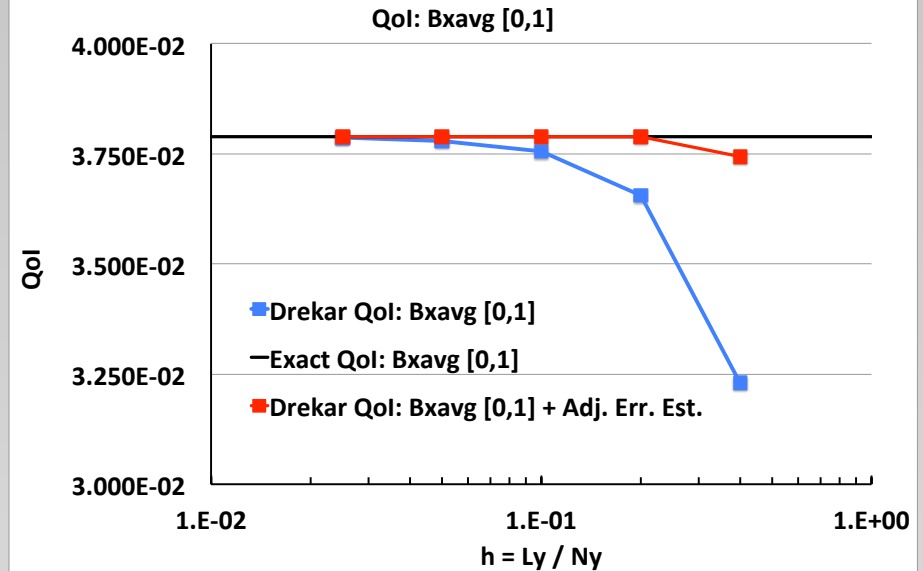
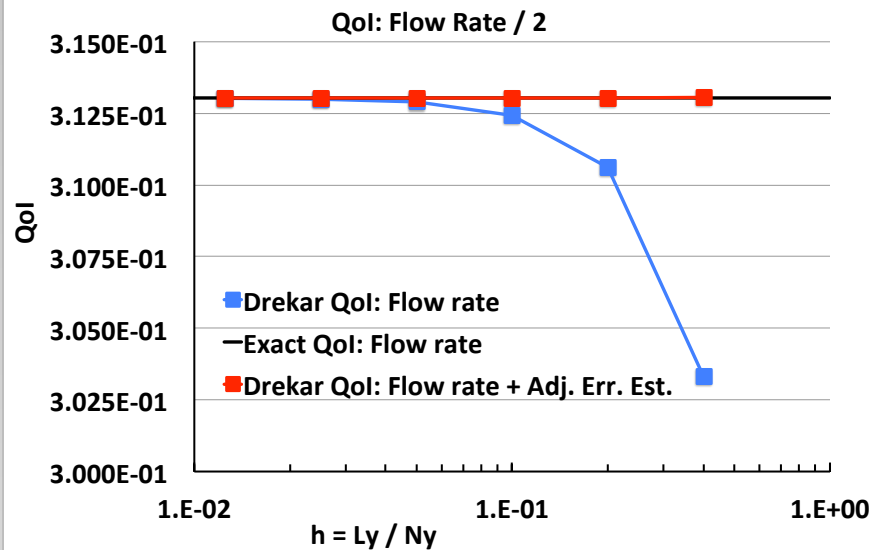
$$B_x = -\frac{G_0 L^2 \mu_0}{\sqrt{\mu \eta}} \frac{1}{Ha} \left(\frac{y}{L} - \frac{1}{\tanh[Ha]} \frac{\sinh[Ha y/L]}{\cosh[Ha]}\right)$$



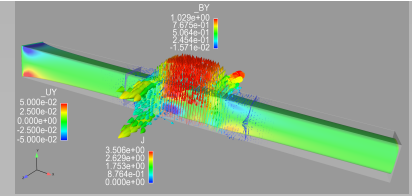
$$Re_m = \frac{VL}{\eta}$$

$$Re = \frac{\rho VL}{\mu};$$

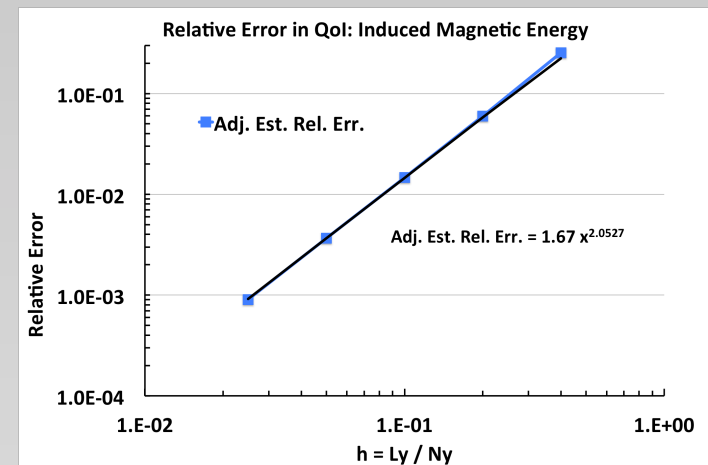
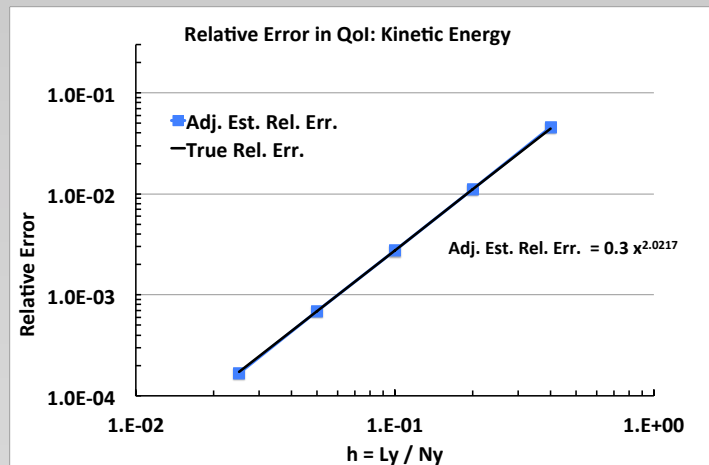
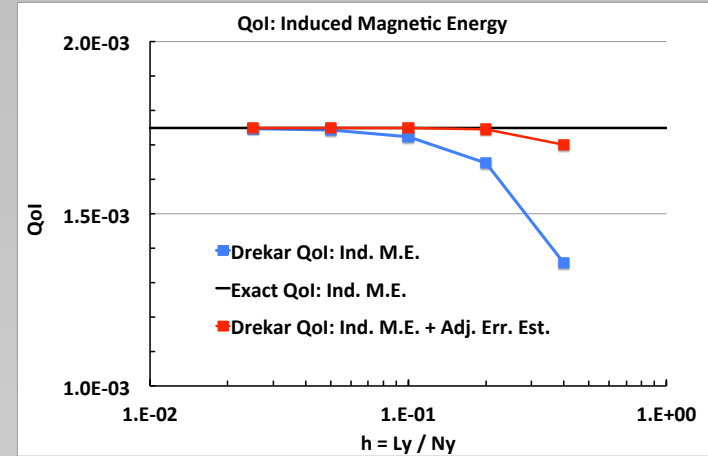
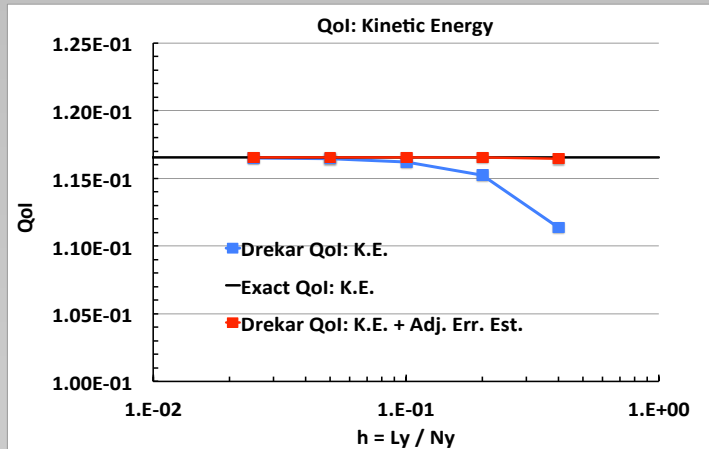
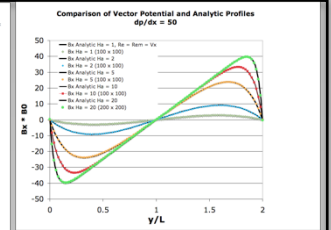
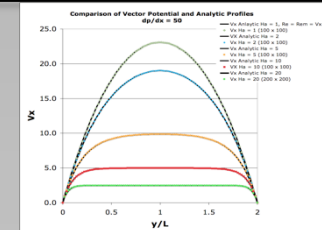
$$Ha = \frac{B_0 L}{\sqrt{\mu \eta}}$$



Initial Adjoint Error Estimate Study for Resistive MHD: Analytic Hartmann Flow – Nonlinear QoI

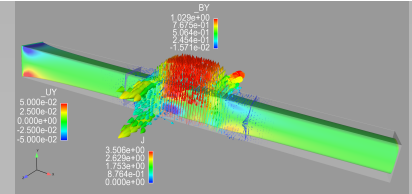


- QoI (1): Kinetic Energy
$$\text{K.E.} = \frac{1}{2} \int_{\Omega} u_x^2 d\Omega$$
- QoI (2): Induced Magnetic Energy:
$$\text{M.E.} = \frac{1}{2} \int_{\Omega} B_x^2 d\Omega$$



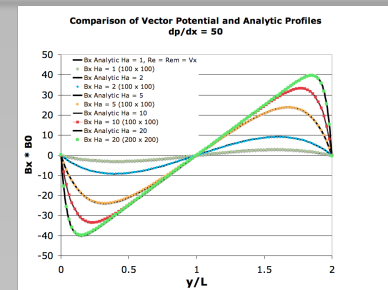
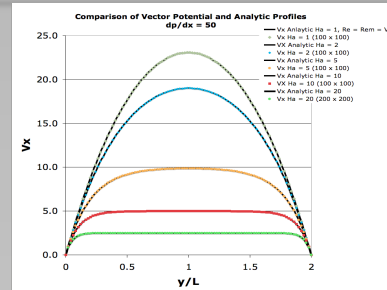
Initial Adjoint Sensitivity Analysis for Resistive MHD: MHD Duct Flows

E.g. Analytic Hartmann Flow – accuracy of derivatives



- QoI (1) Flow: Average Fluid velocity (V_x)

$$\bar{V} = \frac{1}{2} \int_{-1}^1 V_x dy$$



$$Re = \frac{\rho V L}{\mu}; Re_m = \frac{V L}{\eta}$$

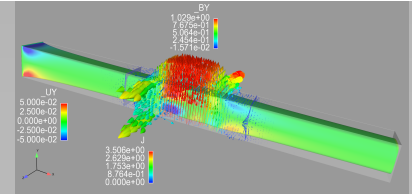
$$Ha = \frac{B_0 L}{\sqrt{\mu \eta}}$$

E.g. Mesh Simulation: 40 elements in duct cross-section

Physical Parameter	Re = 1; Rem = 1, Ha = 1;			Re = 875; Re = 43.7.; Ha = 44.7;		
	Analytic	Adjoint	Rel. Err.	Analytic	Adjoint	Rel. Err.
Pressure Gradient (G_0)	-0.313035	-0.312884	0.048%	-4.37214	-4.36929	0.065%
Dynamic Viscosity (μ)	-0.294487	-0.294383	0.04%	-447.214	446.529	0.15%
Density (ρ)	0.0	-1.2e-7	-----	0.0	1.1e-3	-----
Resistivity (η)	0.018548	0.018501	0.2%	21.3607	21.3623	0.01%
Applied Mag. Ind. (B_0)	-0.037097			-4.27214		

Initial Adjoint Sensitivity Analysis for Resistive MHD: MHD Duct Flows

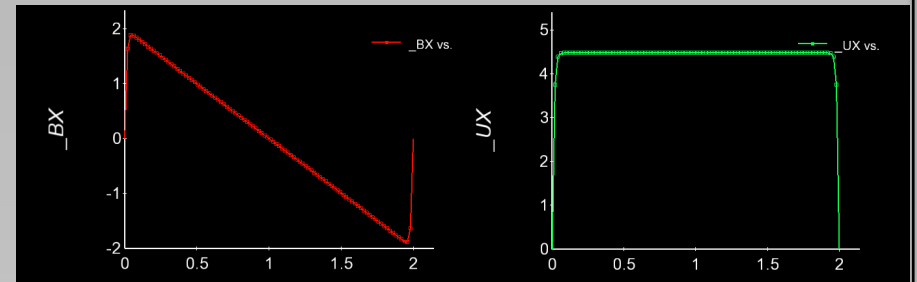
E.g. Analytic Hartmann Flow – accuracy of derivatives



■ QoI (1): Total Energy: Kinetic + Magnetic

$Re = 884$; $Rem = 177$; $Ha = 90$;

$$T.E. = \int_{\Omega} \frac{1}{2} (u_x^2 + u_y^2) d\Omega + \int_{\Omega} \frac{1}{2\mu_0} (B_x^2 + B_y^2) d\Omega$$

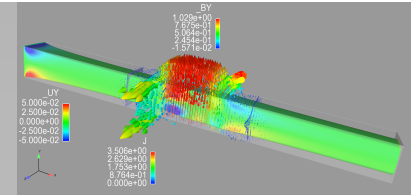


E.g. Mesh Simulation: 40 elements in duct cross-section

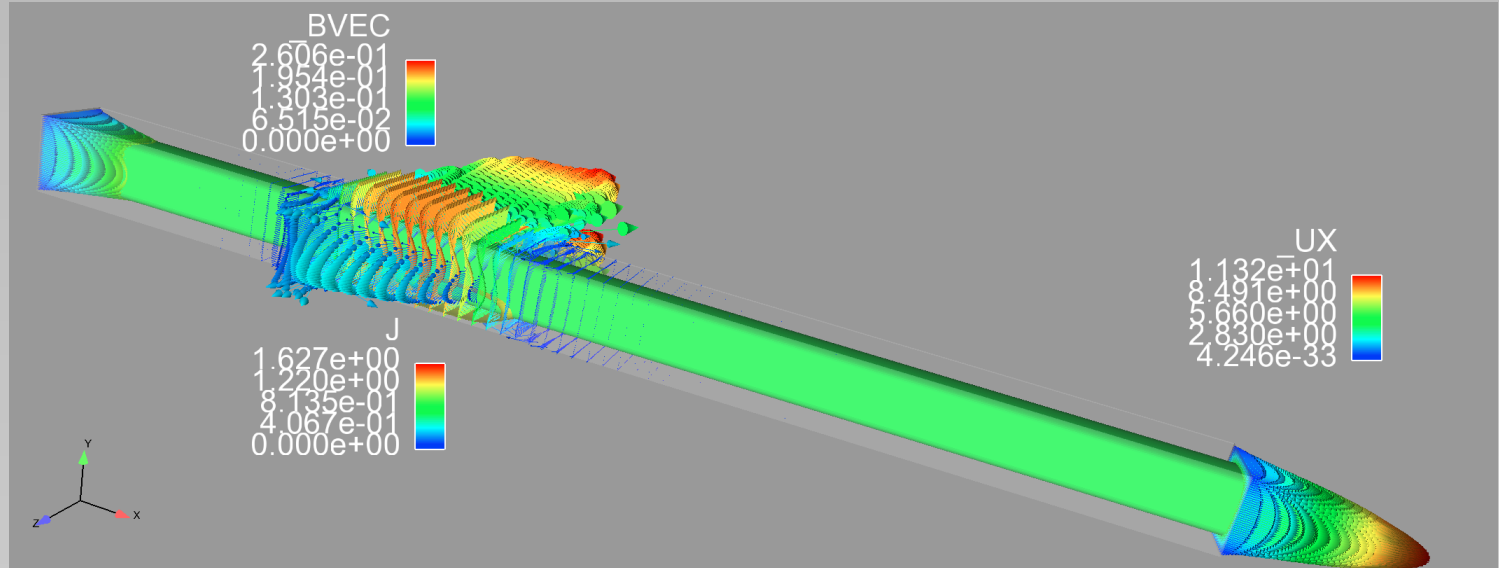
Physical Parameter	Analytic	Uniform Mesh		Non-uniform Boundary Layer Mesh	
		Drekar / Adjoint	Rel. Err.	Drekar / Adjoint	Rel. Err.
QoI: T.E.	21.9318	22.29552	1.66%	21.96336	0.15%
QoI Derivatives:					
Pressure Gradient (G_0)	-20.9318	-21.4356	2.41%	-20.9753	0.21%
Dynamic Viscosity (μ)	-3972.97	-4145.97	4.35%	-3979.72	0.17%
Density (ρ)	0.0	1.1e-1	-----	3.0e-3	-----
Resistivity (η)	778.574	779.613	0.133%	779.988	0.18%
Applied Mag. Ind. (B_0)	-41.4632				

Initial Adjoint Study: Visualization of Adjoint Solution for Resistive MHD

E.g. 3D MHD Generator ($Re \sim 2500$, $Re_m \sim 10$, $Ha = 5$)

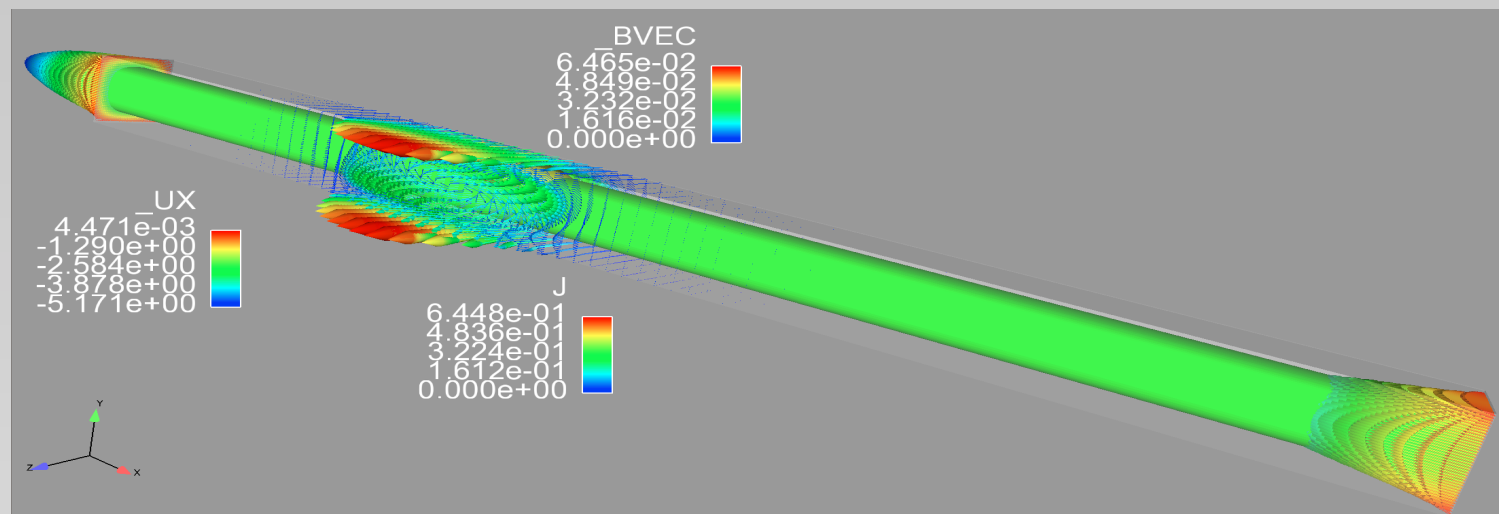


Forward
Solution



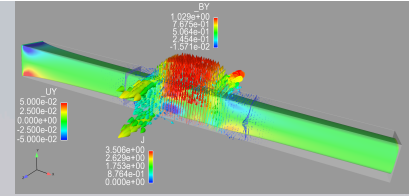
Adjoint
Solution

QoI: $\bar{V}$



Initial Adjoint Error Estimation Study for Resistive MHD: 3D MHD Duct Flows

E.g. 3D MHD Generator ($Re \sim 2500$, $Re_m \sim 10$, $Ha = 5$)



- Qol (1): Average Fluid velocity ($\mathbf{Vx}$)

$$\bar{V} = \frac{\int_{\Omega} V_x d\Omega}{\text{Volume}(\Omega)}$$

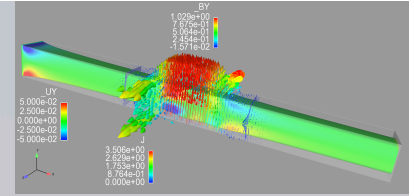
$$Re = \frac{\rho V L}{\mu}; \quad Re_m = \frac{V L}{\eta} \quad Ha = \frac{B_0 L}{\sqrt{\mu \eta}}$$

- State: $Re \sim 2500$, $Re_m \sim 10$, $Ha = 5$;
- Adjoint Error estimation, take reference solution as 400x200x200 element mesh

Nx x Ny x Nz (#unknowns)	Qol: $\bar{V}$	Err. Est.	Pred. Qol	Est. Rel. Err.	Rel. Err. Ref.*
20x10x10 (16K)	5.63814	0.4664	6.1045	8.3%	-3.5%
40x20x20 (128K)	5.40236	0.1154	5.5178	2.1%	0.8%
80x40x40 (1M)	5.41037	0.0159	5.4263	0.3%	0.7%
160x80x80 (8M)	5.44320	0.0040	5.4472	0.07%	0.09%
400x200x200 (128M)*	5.44831	-	-	-	-

Initial Adjoint Error Estimation Study for Resistive MHD: 3D MHD Duct Flows

E.g. 3D MHD Generator ($Re \sim 2500$, $Re_m \sim 10$, $Ha = 5$)



- Qol (1) Flow: Induced Magnetic Energy

$$M.E. = \frac{1}{2\mu_0} \int_{\Omega} (B_x^2 + B_z^2) d\Omega$$

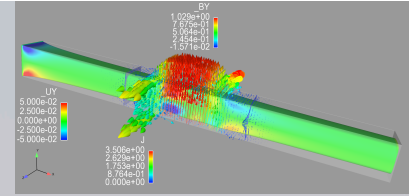
$$Re = \frac{\rho V L}{\mu}; \quad Re_m = \frac{V L}{\eta} \quad Ha = \frac{B_0 L}{\sqrt{\mu \eta}}$$

- State: $Re \sim 2500$, $Re_m \sim 10$, $Ha = 5$;
- Adjoint Error estimation, take reference solution as 400x200x200 element mesh

Nx x Ny x Nz (#unknowns)	Qol: M.E. ($2.0 \cdot 10^4$)	Err. Est. ($2.0 \cdot 10^4$)	Pred. Qol ($2.0 \cdot 10^4$)	Est. Rel. Err.	Rel. Err. Ref.*
40x20x20 (128K)	6.4768	0.1298	6.6085	2.0%	10.2%
60x30x30 (432K)	6.5999	0.2962	6.8961	4.5%	8.5%
80x40x40 (1M)	6.8876	0.2239	7.1114	3.25%	4.51%
100x50x50 (2M)	7.0632	0.1136	7.1769	1.50%	2.07%
160x80x80 (8M)	7.1256	0.0748	7.2004	1.05%	1.21%
400x200x200 (128M)*	7.2128	-	-	-	-

Initial Adjoint Error Estimation Study for Resistive MHD: 3D MHD Duct Flows

E.g. 3D MHD Generator ($Re \sim 2500$, $Re_m \sim 10$, $Ha = 5$)



$$Re = \frac{\rho V L}{\mu}; \quad Re_m = \frac{V L}{\eta} \quad Ha = \frac{B_0 L}{\sqrt{\mu \eta}}$$

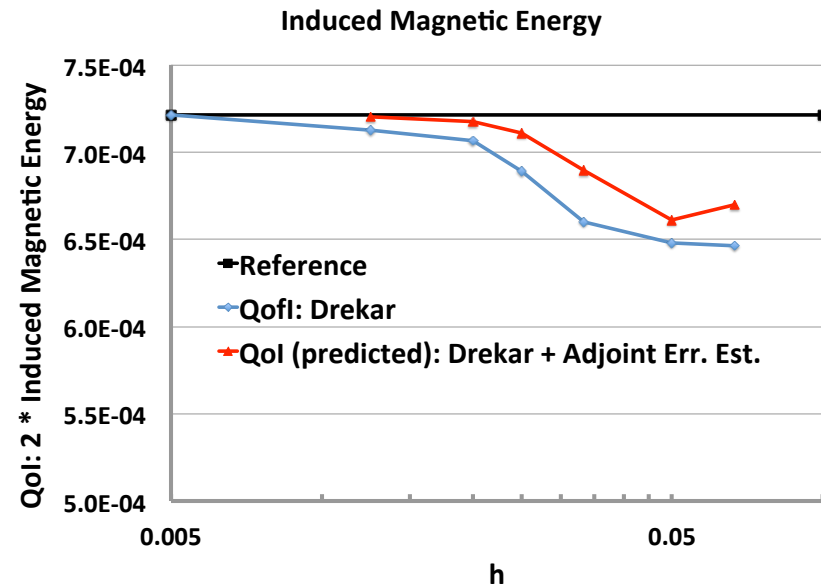
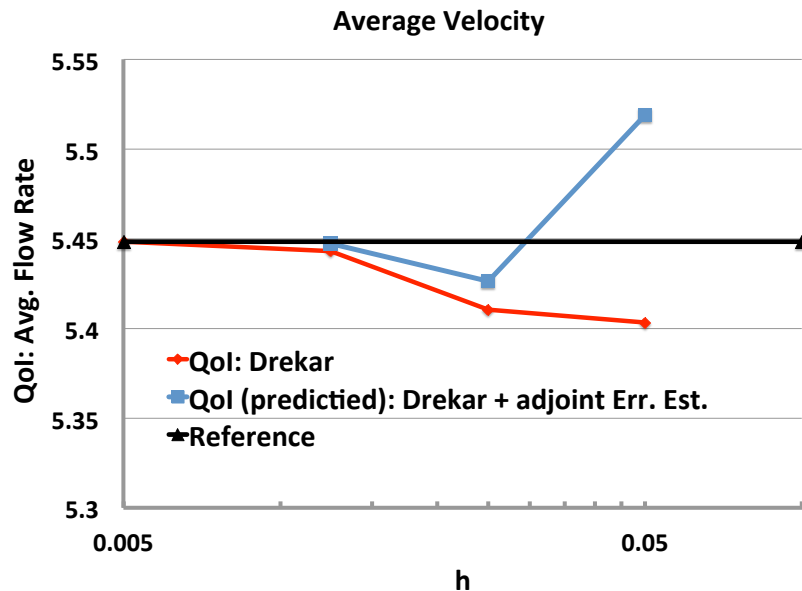
- Qol (1): Average Fluid velocity ($\mathbf{Vx}$)

$$\bar{V} = \frac{\int_{\Omega} V_x d\Omega}{\text{Volume}(\Omega)}$$

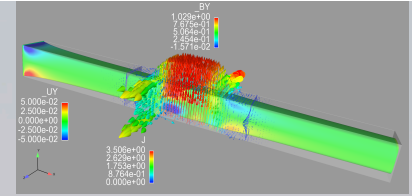
- Qol (2): Induced Magnetic Energy

$$\text{M.E.} = \frac{1}{2\mu_0} \int_{\Omega} (B_x^2 + B_z^2) d\Omega$$

- State: $Re \sim 2500$, $Re_m \sim 10$, $Ha = 5$;
- Adjoint Error estimation, take reference solution as 400x200x200 element mesh



Initial Adjoint Sensitivity Analysis for Resistive MHD: 3D MHD Duct Flows E.g. 3D MHD Generator ($Re \sim 2500$, $Re_m \sim 10$, $Ha = 5$)

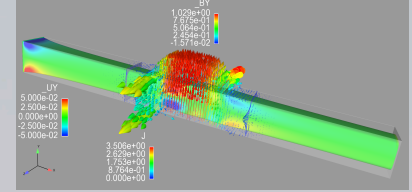


- QoI (1) Flow: Average Fluid velocity ($\mathbf{Vx}$) $\bar{V} = \int_{-1}^1 V_x dy$
- Reference state: $\rho = 1, \mu = 0.002, G_0 = 0.31, \eta = 1, B_0 = 0.2236$
- Parameters in simple numerical sensitivity study (+- 1%, 5%, 10%) μ, G_0 ;
- Local linear Taylor series model (e.g. surrogate model for sampling UQ) $q = \bar{q} + \frac{\partial q}{\partial p}(p - \bar{p}) + H.O.T$

E.g. Coarse Mesh Simulation: $N_x \times N_y \times N_z$: 140x20x20 mesh

Physical Parameter Dynamic Viscosity (μ)	QoI computed from Drekar	QoI Estimated from Adjoint Sensitivity & Linear Model	Relative Error
0.00202 ($\mu+1\%$)	4.61750	4.61703	0.010%
0.00198 ($\mu-1\%$)	4.69811	4.69784	0.006%
0.00210 ($\mu+5\%$)	4.46483	4.45541	0.211%
0.00190 ($\mu-5\%$)	4.86876	4.85945	0.191%
0.00220 ($\mu+10\%$)	4.28845	4.25338	0.82%
0.00180 ($\mu-10\%$)	5.10192	5.06148	0.79%

Initial Adjoint Sensitivity Analysis for Resistive MHD: 3D MHD Duct Flows E.g. 3D MHD Generator ($Re = 2500$, $Re_m = 10$, $Ha = 5$)



- QoI (1) Flow: Average Fluid velocity ($\mathbf{Vx}$) $\bar{V} = \int_{-1}^1 V_x dy$
- Reference state: $\rho = 1, \mu = 0.002, G_0 = 0.31, \eta = 1, B_0 = 0.2236$
- Parameters in simple numerical sensitivity study (+- 1%, 5%, 10%) μ, G_0 ;
- Local linear Taylor series model (e.g. surrogate model for sampling UQ) : $q = \bar{q} + \frac{\partial q}{\partial p}(p - \bar{p}) + H.O.T$

E.g. Coarse Mesh Simulation: $N_x \times N_y \times N_z$: 140x20x20 mesh

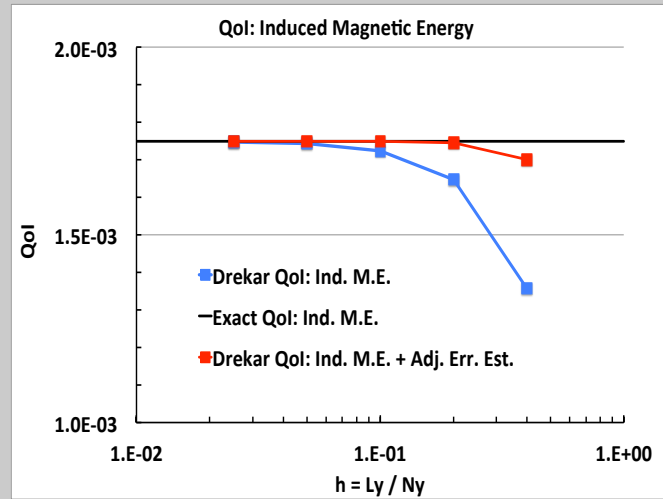
Physical Parameter Pressure Gradient (G_0)	QoI computed from Drekar	QoI Estimated from Adjoint Sensitivity & Linear Model	Relative Error
0.3131 (G_0 +1%)	4.70082	4.70288	0.04%
0.3069 (G_0 -1%)	4.61401	4.61198	0.04%
0.3255 (G_0 +5%)	4.87404	4.88466	0.22%
0.2945 (G_0 -5%)	4.43997	4.43020	0.17%
0.341 (G_0 +10%)	5.14753	5.11189	0.69%
0.279 (G_0 -10%)	4.22159	4.19842	0.55%

Example: Steady MHD Duct Flow (Hartmann Analytic Solution)

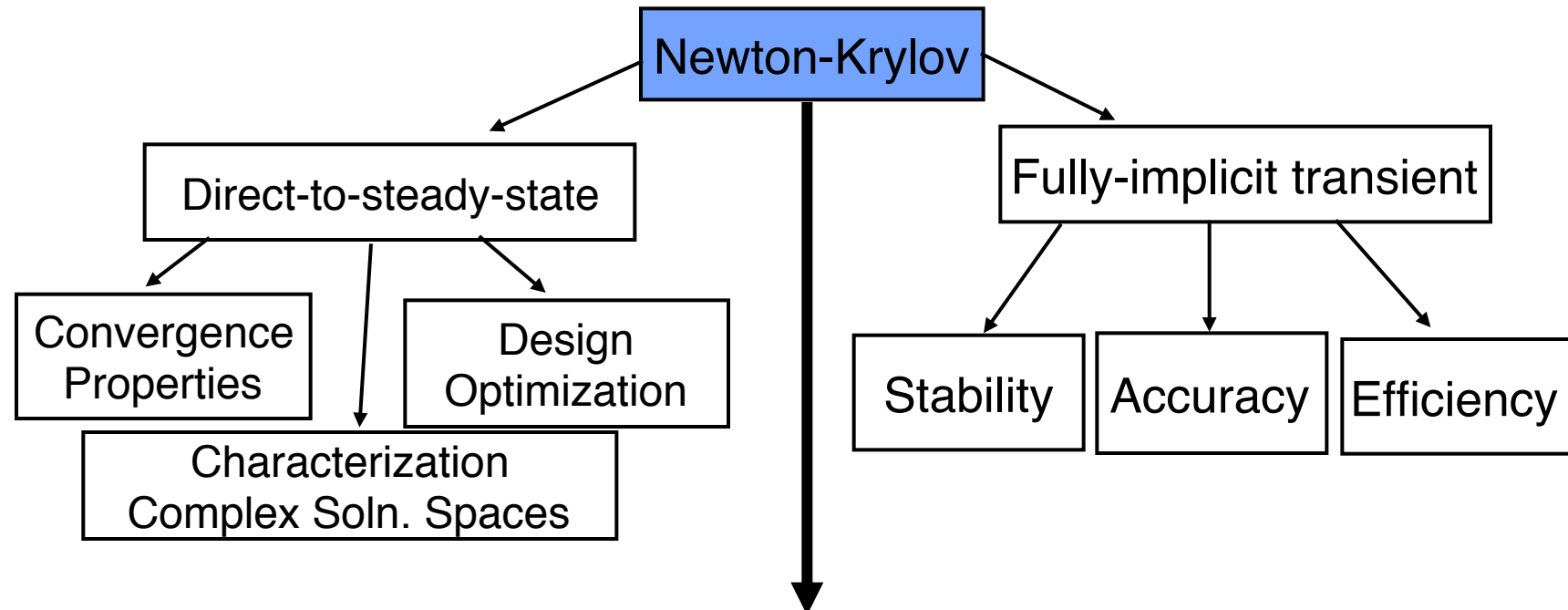
Example: Accuracy of Adjoint Error
Estimate (Re=Rem=Ha =1)

Qol: Induced Magnetic Energy

$$\text{M.E.} = \frac{1}{2} \int_{\Omega} B_x^2 d\Omega$$



Why Newton-Krylov Methods?

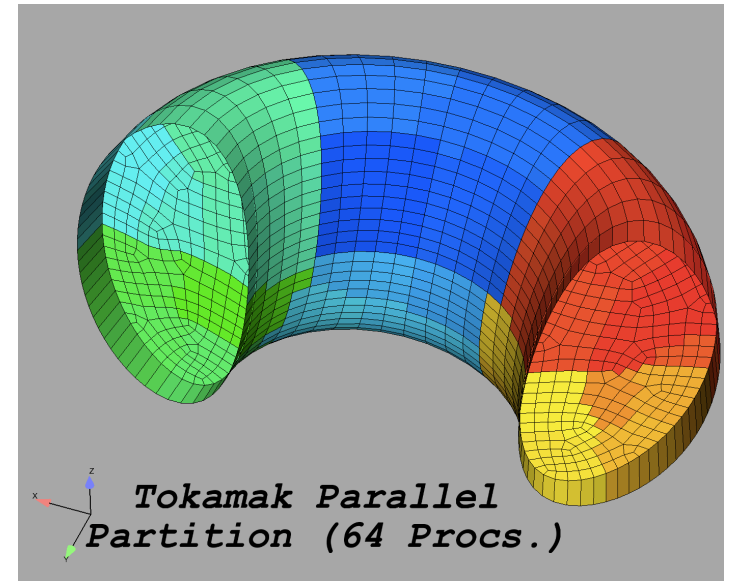


Preconditioning

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)

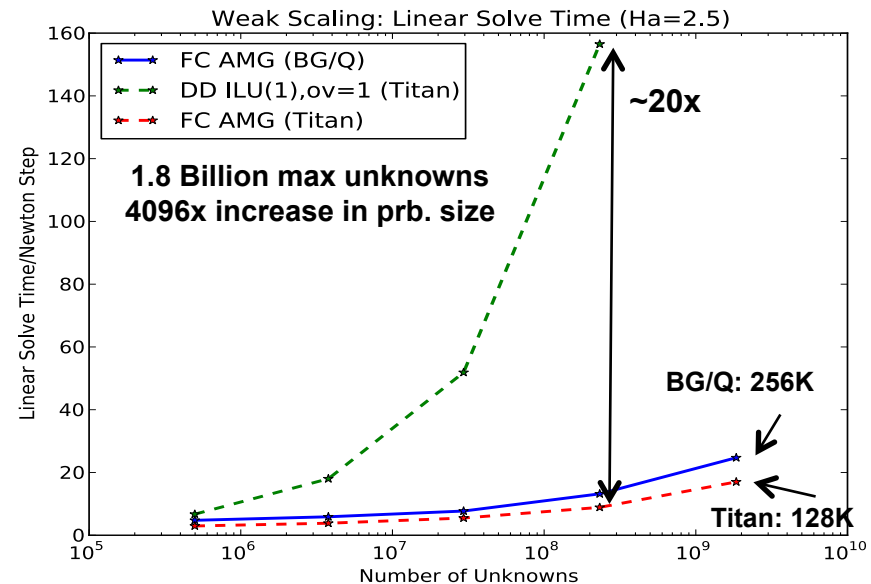
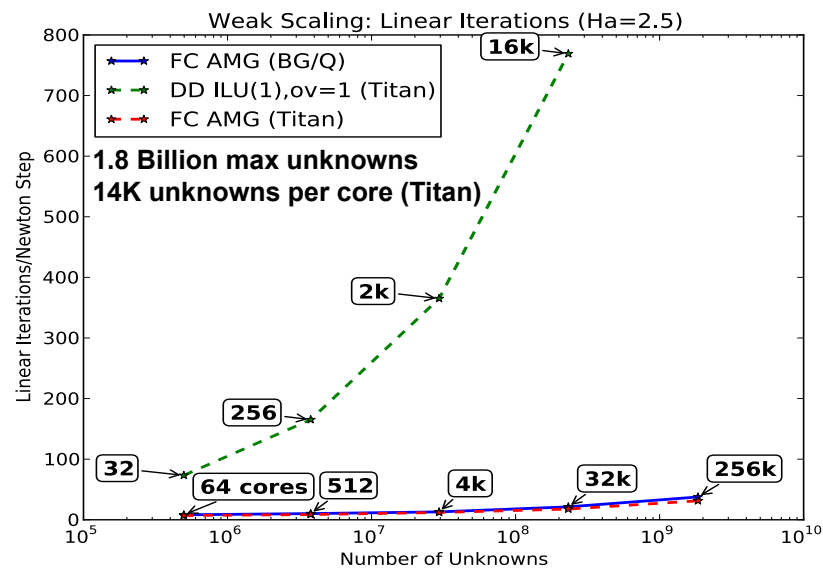
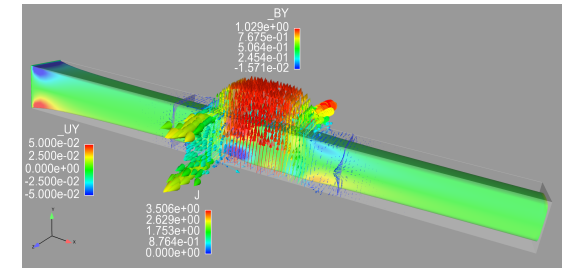
Fully-coupled Algebraic Multilevel methods

- 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

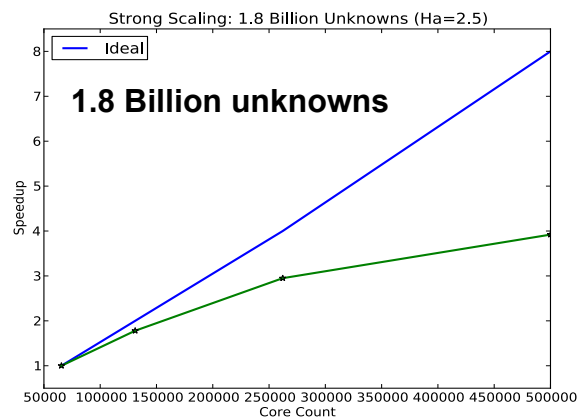
3. Approximate Block Factorization / Physics-based (Teko package)

- 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

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

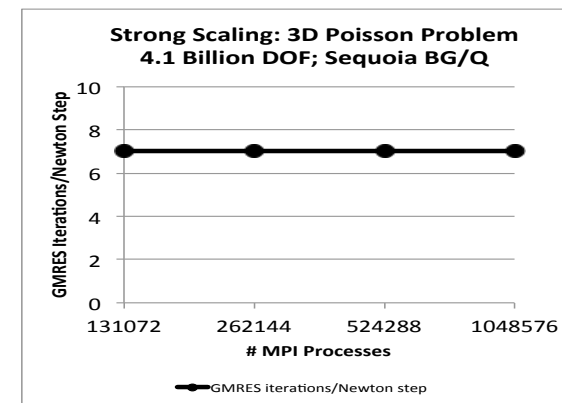


MHD Recently run on 1/2 M cores of BG/Q



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

4 Billion element/unknown Solution of Poisson Eq. 1M cores

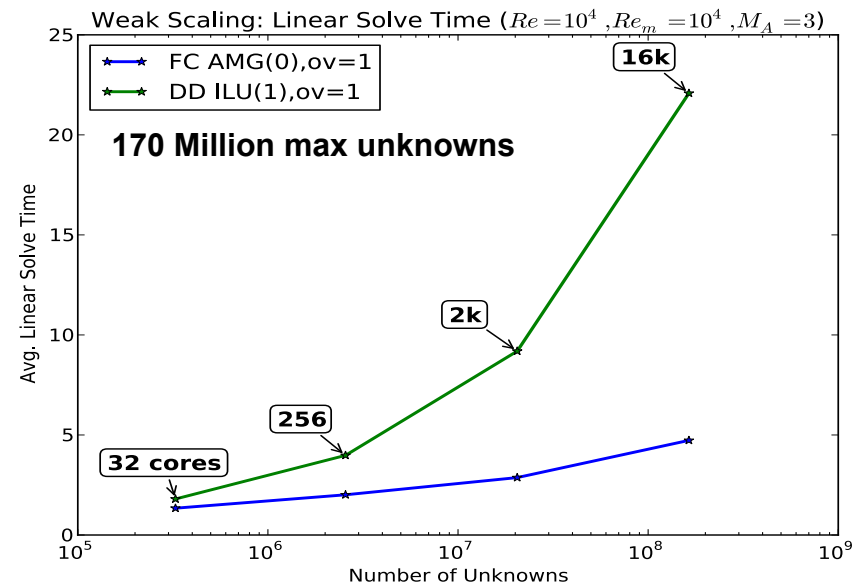
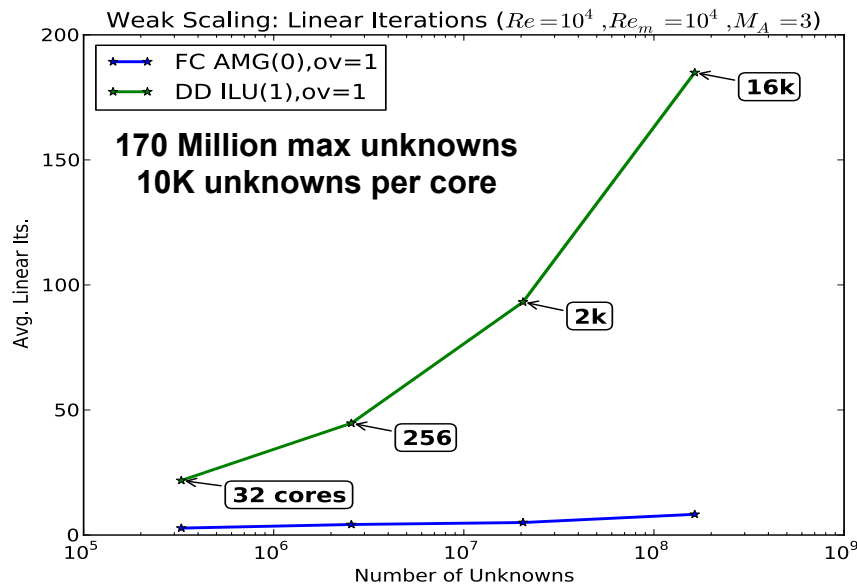
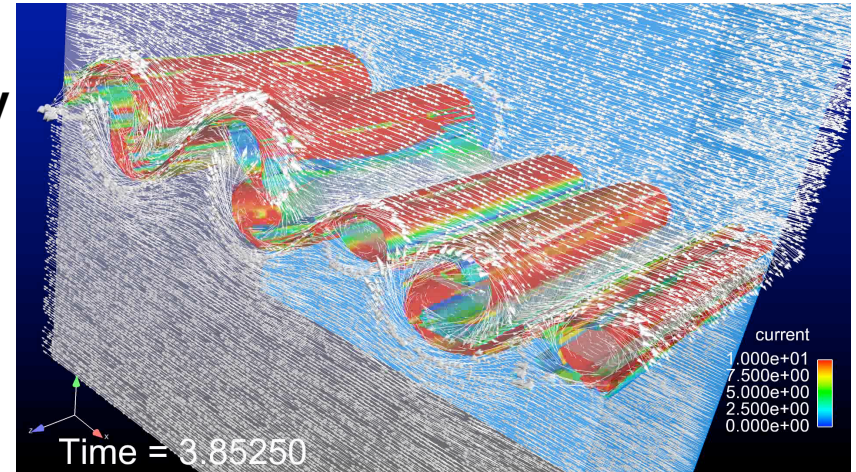


(DOE/ORNL Titan Cray XK7: Joule Metric)

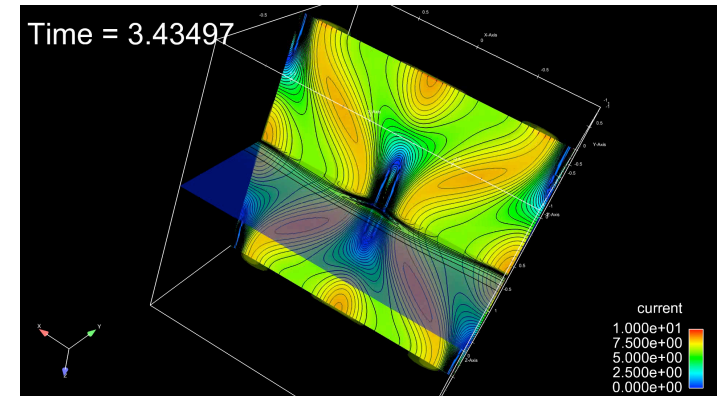
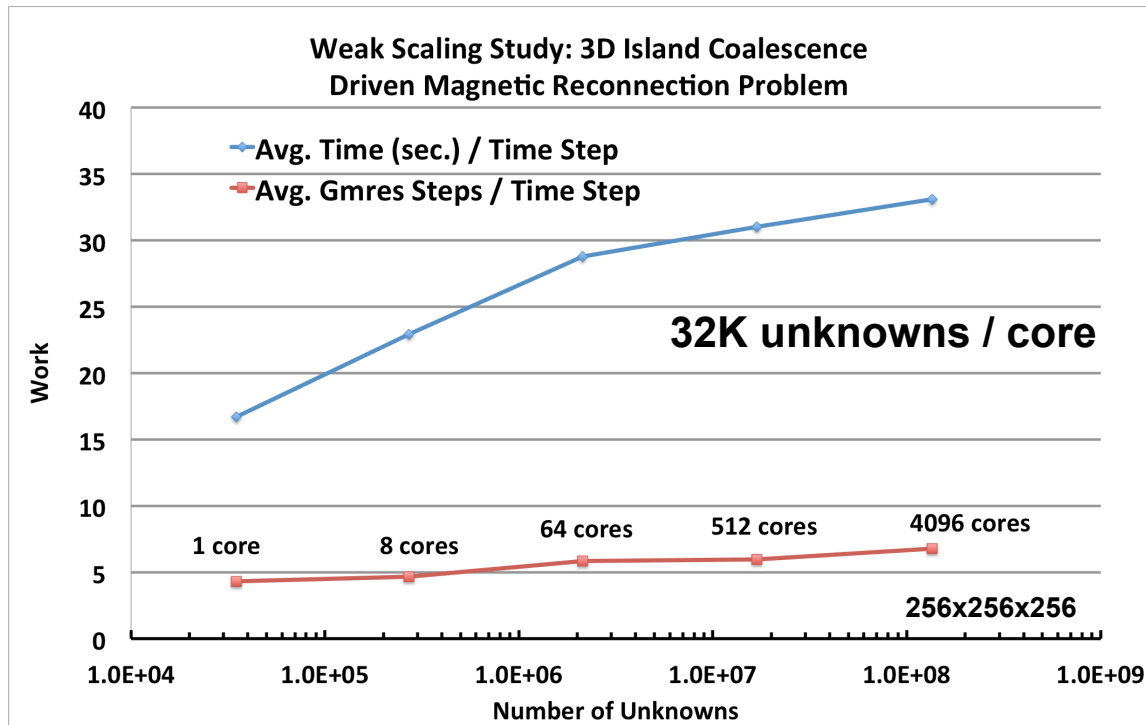
Initial Scaling Study for Cray XK7.

3D Hydromagnetic Kelvin-Helmholtz Instability

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



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



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, $dt = 0.0333$.

Highlight: Scalable FC-AMG and ABF Preconditioning for resistive MHD

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

Resistive MHD Model in Residual Notation

$$\begin{aligned}
 \mathbf{R}_u &= \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot [\rho \mathbf{u} \otimes \mathbf{u} - (\mathbf{T} + \mathbf{T}_M)] + 2\rho \Omega \times \mathbf{u} - \rho \mathbf{g} = \mathbf{0}; & \mathbf{T} &= - \left(P + \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \right) \mathbf{I} + \mu [\nabla \mathbf{u} + \nabla \mathbf{u}^T] \\
 R_P &= \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 & \mathbf{T}_M &= \frac{1}{\mu_0} \mathbf{B} \otimes \mathbf{B} - \frac{1}{2\mu_0} \|\mathbf{B}\|^2 \mathbf{I} \\
 R_e &= \frac{\partial(\rho e)}{\partial t} + \nabla \cdot [\rho \mathbf{v} e + \mathbf{q}] - \mathbf{T} : \nabla \mathbf{v} - \eta \left\| \frac{1}{\mu_0} \nabla \times \mathbf{B} \right\|^2 = 0 \\
 \mathbf{R}_B &= \frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot [\mathbf{u} \otimes \mathbf{B} - \mathbf{B} \otimes \mathbf{u} - \frac{\eta}{\mu_0} (\nabla \mathbf{B} - (\nabla \mathbf{B})^T) + \psi \mathbf{I}] = \mathbf{0} & \mathbf{B} &= \nabla \times \mathbf{A} \\
 R_\psi &= \nabla \cdot \mathbf{B} = 0 & R_{A_z} &= \frac{\partial A_z}{\partial t} + \mathbf{u} \cdot \nabla A_z - \frac{\eta}{\mu_0} \nabla^2 A_z + E_z^0 = 0.
 \end{aligned}$$

$\xrightarrow{2D}$

We consider a primitive variable discretization for incompressible, low flow-Mach number approximations, anelastic approx. and low flow-Mach number compressible flows

General Structure of Newton System:

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

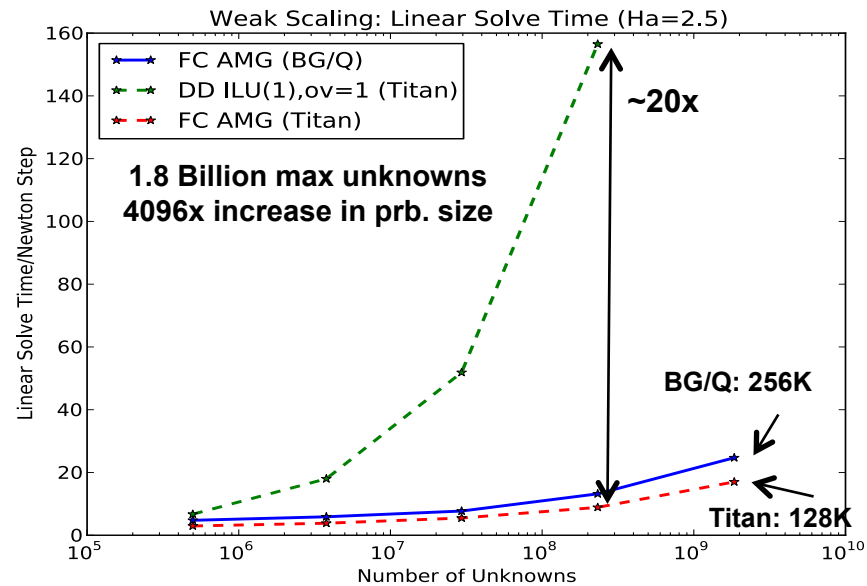
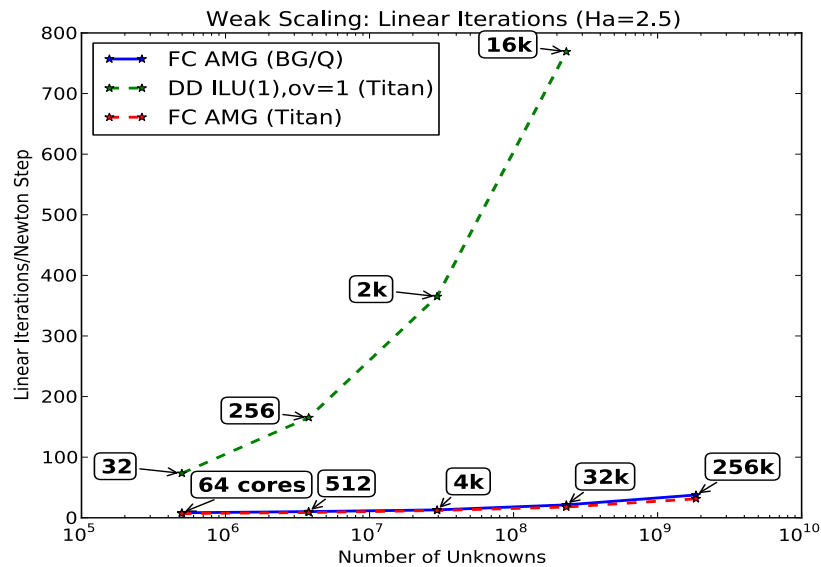
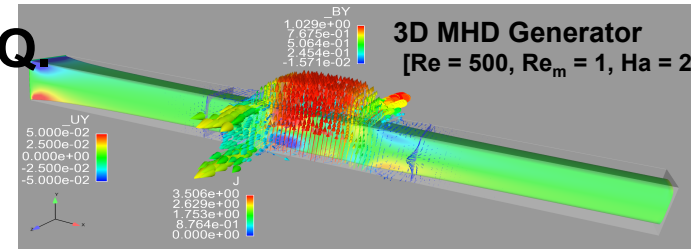
Note: For non-stabilized form

Incompressible, low-flow Mach
approximation $C_u = 0$

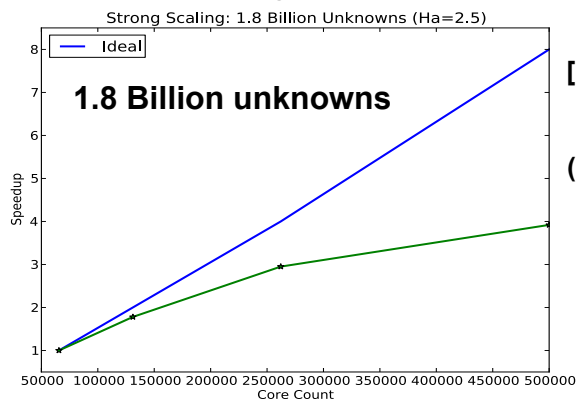
Elliptic constrained generalized
Lagrange multiplier $C_B = 0$

Initial Scaling Studies for Cray XK7 AND BG/Q.

SFE, Q1 interpolation, $\square\square\square\square$; C_u and C_B weighted
Laplacian matrix;

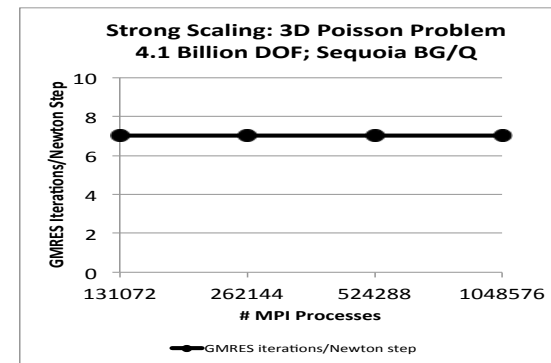


MHD Recently run on 1/2 M cores of BG/Q



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

4 Billion element/unknown Solution of Poisson Eq. 1M cores



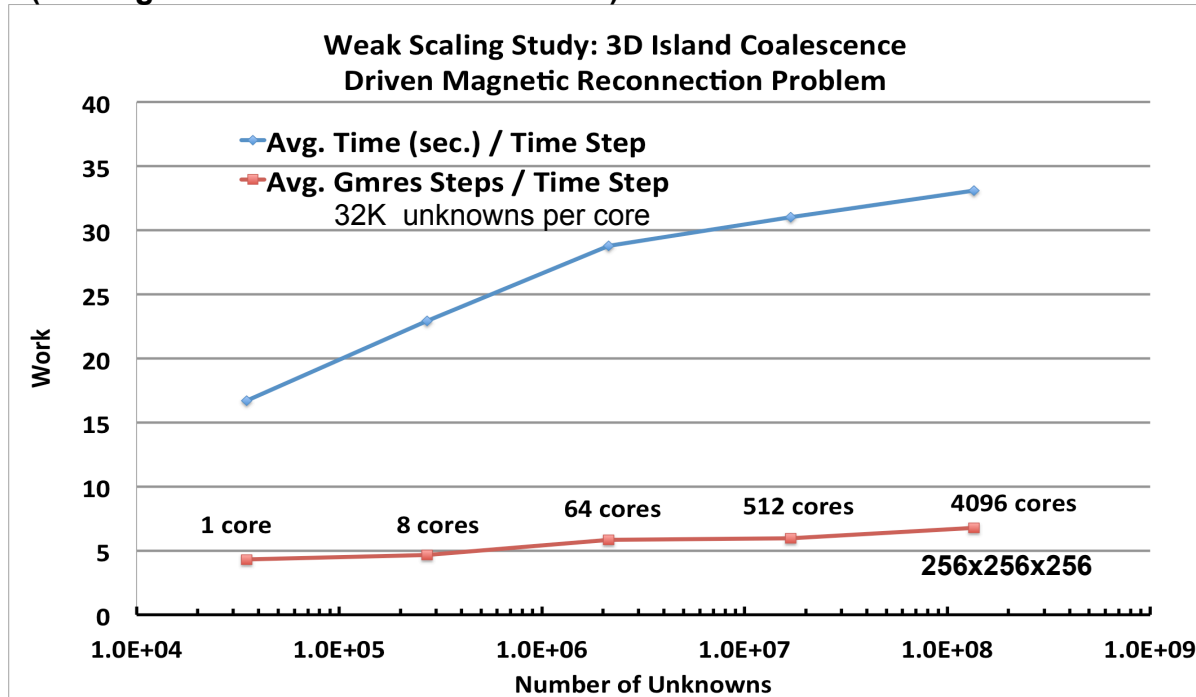
Shadid, Pawlowski, Cyr, Tuminaro, Chacon, Scalable Implicit 3D Resistive MHD with
Stabilized FE Methods and Fully-coupled Multilevel Preconditioners, in preparation

(DOE/ORNL Titan Cray XK7: Joule Metric)



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

(Scaling of total time with I/O included)

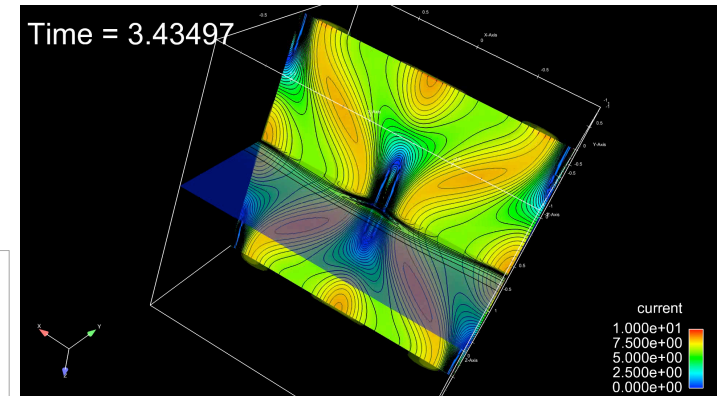


Analysis (coarse graph-based aggregation):

- Sala; *Math. Modeling and Numer. Anal.*, 2004
- Sala, Shadid, Tuminaro; *SIAM J. Matrix Analysis*, 2006

Numerical Studies for NS, TR and MHD Systems:

- Shadid et. al. *CMAME.*, 2006
- Lin, Sala, Shadid, Tuminaro; *IJNME* 2006
- Lin, Shadid, Tuminaro, Marzio Sala, *IJNME* 2010
- Lin, Shadid, et. al. *IJNMF* 2010
- Shadid, Pawlowski, Banks, Chacon, Lin, Tuminaro, *JCP* 2010
- Lin, *IJNME*, 2012
- Cyr, Shadid and Tuminaro, *JCP* 2012
- Shadid, Pawlowski, Cyr, Tuminaro, Chacon, 2014, in preparation



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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.

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: 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:

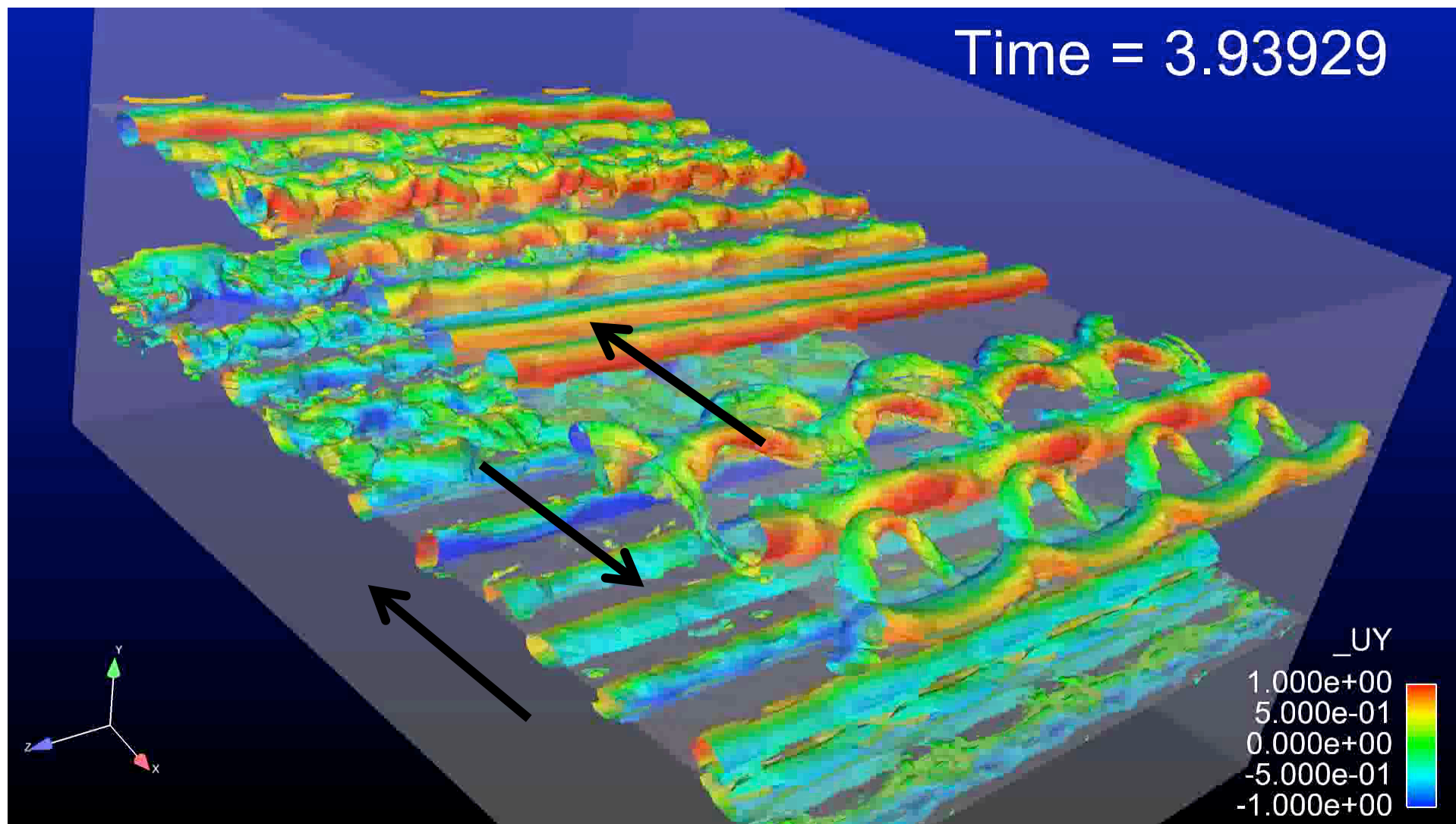
Physics-based: Understand stiff physics, develop asymptotic analytic analysis to simplified system(s) while approximating critical operators to maintain stiff coupling in approximate Schur complement(s)

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)

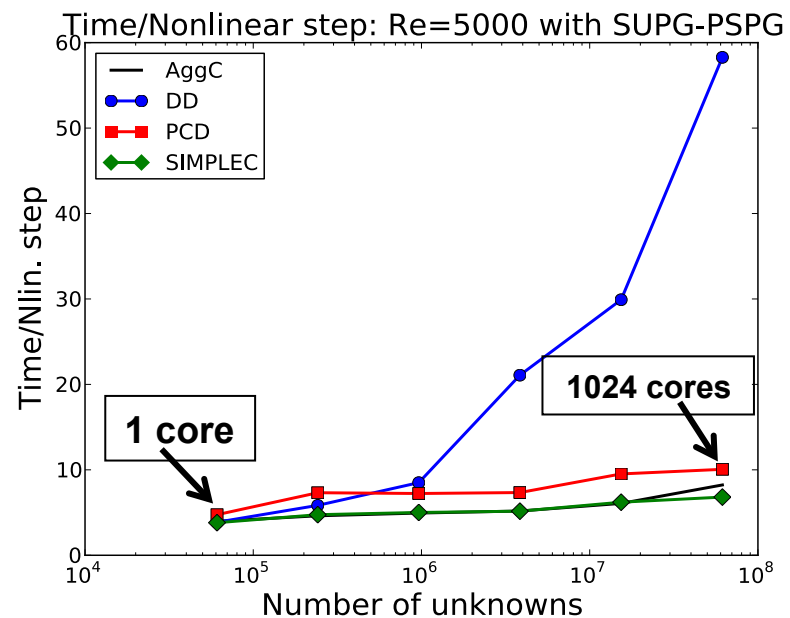
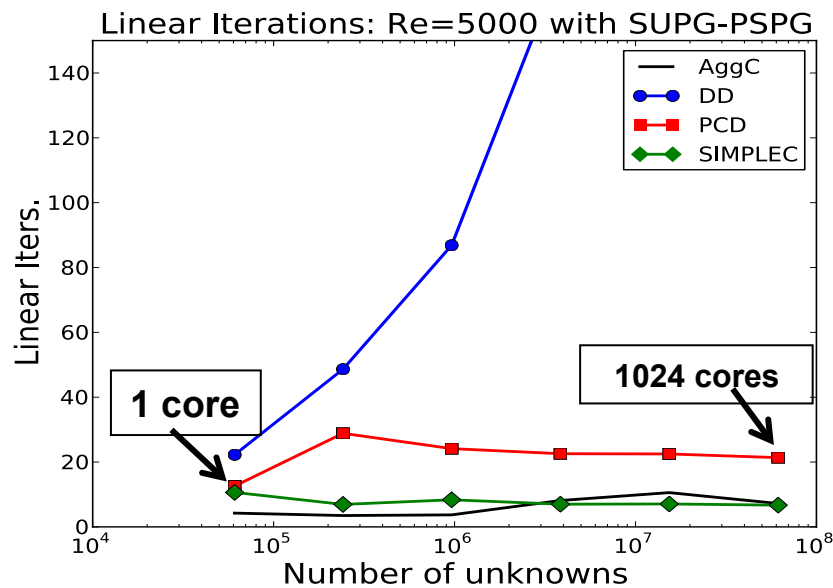
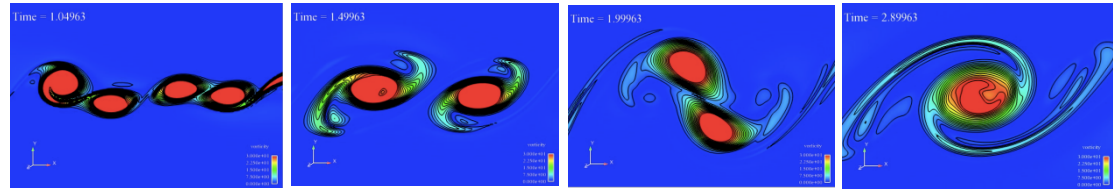
Step back to CFD for a moment to

Introduce block approximate factorization (physics-based) preconditioners

**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)

Now Return to MHD

Block approximate factorization (physics-based) preconditioners

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

E.g. Primitive-Variable MHD a New Nested Schur Complement (2D vector potential)

1) Fully-implicit enables solution of incompressible, anelastic, low-Mach approximation, low-flow Mach compressible systems. However physics coupling is challenging

e.g. Mixed FE,
Staggered FV for other
than compressible

$$\begin{bmatrix} F & B^T & Z \\ B & 0 & 0 \\ Y & 0 & D \end{bmatrix}$$

e.g. Stabilized FE, or
compressible

$$\begin{bmatrix} F & B^T & Z \\ B & C & 0 \\ Y & 0 & D \end{bmatrix}$$

2) Consider Block LU factorization

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

where

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

(C⁻¹ doesn't need to exist)

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

- 3x3 system leads to embedded Schur complements (embedding is independent of ordering)
- How are S and P to be effectively approximated?
- Straight forward approach: approximate operators in Schur complement to produce diagonal inverses
- Use alternate approximate block factorizations (ABF)

Overview of more Detailed Mathematical Analysis of Residual-based Defect-Correction ABF Preconditioner

- 1) Developed a new residual defect-correction factorization procedure that strongly couples operators producing the Alfven wave and reduces to two 2x2 blocks for the ABF:

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

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

- 2) Our previous extensive work for NS Schur complement lead to evaluated and developed diagonal (Pressure Proj., SIMPLE(R)), Press-Conv-Diff (PCD) and Least Squares comutator (LSC) type approaches for

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

Pressure Projection: $\mathcal{S} = -B\hat{F}^{-1}B^T \approx -B(\Delta t)IB^T \approx -(\Delta t)L$

Press-Conv-Diff (PCD): $\mathcal{S} = -B\hat{F}^{-1}B^T \approx -F_P^{-1}BB^T \approx -F_P^{-1}L$

Overview of more Detailed Mathematical Analysis of Residual-based Defect-Correction ABF Preconditioner

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- 2) Our previous extensive work for NS Schur complement lead to evaluated and developed diagonal (SIMPLE), Press-Conv-Diff (PCD) and Least Squares comutator (LSC) type approaches for

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

- 3) Additionally the similar structure of S and P, an order-of-magnitude analysis and a stiff-wave analysis of the momentum-magnetics sub-block carried out, suggested diagonal, comutator, and LSC approaches for

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

- 4) Analysis of the Spectrum for our New residual-based defect-correction primitive-variable MHD Preconditioner.

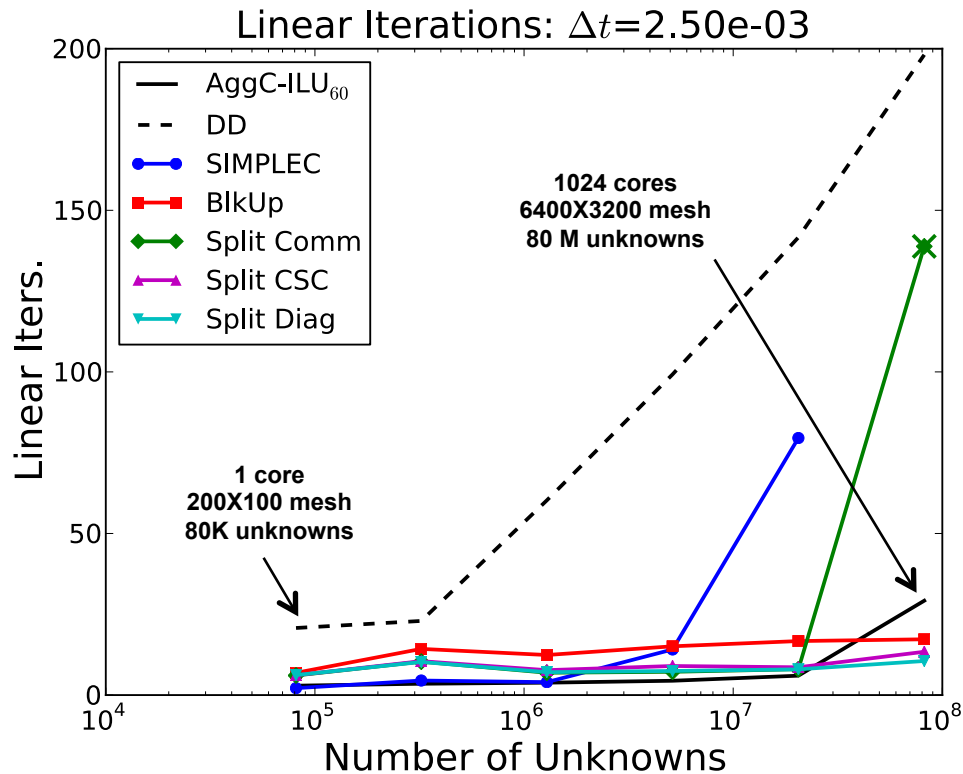
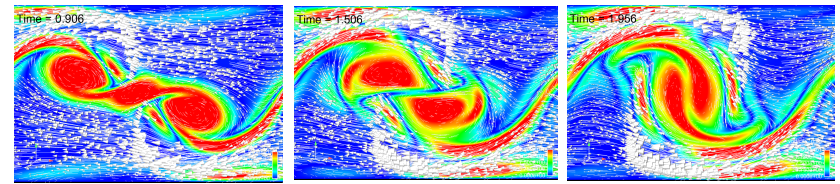
$$\begin{bmatrix} F & B^T & Z \\ B & C & 0 \\ Y & 0 & D \end{bmatrix} \begin{bmatrix} F & B^T \\ B & C \\ & & I \end{bmatrix}^{-1} \begin{bmatrix} F & & \\ & I & \\ & & I \end{bmatrix} \begin{bmatrix} F & & Z \\ & I & \\ Y & & D \end{bmatrix}^{-1} = \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ K_u & K_p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

Mathematical Analysis:

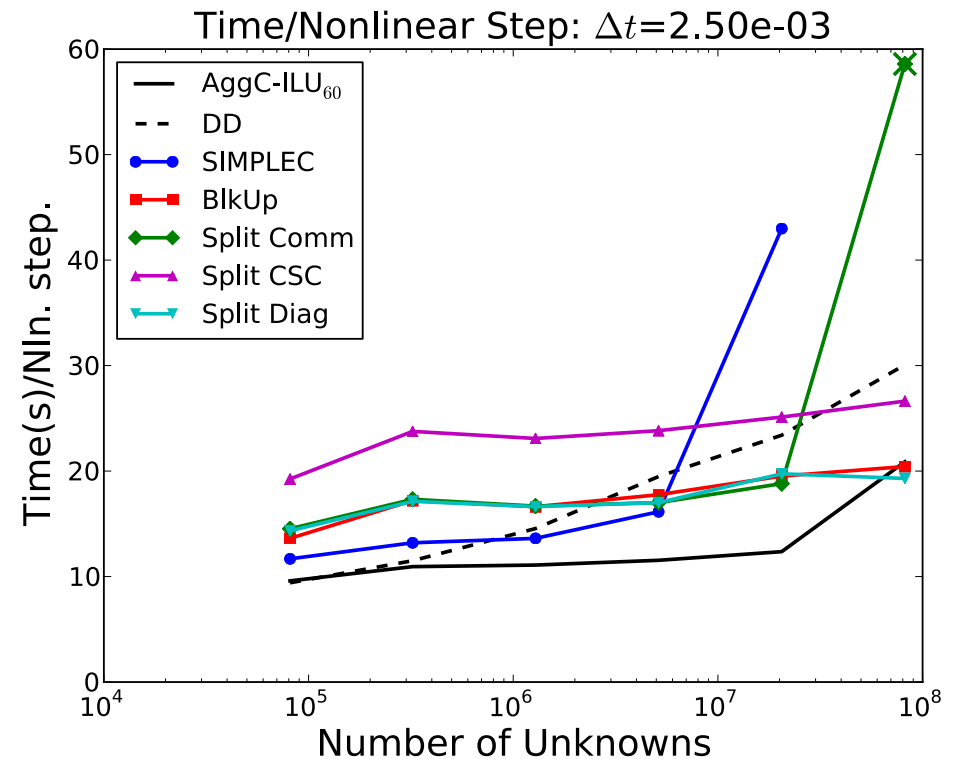
- Derivation of prec. operator above implies large number of e-values equal to unity.
- A combined analytical and numerical study of spectrum carried out. Result indicated encouraging bound on eigenvlaue spectrum. Confirmed with numerical results.

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.



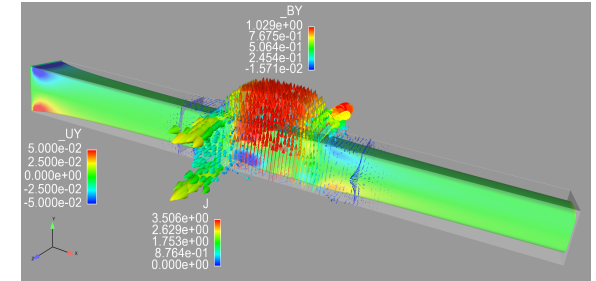
Quad-core Nehalems with Infini-band SNL Red Sky

Cyr, Shadid, 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

E. C. Cyr, J. N. Shadid, and R. S. Tuminaro, "Teko an abstract block preconditioning capability with concrete example applications to Navier-Stokes and resistive MHD," in preparation, 2013.

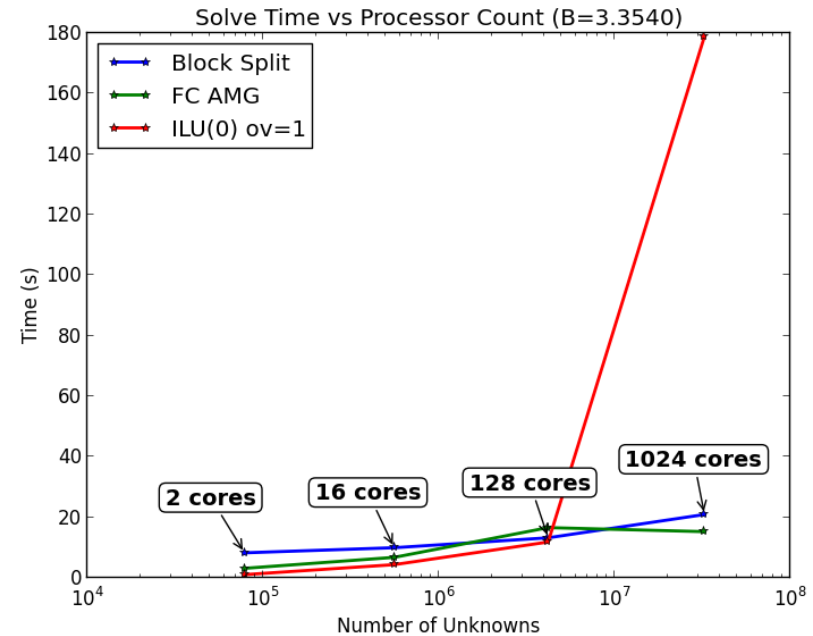
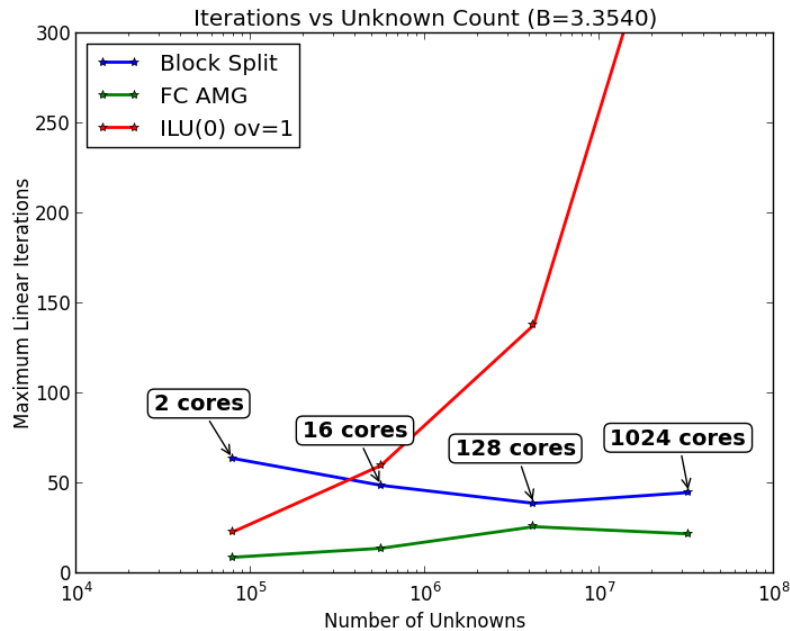


Extensions to 3D: Initial Approximate Block Preconditioning 3D MHD Generator [Re = 500, Re_m = 1, Ha = 2.5], SFE



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

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



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

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

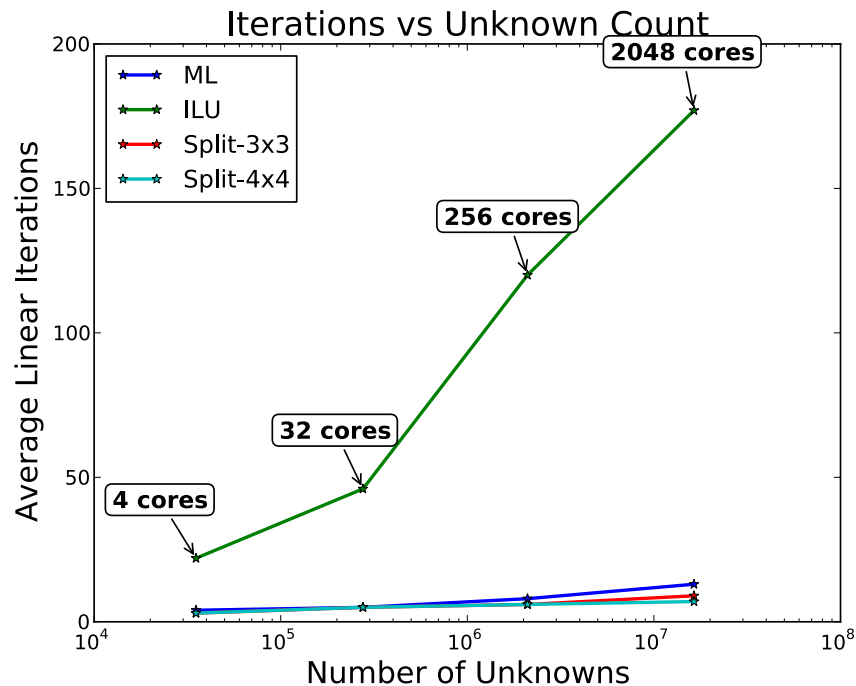
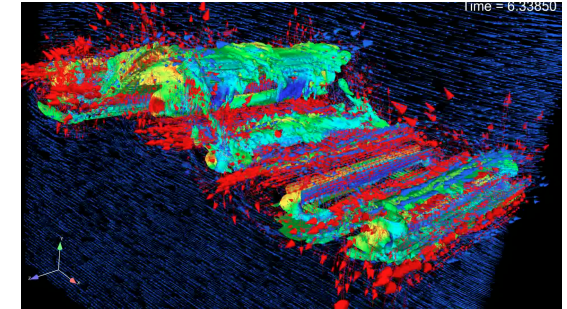
$M_1 \tilde{x} = b$; $M_2(\hat{x} - \tilde{x}) = (b - \mathcal{J}\tilde{x})$; leads to this ABF $\hat{x} = M_2^{-1}(M_1 + M_2 - \mathcal{J})M_1^{-1}b$

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

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

- 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 $P = F_B - Y\hat{F}_m^{-1}Z$
- Eigen-structure analysis to be carried out.

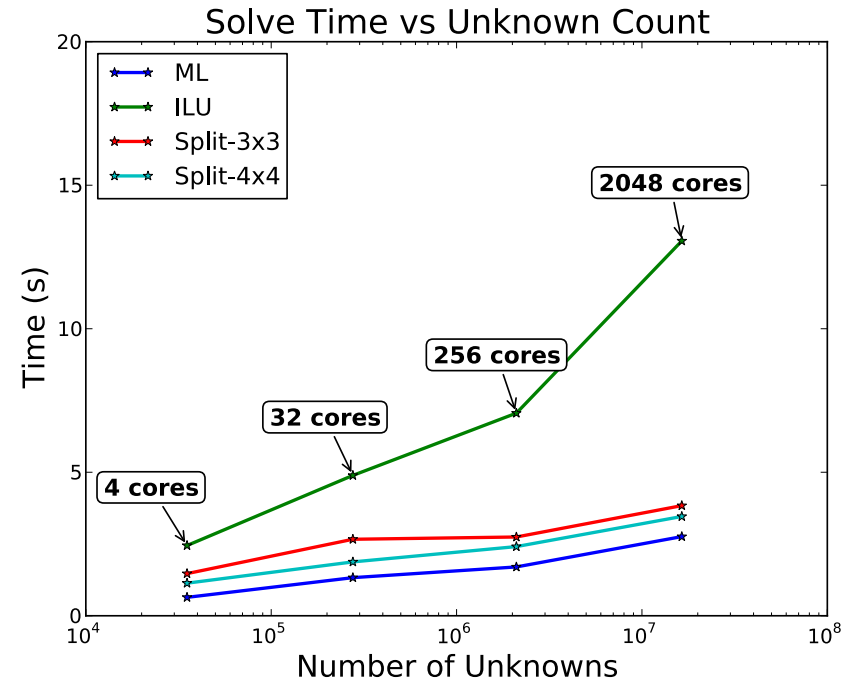
Extensions to 3D: Initial Approximate Block Preconditioning
3D HMKH [Re =10⁴, Rem=10⁴, MA = 3; CFL ~0.125], SFE
FC-AMG – ILU(0), V(3,3); 3x3, 4x4 SIMPLEC and Gauss-Seidel



Fully coupled Algebraic

ML: Uncoupled AMG with repartitioning

DD: Additive Schwarz Domain Decomposition



Block Preconditioners

Split-3x3: 3x3 (SIMPLEC everywhere)

Preliminary Split-4x4: 4x4

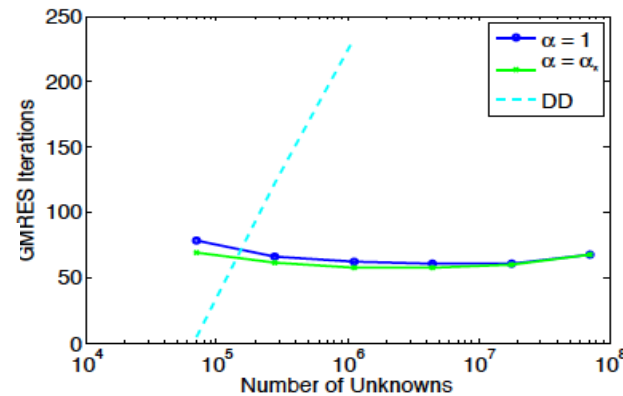
ABF preconditioners scale algorithmically, more relevant for mixed and physics-compatible discretizations

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

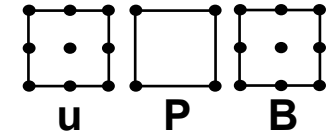
Exact Penalty Formulation: (Q2/Q1 Navier-Stokes, Q2 B field; see e.g. Gunzburger)

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

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



Mixed basis*:



Phillips, Elman, Cyr, Shadid, Pawlowski, A Block Preconditioner for an Exact Penalty Formulation for Stationary MHD, submitted to SISC

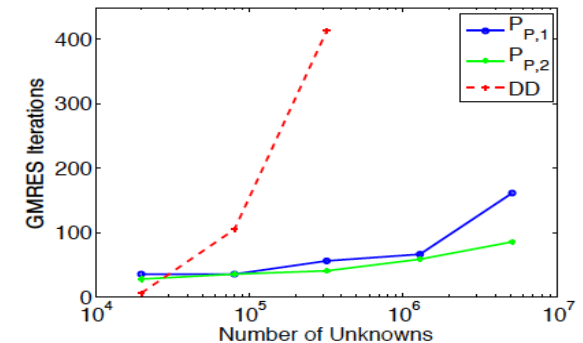
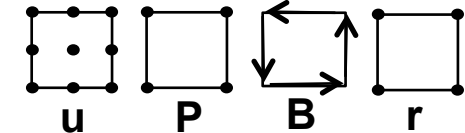
Shotzau Formulation: (Q2/Q1 Navier-Stokes, B -edge, Q1 Lagrange Multiplier)

Structure of preconditioner and Maxwell ABF

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

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

Mixed basis*:



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



Focus on Nonlinear contributions to flux terms: VMS induced cross term fluxes (sub-grid to resolved scales)

$$\mathcal{N}_{\mathbf{v}}^{(1)} = \rho (\mathbf{v}^h \otimes \mathbf{v}'$$

$$\mathcal{N}_{\mathbf{B}}^{(1)} = (-\mathbf{v}^h \otimes \mathbf{B}' + \mathbf{B}' \otimes \mathbf{v}^h)$$

Used as VMS FE MHD turbulence model with Assad Oberai, David Sondak (RPI)

- Includes subgrid effects ($\mathbf{u}'$)
- Allows for the possibility of local inverse energy cascade
- Cross stresses ($\mathbf{u}^h \otimes \mathbf{u}'$) well-represented
(Wang and Oberai 2010)
- Reynolds stresses ($\mathbf{u}' \otimes \mathbf{u}'$) not adequately modeled
(Wang and Oberai 2010)
⇒ Eddy viscosity model?
- Mix the VMS models with an eddy viscosity model

$$\mathcal{A}(\mathbf{W}^h, \mathbf{u}^h + \mathbf{u}') + (\nabla^s \mathbf{w}^h, 2\nu_T \nabla^s \mathbf{u}^h) + (\nabla^a \mathbf{c}^h, 2\lambda_T \nabla^a \mathbf{B}^h) = (\mathbf{W}^h, \mathbf{F}^h)$$

Eddy diffusivities

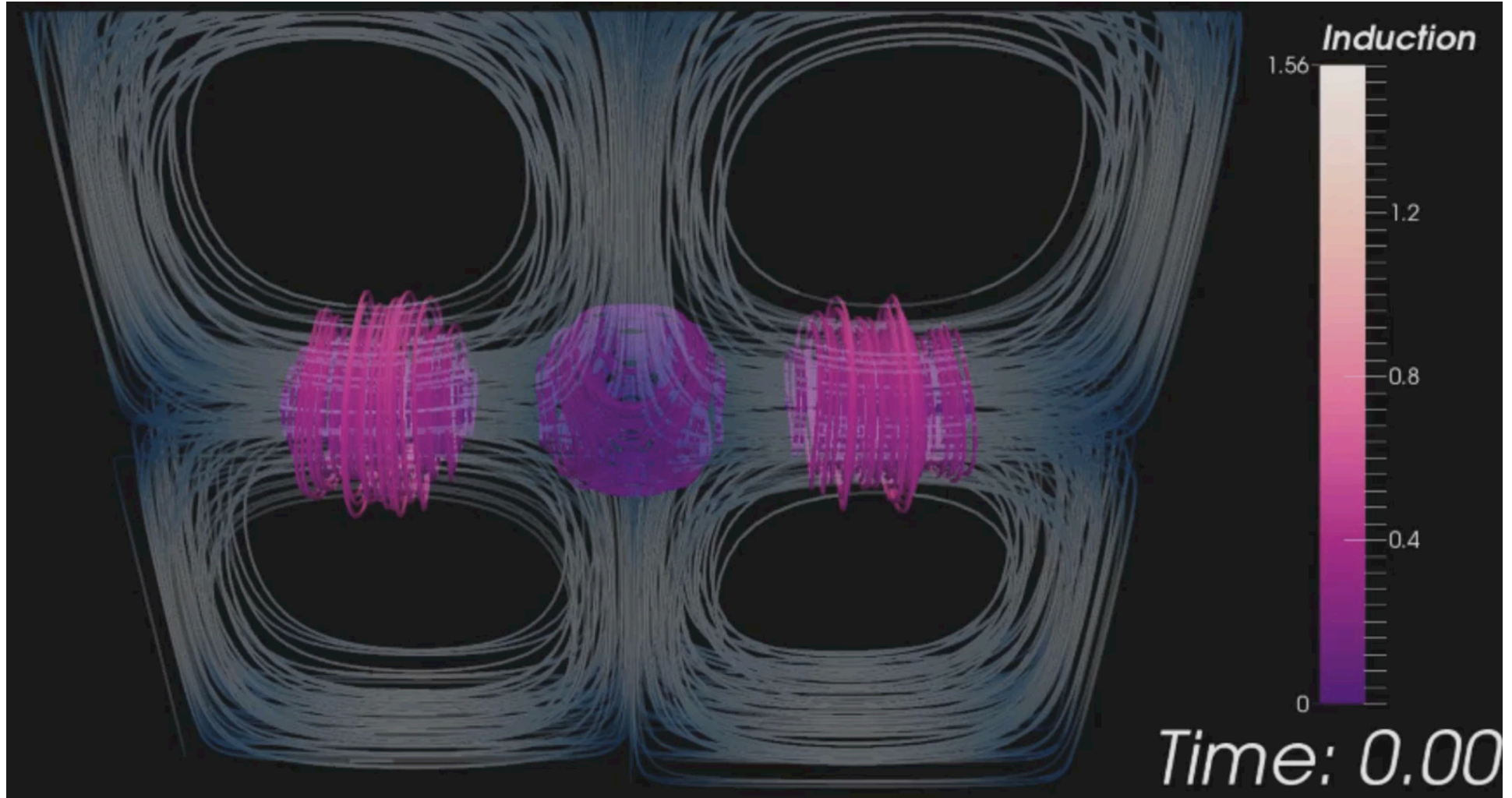
$$\nu_T = \lambda_T = \overline{C} h \sqrt{|\mathbf{u}'|^2 + \frac{1}{\mu_0 \rho} |\mathbf{B}'|^2}, \quad \overline{C} = 0.0398$$

Oberai and Sondak, Spectral
VMS MHD Turbulence, 2012



MHD Turbulence Modeling

Taylor–Green MHD Vortex Decay: $Re = 5100$ (Drekar FE VMS Resistive MHD Model)



With:

Prof. Assad Oberai (RPI),

David Sondak (DOE Office of Science Graduate Fellowship, recent Ph. D. – RPI)



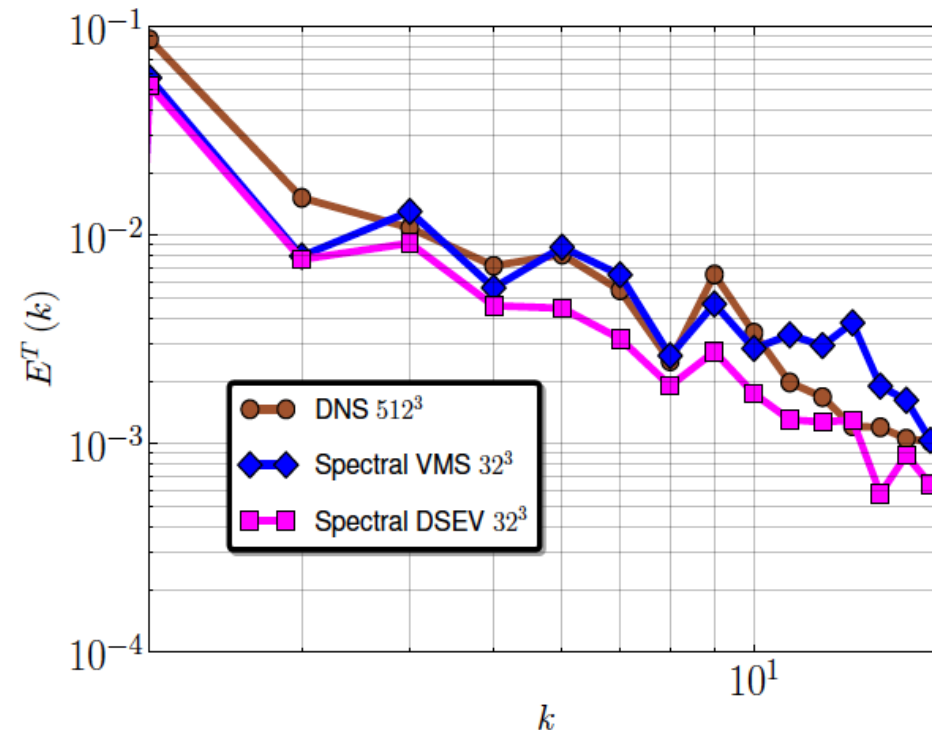
Homogeneous, Isotropic Turbulence

VMS Spectral Method

- Momentum and induction cross correlation terms
- Periodic boundary conditions
⇒ Only nonlinear terms
- Adds to stability of method

Further Explorations

- Detailed turbulence statistics
- Subgrid dynamo and VMS
- Helical flows
- Vary Pr_m



The VMS-based model performs very well. The dynamic Smagorinsky model is overly dissipative.

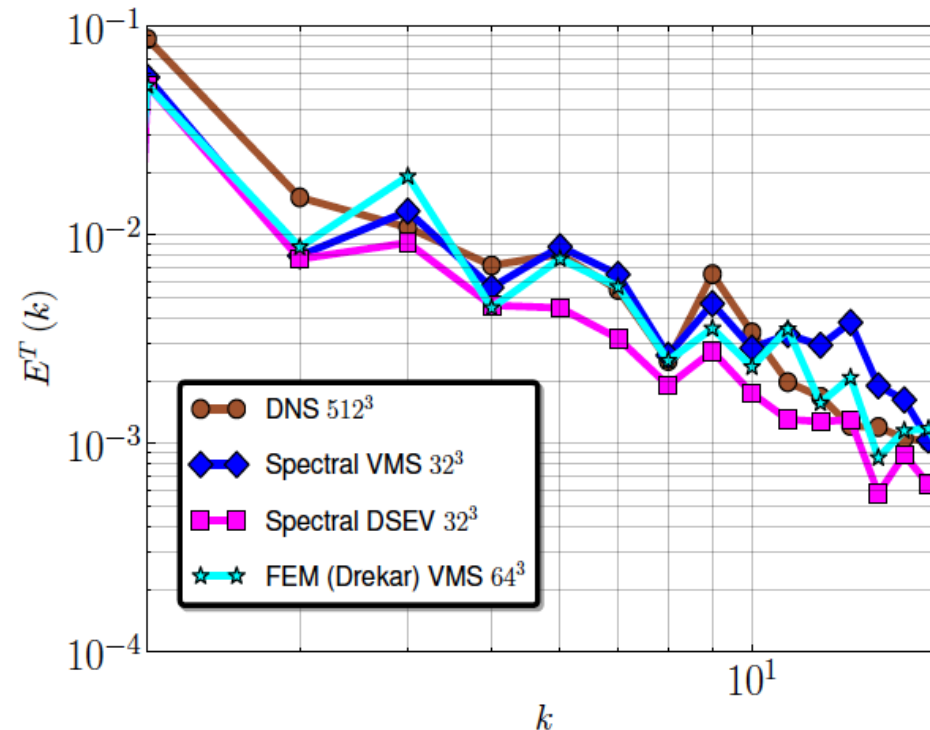
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- Vary Pr_m



The FEM solution with linear elements using the VMS model also performs very well.

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, ..])**
{Talks by Eric Cyr, Howard Elman, Edward Phillips}
 - **Initial scaling of NK/FC-AMG linear solver to near extreme-scale (256K, 1/2 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 systems (w/Oberai, Sondak – RPI).

Recent Related Publications:

- J. N. Shadid, R. P. Pawlowski, J. W. Banks, L. Chacon, P. T. Lin, R. S. Tuminaro, “Towards a Scalable Fully-Implicit Fully-coupled Resistive MHD Formulation with Stabilized FE Methods”, JCP, 229, 20, 7649 – 7671, 2010
- Paul T. Lin, John N. Shadid, Ray S. Tuminaro, Marzio Sala, Gary L. Hennigan, Roger P. Pawlowski, “A Parallel Fully-Coupled Algebraic Multilevel Preconditioner Applied to Multiphysics PDE Applications: Drift-diffusion, Flow/transport/reaction, Resistive MHD”, IJNMF, Volume 64, issue 10-12, pp 1148-1179, (2010)
- P. T. Lin, and J. N. Shadid, “Multi-socket/Multicore Parallel Performance of Semiconductor Device Simulations using MPI-only”, JCP, 229, pp. 6804-6818, 2010
- P. T. Lin, J. N. Shadid, M. Sala, R. S. Tuminaro, “Performance of a Petrov-Galerkin Algebraic Multilevel Preconditioner for Finite Element Modeling of the Semiconductor Device Drift-Diffusion Equations”, Int. J. Num. Meth. Eng., 84, 448 – 469, 2010
- E. C. Cyr, J. N. Shadid, R. S. Tuminaro, R. P. Pawlowski, and L. Chacon, “A new approximate block factorization preconditioner for 2D incompressible (reduced) resistive mhd,” 35:B701-B730, 2013
- E. Cyr, J. N. Shadid, and T. Wildey, “A Posteriori Analysis of Stabilized Finite Element Methods”, (in revision for SISC).
- Chaudhry, Estep, Ginting, Shadid, Tavener, Adjoint based a posteriori analysis of IMEX time integration schemes for partial differential equations, Submitted to SISC
- E. C. Cyr, J. N. Shadid, and T. Wildey, Efficient Backward-in-time Adjoint Integration Employing Data Compression, (in preparation)
- J. N. Shadid, R. P. Pawlowski, Dana Knoll, Luis Chacon, Paula Weber, Eric Cyr, “High Lundquist number plasmoid instability in the driven magnetic reconnection island coalescence problem”, (in preparation)

The End