SAND2022-6857C

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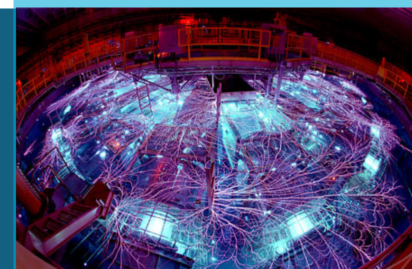
# Scalable Solution of Implicit Continuum Models for Challenging Plasma Physics Systems



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U.S. DEPARTMENT OF ENERGY Office of Science

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# Collaborators

## Long-time-scale Collaborators:

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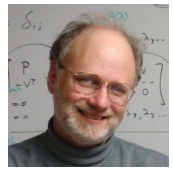
Ray Tuminaro

Luis Chacon: (LANL)



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## Current Research Team:

Jesus Bonilla
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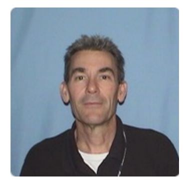
Sidafa Conde

Michael Crockatt

Peter Ohm (PD)

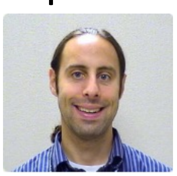
Edward Phillips



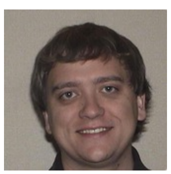
Tom Smith

Ignacio Tomas (PD)

## Important Past Collaborators:



Eric Cyr



Sean Miller
(AMD)

Sibu Mabuza
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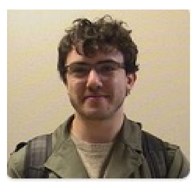


Ari Rappaport
(Ph.D student Inria Paris
and Sorbonne Université )

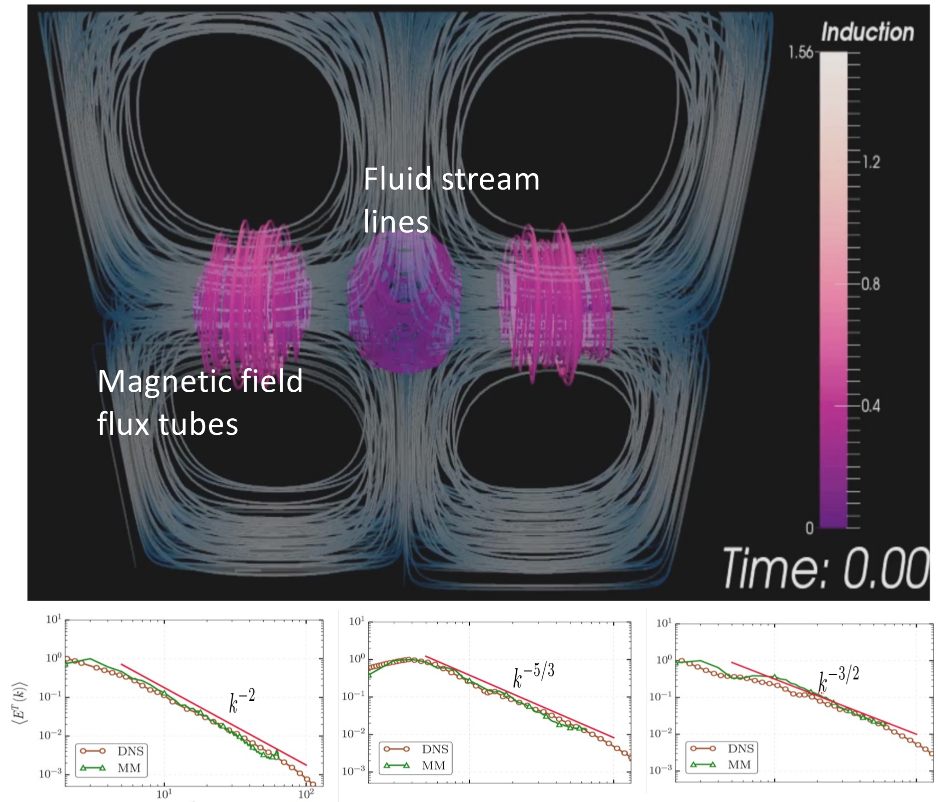
# Outline

- General Scientific and Mathematical/Computational Motivation
- Comments on Multiple-time-scale Plasma Systems
  - Magnetic Confinement Fusion: Tokamak Device
  - Magnetic Inertial Fusion: Z-pinch (not discussed but a strong motivation)
- Brief Description of Continuum PDE Models (Kinetic, Navier-Stokes (NS), MHD, multifluid plasma)
- Why Newton-Krylov Methods and Implicit/IMEX Time Integration?
- Illustrations of Scalable Solution
  - CFD
    - Fully-coupled system AMG (Stabilized Continuous Galerkin [CG] FE)
  - Resistive MHD
    - Fully-coupled system AMG (Stabilized Continuous Galerkin [CG] FE)
    - Approximate Block Factorization & AMG sub-block solvers (CG FE Structure Preserving discretizations)
  - Multifluid EM Plasmas (Approximate Block Factorization & AMG sub-block solvers)
- Preliminary Results for Tokamak Related Simulations (if time permits)
- Concluding Remarks

# Motivation: Science/Technology

***Resistive and extended MHD models are used to study important multiple-time/ length-scale multiphysics plasma physics systems***

- **Astrophysics and Planetary-physics:**
  - **Magnetic reconnection, instabilities,**
  - **Solar flares, Coronal Mass Ejections.**
  - **Earth's magnetospheric sub-storms,**
  - **Aurora, Planetary-dynamos.**
- **Fusion & High Energy Density Physics:**
  - **Magnetic Confinement [MCF] (e.g. ITER),**
  - **Inertial Confinement [ICF] (e.g. Z-pinch, NIF).**




**MHD VMS–LES MHD Turbulence Modeling Taylor-Green Vortex Decay. Illustration of non-universality of total MHD energy turbulent decay spectrum [with D. Sondak (Harvard), A. Oberai (USC)]**

## General Mathematical / Computational Science Motivation:

***Achieving Roust Scalable Simulations of Strongly Coupled Nonlinear Multiple-time-scale Multiphysics Systems to Enable***

- Predictive, Accurate, and Efficient Longer Time-scale Computational Simulations
- Beyond Forward Simulation: Design/Optimization/UQ
- Physics / Mathematical Model Validation, Experimental Data Interpretation & Inference

# 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,**

Explicit methods

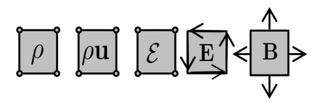
- **consist of a set of widely separated time-scales that produce a stiff system response,**
- **nearly balance to evolve system on dynamical time-scales that are long relative to component time scales,**
- **or balance to produce steady-state behavior.**

Some implicit aspect required

**E.g. Fusion Reactors (Tokamak -ITER; Pulsed - NIF & Z-pinch); Fission Reactors (GNEP); Astrophysics; Combustion; Chemical Processing; Fuel Cells; etc.**

# *Our Mathematical Approach - develop:*

- **Stable, higher-order accurate implicit/IMEX formulations for multiple-time-scale systems**
- **Stable and accurate unstructured FE spatial discretizations. Options enforcing key mathematical properties (e.g. structure preserving forms: div B = 0; positivity $\rho$ , P; DMP)**

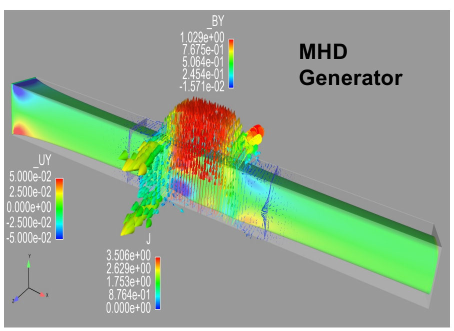


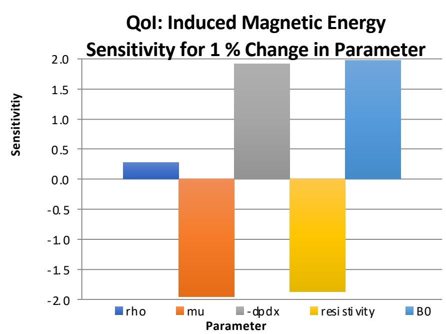

Structure Preserving FE

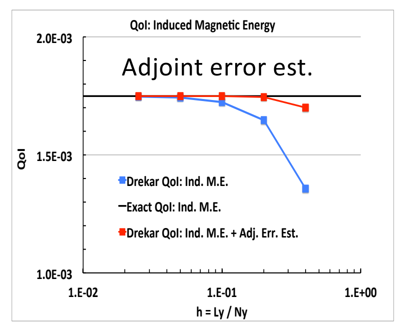
- **Robust, efficient fully-coupled nonlinear/linear iterative solution based on Newton-Krylov methods**
- ***Scalable and efficient multiphysics preconditioners utilizing physics-based and approximate block factorization/Schur complement preconditioners with multi-level (AMG) sub-block solvers***

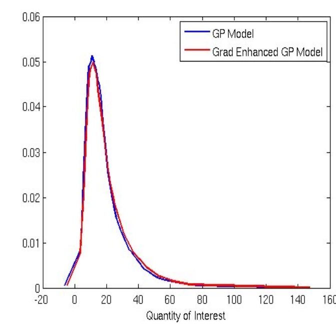
**=> Also enables beyond forward simulation: Design/Optimization/UQ ( e.g. Adjoints - error estimates, sensitivities; surrogate modeling (E.g. GP), …)**

[e.g. Steady state adjoint analysis of MHD duct flows; Hartmann problem, MHD Generator]



# E.g. Multiple-time-scale Multiphysics System: Magnetic Confinement Fusion

<u>Goal for Fusion Device:</u>

- Attempt is to achieve temperature of ~100M deg K (6x Sun temp.) ,
- Energy confinement times O(1 - 10) min. are desired.
- Understanding and controlling instabilities/disruptions in plasma confinement is critical

**Strong external magnetic fields used for:**

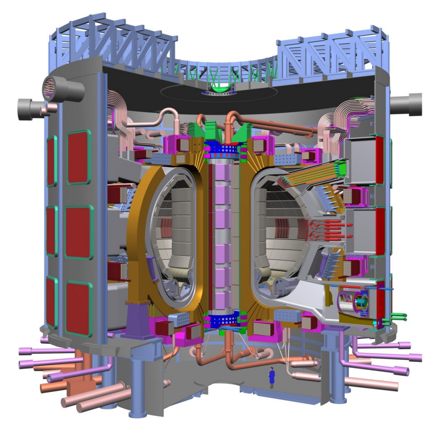
- Resistive heating of the plasma (along with RF-EM waves, ..)

- Confinement of the hot plasma to keep it from striking the wall

  - Plasma disruptions can cause break of confinement, huge plasma thermal energy loss, and discharge of very large electrical currents (~20MA) to surface and damage the device.

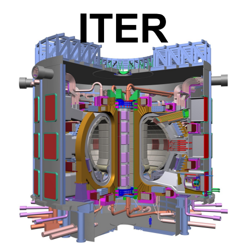
  - ITER can sustain only a limited number of significant disruptions, O(1 – 5).

(ITER)

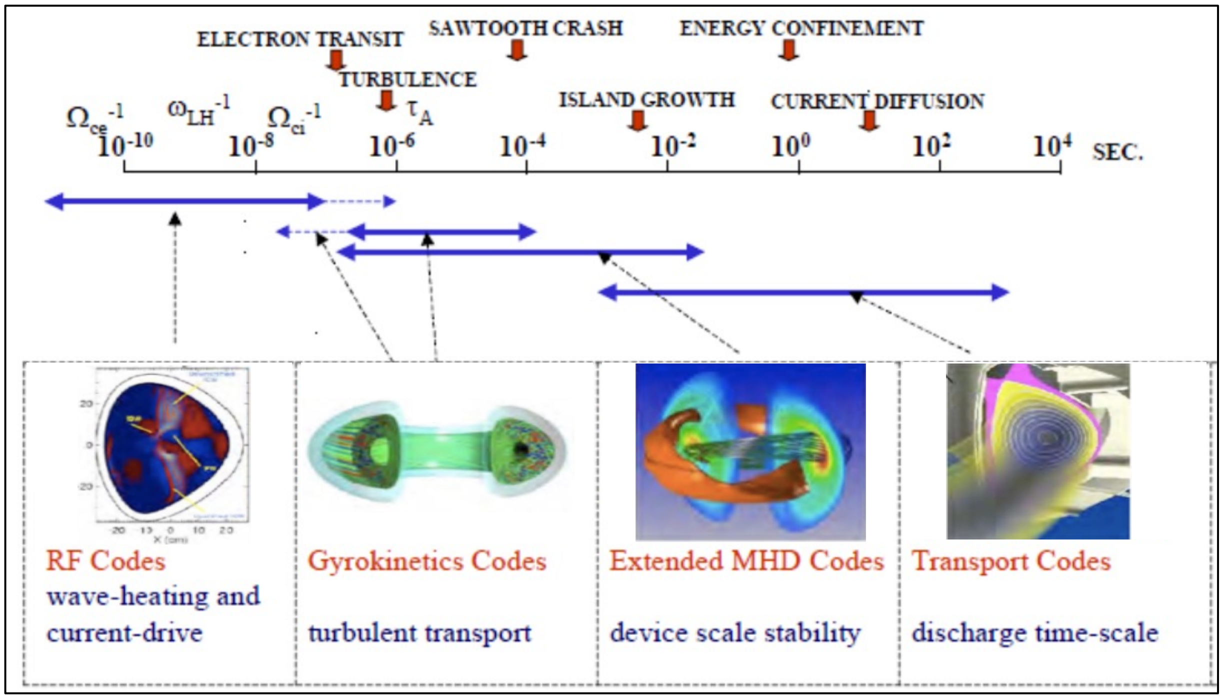


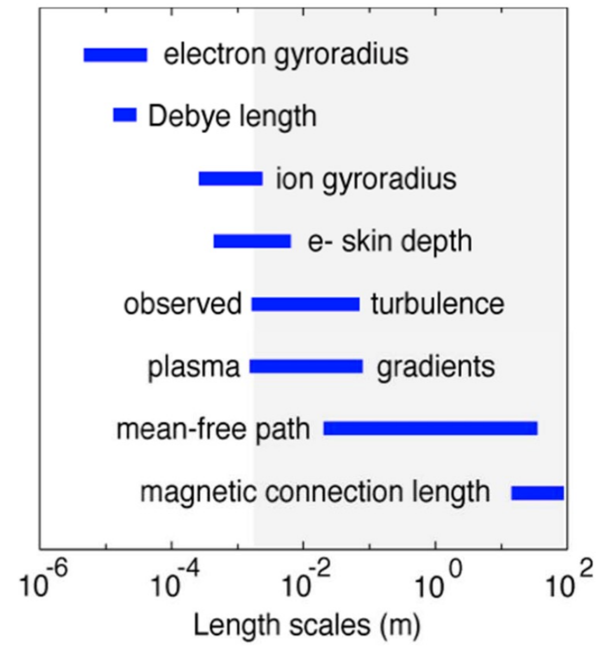
International Thermonuclear Experimental Reactor [under construction, Cadarache facility France]

# E.g. Multiple-time-scale Multiphysics System: Magnetic Confinement Fusion (MCF)



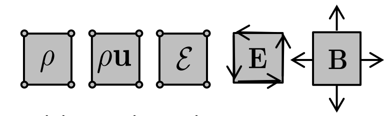

**MCF Devices (e.g. ITER) are characterized by large-range of time and length-scales**




**DOE Office of Science ASCR/OFES Reports: Fusion Simulation Project Workshop Report, 2007, Integrated System Modeling Workshop 2015**

# 5 Moment Full Maxwell EM Multifluid Plasma Model: Multiple Atomic Species [e.g. structure preserving formulation]




Nodal FE Hydro and Structure-preserving discretization for EM

| | **Conservation / Balance Eqn.** |
|---|---|
| Mass[0] | $\partial_t \rho_s + \nabla \cdot (\rho_s \mathbf{u}_s) = \mathcal{C}_s^{[0]} + \mathcal{S}_s^{[0]}$ |
| Momentum[1] | $\partial_t (\rho_s \mathbf{u}_s) + \nabla \cdot (\rho_s \mathbf{u}_s \otimes \mathbf{u}_s + p_s \underline{\mathbf{I}} + \underline{\boldsymbol{\Pi}}_s) = q_s n_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) + \boldsymbol{\mathcal{C}}_s^{[1]} + \boldsymbol{\mathcal{S}}_s^{[1]}$ |
| Total Energy[2] | $\partial_t \mathcal{E}_s + \nabla \cdot [(\mathcal{E}_s + p_s)\mathbf{u}_s + \mathbf{u}_s \cdot \underline{\boldsymbol{\Pi}}_s + \mathbf{h}_s] = q_s n_s \mathbf{u}_s \cdot \mathbf{E} + \mathcal{C}_s^{[2]} + \mathcal{S}_s^{[2]}$ |
| Charge / Current | $q = \sum_s q_s n_s$     $\mathbf{J} = \sum_s q_s n_s \mathbf{u}_s$ |
| Maxwell's Eqn. | $\frac{1}{c^2}\partial_t \mathbf{E} - \nabla \times \mathbf{B} + \mu_0 \mathbf{J} = \mathbf{0}$    $\nabla \cdot \mathbf{E} = \frac{q}{\epsilon_0}$ <br> $\partial_t \mathbf{B} + \nabla \times \mathbf{E} = \mathbf{0}$    $\nabla \cdot \mathbf{B} = 0$ <br> Important involutions that the continuous system satisfies. Structure-preserving methods enforce these in an appropriate discrete sense. |

Braginskii, Rev. Plasma Phys. 1965; E. T. Meier and U. Shumlak PoP, 2012;

# A Reduced length-scale/time scale representation; Basic single fluid Resistive MHD [e.g. 3D H(grad) Variational Multiscale (VMS) Stabilized FE]

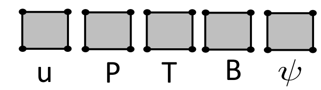



Illustration how Resistive MHD differs from CFD:

- Magnetic Stress
- Work due to Magnetic stress
- Magnetic Induction Evolution Eq. and GLM Solenoidal Constraint Eq.

Resistive MHD Model in Conservative Form

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

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

$$\frac{\partial \Sigma_{tot}}{\partial t} + \nabla \cdot [(\rho e + \frac{1}{2}\|\mathbf{v}\|^2)\mathbf{v} - (\mathbf{T} + \mathbf{T_M}) \cdot \mathbf{v} + \mathbf{h}] = 0$$

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

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

We use elliptic cleaning and VMS stabilization for smooth problems

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

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

$$\Sigma_{tot} = \rho e + \frac{1}{2}\rho\|\mathbf{u}\|^2 + \|\mathbf{B}\|^2/2\mu_0$$

- Divergence free involution enforced as constraint with a Lagrange multiplier (Elliptic, parabolic, hyperbolic) [Dedner et. al. 2002; Elliptic: Codina et. al. 2006, 2011, JS et. al. 2010, 2016]
  - Only weakly divergence free in FE implementation (stabilization of B - $\psi$ coupling )
- Relationship with projection (Brackbill and Barnes 1980), and elliptic divergence cleaning (Dedner et. al, 2002), (JS et al. 2016).
- Issue with $C^0$ FE for domains with re-entrant corners / soln singularities [Costabel et. al. 2000, 2002, Codina, 2011, Badia et. al. 2014]

# Why Newton-Krylov Methods?

Newton-Krylov

Direct-to-steady-state | Fully-implicit / IMEX transient

**Convergence properties**

- **Strongly coupled multi-physics often requires a strongly coupled nonlinear solver**
- **Quadratic convergence near solutions (backtracking, adaptive convergence criteria)**
- **Often only require a few iterations to converge, if close to solution, independent of problem size**

$$\mathbf{F}(\mathbf{x},\lambda_1,\lambda_2,\lambda_3,..)=\mathbf{0}$$

Inexact Newton-Krylov

Solve $Jp_k = -F(x_k)$; until $\dfrac{\|Jp_k + F(x_k)\|}{\|F(x_k)\|} \le \eta_k$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \Theta \mathbf{p}_k$$

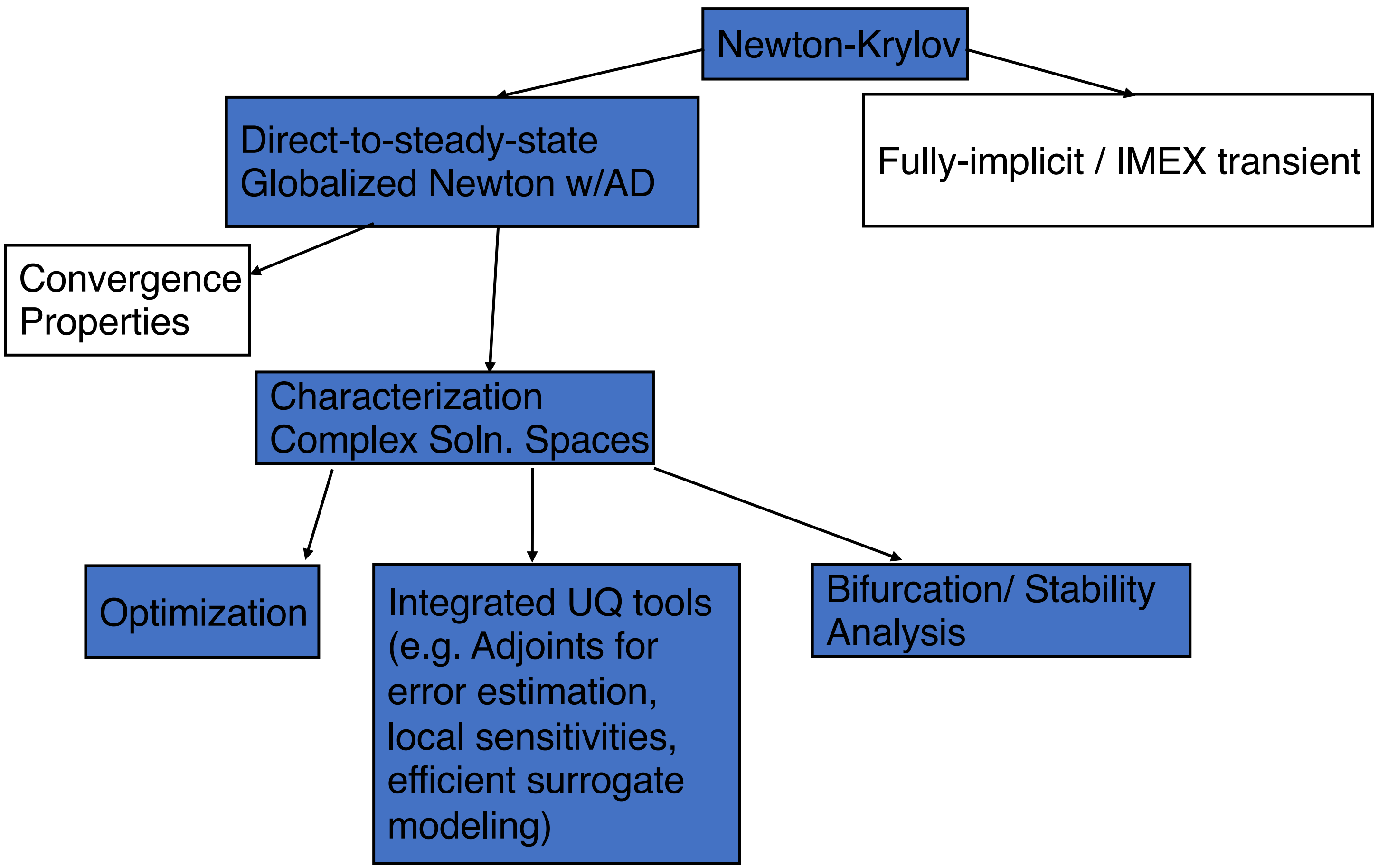
Jacobian Free N-K Variant

$$\mathbf{M}\mathbf{p}_k = \mathbf{v}$$

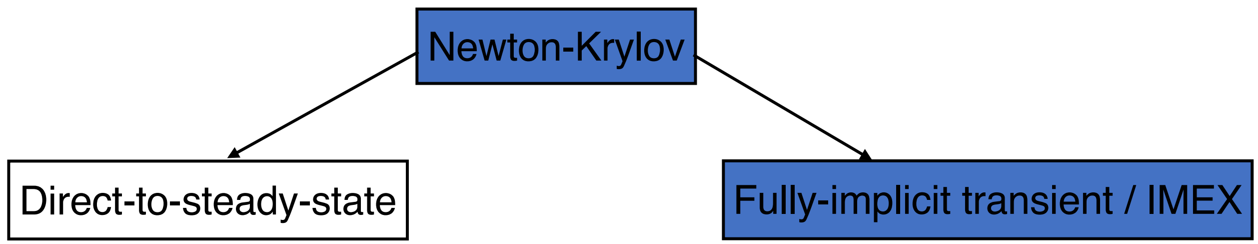
$$\mathbf{J}\mathbf{p}_k = \frac{\mathbf{F}(\mathbf{x}+\delta\mathbf{p}_k) - \mathbf{F}(\mathbf{x})}{\delta}\ ; \text{ or by AD}$$

See e.g. Knoll & Keyes, JCP 2004

# Why Newton-Krylov Methods?



# Why Implicit / IMEX Newton-Krylov Methods?




$$\mathbf{F}(\dot{\mathbf{x}},\mathbf{x},\lambda_1,\lambda_2,\lambda_3,..)=\mathbf{0}$$

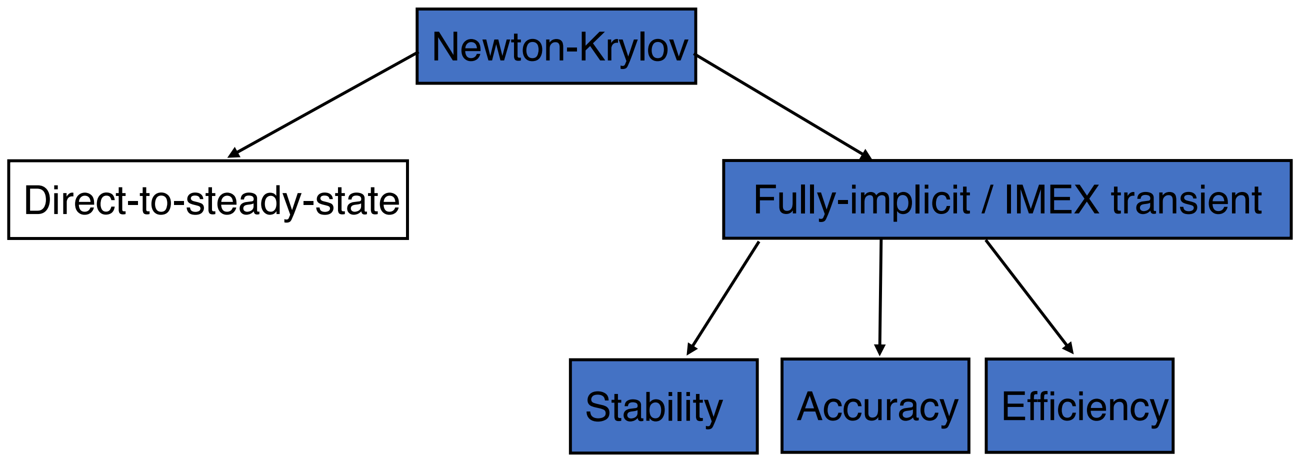
*e.g.*

$$\left.\frac{\partial c}{\partial t}\right|^{n+1}+\nabla\bullet\left(\left[\rho c\mathbf{u}\right]^{n+1}\right)-\nabla\bullet\left[D^{n+1}\nabla c^{n+1}\right]+S_c^{n+1}=0$$

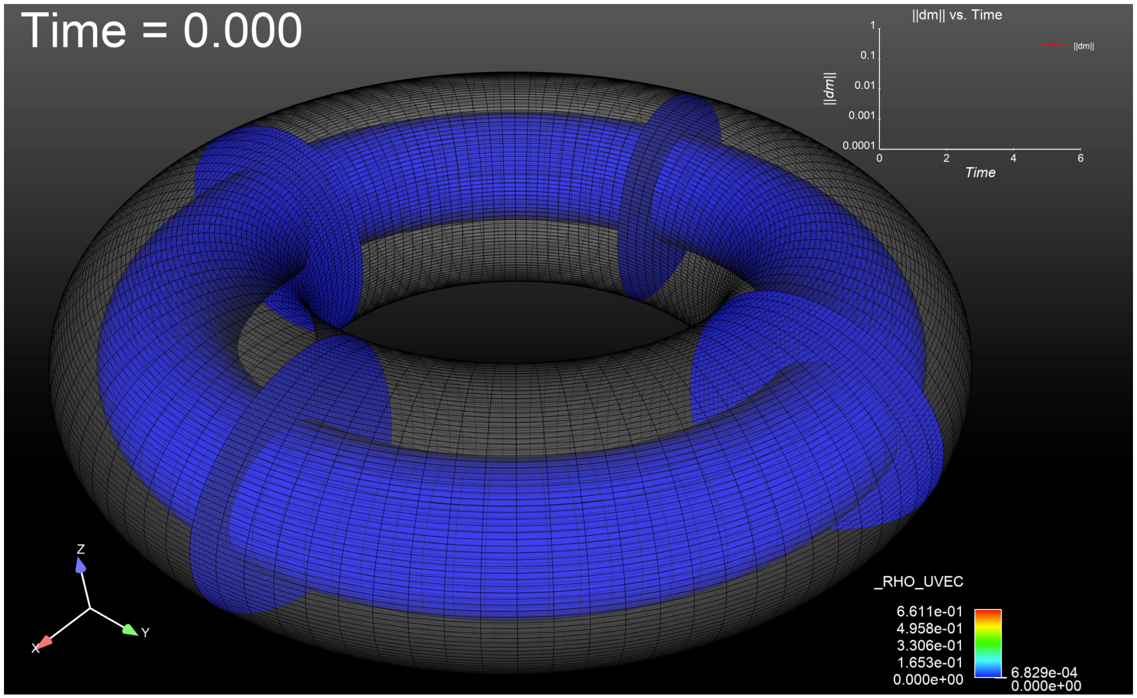
Stability, Accuracy and Efficiency

- Stable (stiff systems)
- High order methods (e.g. BDF, DIRK, IMEX, etc.)
- Variable order techniques
- Local and global error control possible
- Can be stable, accurate, and efficient when run at the dynamical time-scale of interest in appropriate multiple-time-scale systems (e.g. Knoll et. al., Brown and Woodward., Chacon and Knoll, S., Ober, JS. and Ropp)

# Why Implicit / IMEX Newton-Krylov Methods?



# Resistive MHD: Soloveev Analytic Equilibrium Nonlinear Disturbance Saturation (VMS Q1).




Kink and interchange instability.

MHD Wave speeds

$\|\mathbf{u}\|, \|\mathbf{u}\| \pm c_s, \|\mathbf{u}\| \pm c_a, \|\mathbf{u}\| \pm c_f, \pm c_h$ Here $c_h$ is $\infty$ for elliptic divergence cleaning

Approx. Computational Time Scales:

- B Divergence Const. ($\nabla \cdot \mathbf{B} = 0$): $1/\infty = 0$
- Fast Magnetosonic Wave ($c_f$): $10^{-4}$ to $10^{-7}$
- Alfven Wave ($c_a$): $10^{-4}$ to $10^{-7}$
- Slow Magnetosonic Wave ($c_s$): $10^{-2}$ to $10^{-3?}$
- Sound Wave (c): $10^{-1}$ to $10^{-3}$

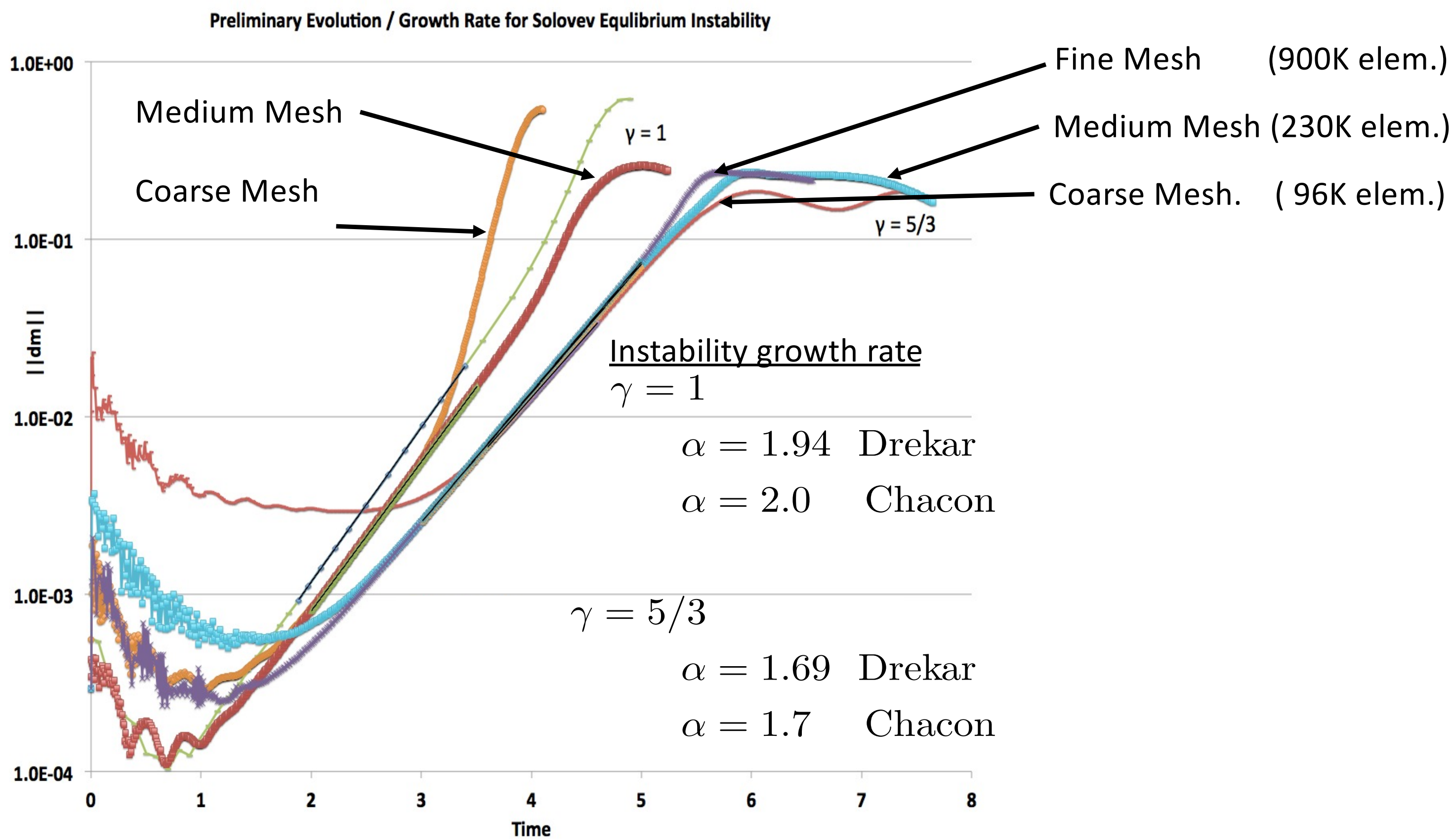
- Advection ($c_{v\ max}$): $\sim 10^{-2}$
- Diffusion: $10^{-3}$ to $10^{-2}$

•Macroscopic Dynamic Time-scale:

unstable mode: O(1)

Fully-implicit (BDF2, SDIRK22)
Max CFL:

$CFL_{div} = \infty$
$CFL_{cf} \sim 10^4$
$CFL_{cA} \sim 10^4$
$CFL_{cs} \sim 1$
$CFL_{c} \sim 1$
$CFL_{cv} \sim 0.1$



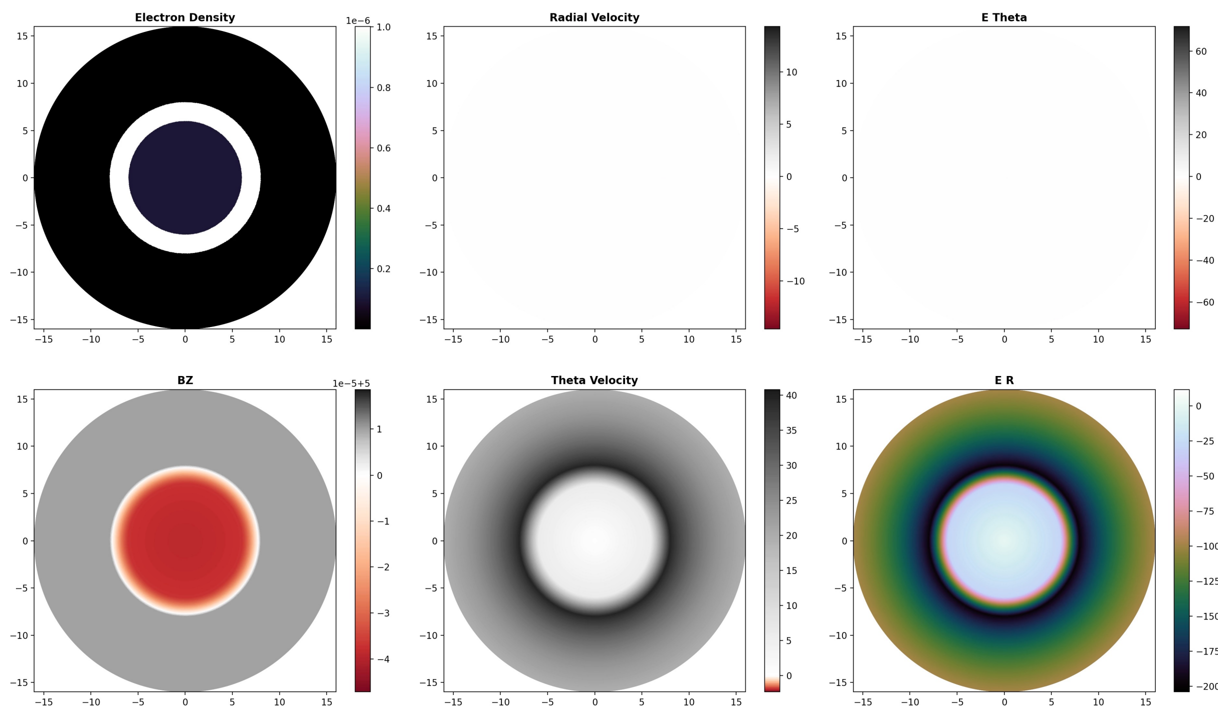

Isentropic EoS

$$\frac{P}{P_0} = (\frac{\rho}{\rho_0})^{\gamma}$$

[Comparisons with L. Chacon and PIXIE 3D code (LANL)]

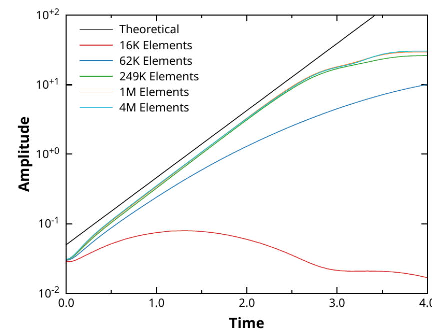
# Multifluid Simulation of a Diocotron Instability of an Electron Beam In a Uniform Axial Magnetic Field

## Comparison with Linear Stability Theory [1,2,3]

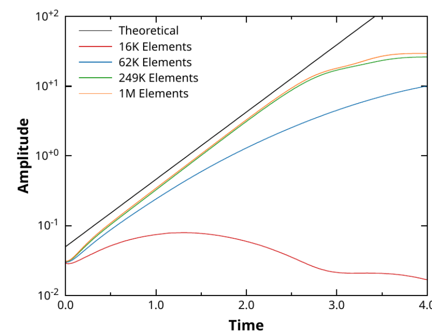



[1]Ronald C Davidson. Physics of Nonneutral Plasmas. World Scienti c Publishing, 2001.
[2] W. Knauer. Diocotron instability in plasmas and gas discharges. Journal of Applied Physics, 37(2):602{611, 1966.
[3] J. Petri. Relativistic stabilisation of the diocotron instability in a pulsar and cylindrical electrosphere. Astronomy & Astrophysics, 469(3):843{855, 2007.

Diocotron instabilities are driven by velocity shear created by ExB drift velocities in non-neutral electron columns. A sufficiently strong shear in this rotational velocity drives the development of the cylindrical diocotron instability.




Multifluid growth rate vs mesh resolution




Generalized Ohm's law without electron inertia

# Illustration of Time-scales and an IMEX Partition for Multi-fluid Plasma System Model

**Ionization/recombination**

| | |
|---|---|
| Density | $\partial_t \rho_s + \nabla\cdot(\rho_s \mathbf{u}_s) = -\rho_s n_e (I_s + R_s) + m_s n_e (n_{s-1} I_{s-1} + n_{s+1} R_{s+1})$ |
| Momentum | $\partial_t(\rho_s \mathbf{u}_s) + \nabla\cdot(\rho_s \mathbf{u}_s \otimes \mathbf{u}_s + p_s \underline{\mathbf{I}} + \underline{\Pi}_s) = q_s n_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) + \sum_{t \neq s} \alpha_{s;t} \rho_s \rho_t (\mathbf{u}_t - \mathbf{u}_s)$ $- \rho_s \mathbf{u}_s n_e (I_s + R_s) + \frac{m_s}{m_{s-1}} n_e \rho_{s-1} \mathbf{u}_{s-1} I_{s-1} + (n_e \rho_{s+1} \mathbf{u}_{s+1} + n_{s+1} \rho_e \mathbf{u}_e) R_{s+1}$ |
| Energy | $\partial_t \mathcal{E}_s + \nabla\cdot[(\mathcal{E}_s + p_s)\mathbf{u}_s + \mathbf{u}_s \cdot \underline{\Pi}_s + \mathbf{h}_s] = q_s n_s \mathbf{u}_s \cdot \mathbf{E} + \sum_t \ldots (T_t - T_s) + m_t (\mathbf{u}_t - \mathbf{u}_s)^2]$ $- \mathcal{E}_s n_e (I_s + R_s) + \frac{m_s}{m_{s-1}} n_e \mathcal{E}_{s-1} I_{s-1} + (n_e \mathcal{E}_{s+1} + n_{s+1} \mathcal{E}_e) R_{s+1}$ |
| Charge and Current | $q = \sum_s q_s n_s$ $\qquad \mathbf{J} = \sum_s q_s n_s \mathbf{u}_s$ |
| Maxwell's Equations | $\frac{1}{c^2}\partial_t \mathbf{E} - \nabla\times\mathbf{B} + \mu_0 \mathbf{J} = \mathbf{0}$ $\qquad \nabla\cdot\mathbf{E} = \frac{q}{\epsilon_0}$ <br> $\partial_t \mathbf{B} + \nabla\times\mathbf{E} = \mathbf{0}$ $\qquad \nabla\cdot\mathbf{B} = 0$ |

**Cyclotron frequency**

**Collisional**

**Strong off diagonal coupling for plasma oscillation**

**Light wave off diagonal coupling**

**IMEX RK: Time Integration**

$$\mathrm{M}\dot{\mathrm{U}} + \mathbf{F} + \mathbf{G} = 0$$

Explicit Hydrodynamics (slow)

Implicit EM, EM sources, sources for species interactions (fast)

Other work on multifluid plasma formulations, solution algorithms:

See e.g.
Abgral et. al.;
Barth;
Kumar et. al.;
Laguna et. al.;
Rossmanith et. al.;
Shumlak et. al.;
B. Srinivasan et. al.;

S. T. Miller, E. C. Cyr, JS, R. M. J. Kramer, E. G. Phillips, S. Conde, R. P. Pawlowski, IMEX and exact sequence discretization of the multi-fluid plasma model. JCP, 2019

## Multifluid Model: Implicitness and IMEX used to handle Multiple-time-scales

Illustration for a particular example (e.g. high resolution mesh ( small $\Delta x$ ) and lower density plasmas)

$$\tau_{EM} \leq \tau_{\omega_{pe}} \leq \tau_{\omega_{ce}} \leq \tau_{\omega_{pi}} \leq \tau_{\omega_{ci}} \leq \tau_{ce} \leq \tau_{ue} \leq \tau_{ci} \leq \tau_{ui}$$

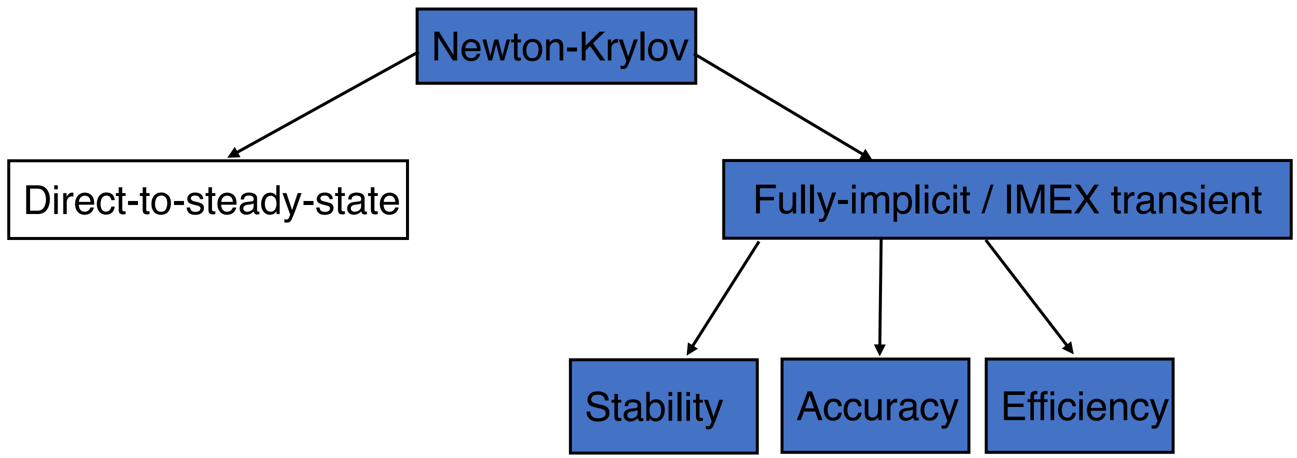
$\Delta t_{dyn}$ (at $\tau_{EM}$): Fully EXPLICIT

$\Delta t_{dyn}$ (at $\tau_{ue}$): ← IMPLICIT | EXPLICIT →

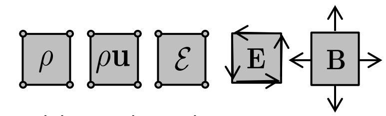
$\Delta t_{dyn}$ (at $\tau_{ui}$): Fully IMPLICIT

Of course stability *does not imply accuracy*.

# Why Implicit / IMEX Newton-Krylov Methods?

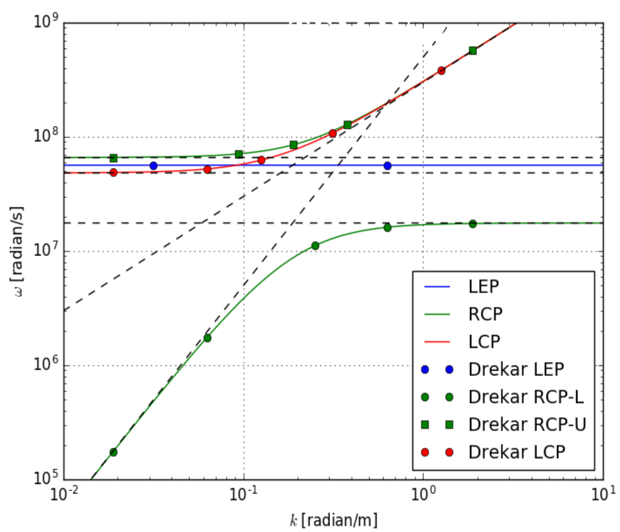


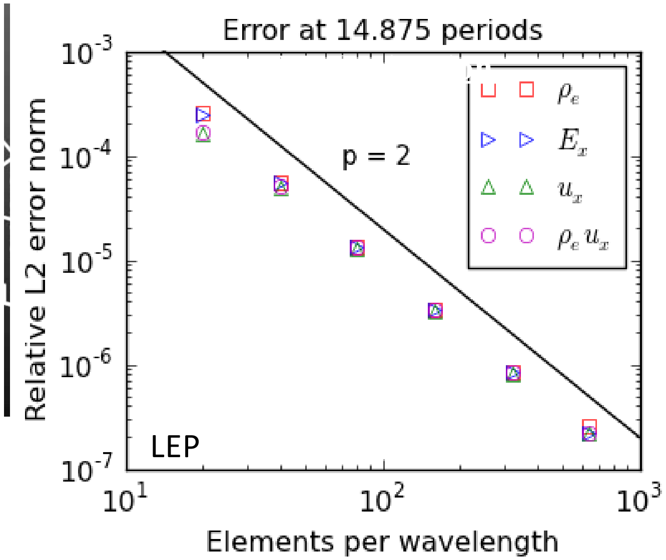
# Demonstration / Verification of Implicit Solution for Longitudinal Electron Plasma (LEP) Oscillation with a Highly Under-resolved TEM Wave (SDIRK22)




Nodal FE Hydro and Structure-preserving discretization for EM

$$\Delta t = 0.1 * \tau_{\omega_{pe}} \approx 10^4 * \tau_{EM} \quad \text{(on 3200 fine mesh)}$$

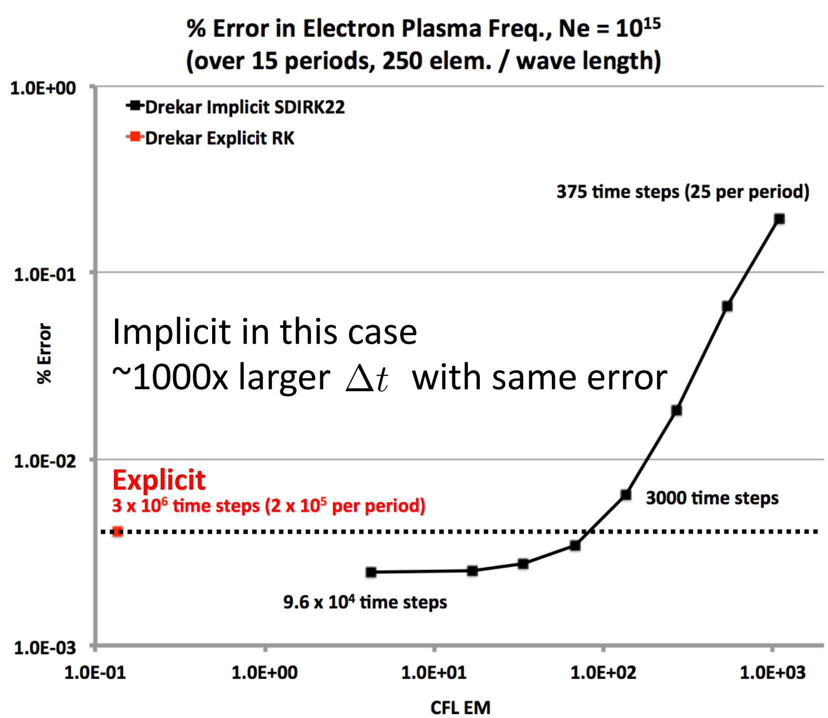


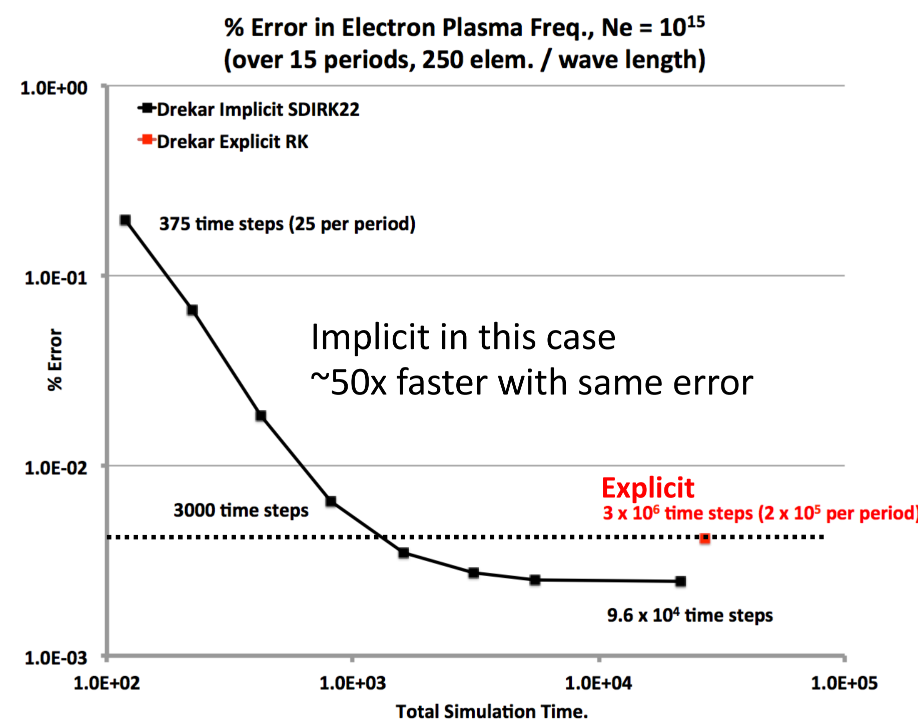




LEP: Longitudinal Electron Plasma Wave
RCP: Right Hand Circularly Polarized Wave
LCP: Left Hand Circularly Polarized Wave
(Cold plasma)

Verification effort with Niederhaus, Radtke, Bettencourt, Cartwright, Kramer, Robinson and ATDM EMPIRE Team

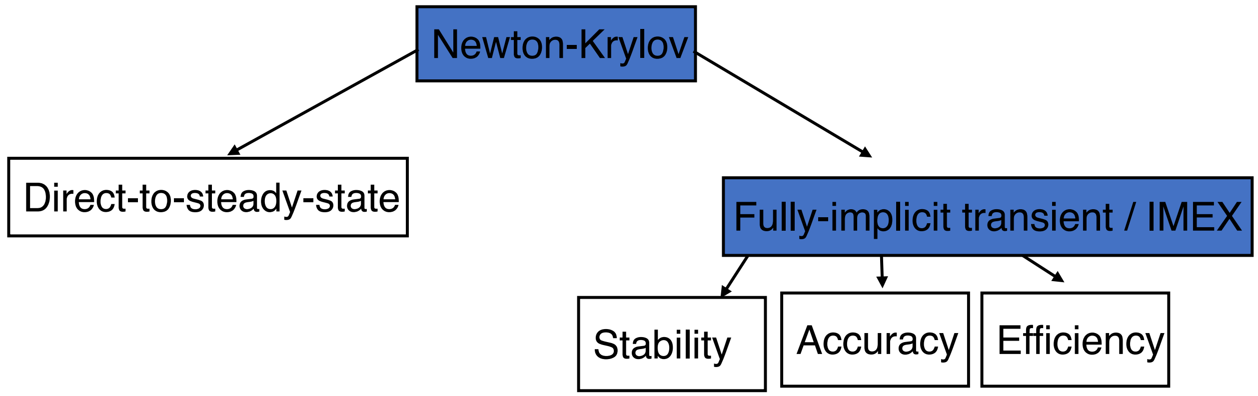
Demonstration of Accuracy for Implicit Solution Methods for Langmuir wave (i.e. Longitudinal Electron Plasma [LEP] Oscillation): Fast time-scale unresolved transverse EM (light) waves (Ne = $10^{15}$)




Note: Explicit solver is not highly optimized. Explicit is 20x – 30x faster per time step.

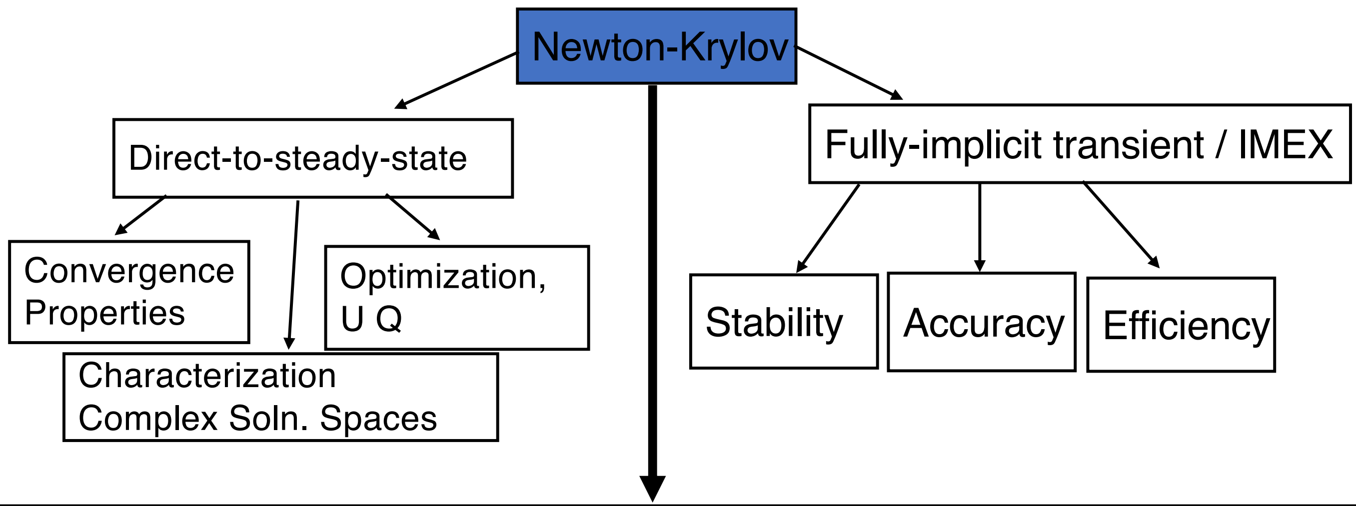
# Why Implicit / IMEX Newton-Krylov Methods?




What I am not implying: Fully-implicit / IMEX is the only way to get these properties

What I am implying: Fully-implicit / IMEX are excellent ways to get these properties along with a number of other benefits when applied to multiple-time-scale multiphysics systems

# Why Implicit/IMEX Newton-Krylov Methods?

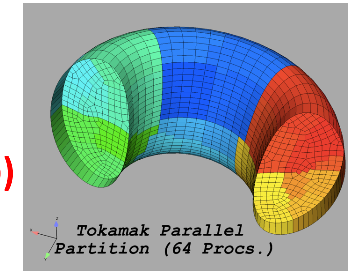



Very Large Problems -> Parallel Iterative Solution of Sub-problems

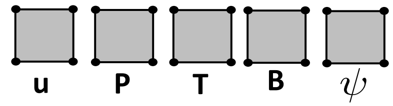
<u>Krylov Methods (e.g. GMRES) - Robust, Scalable and Efficient Parallel Preconditioners</u>

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

# Scalable Preconditioning for Systems



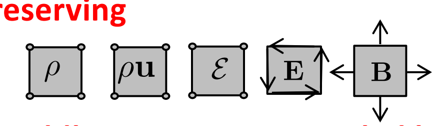

1. **Fully-coupled Algebraic Multilevel (AMG) Methods: (ML & Muelu; Tuminaro, Hu et. al.))**
   - **Consistent set of DOF-ordered blocks at each node (e.g. CG VMS/Stabilized FE)**




   - **Uses non-zero block graph structure of Jacobian**
   - **Additive Schwarz DD ILU(k) as smoothers (Jacobi & GS possible for transients)**
   - **Can provide optimal algorithmic scalability**

**2. Approximate Block Factorization / Physics-based (Teko; Cyr, JS, Tuminaro, Phillips)**

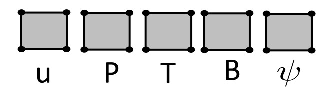
- **Applies to mixed interpolation (FE), staggered (FV), and structure preserving discretization approaches using segregated unknown blocking**




- **Applies to systems where coupled AMG is difficult or might fail (e.g saddle pt. systems, coupled hyperbolic eqns.)**
- **Enables specialized optimal AMG, e.g. H(grad), H(curl) for disparate discretization spaces.**
- **Can provide optimal algorithmic scalability for coupled systems**

**3. Monolithic Multigrid Enabled by Schur-complement Structure Aware Smoothers (Vanka et. al, Farrell et. al, MacLachlan et. al., ….)**

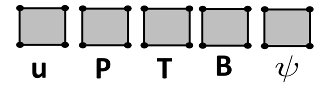
# A Few Examples of Scalability of Full System Projection AMG for 3D Variational Multiscale Stabilized Resistive MHD




## Important for

- scalable solver for uniform / consistent (DOF) of discretizations
- Sub-block system solvers for approximate block factorizations / physics based approaches

# 3D H(grad) Variational Multiscale (VMS) / AFC formulation




**Resistive MHD Model in Residual Notation**

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

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

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

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

$$\frac{\partial \Sigma_{tot}}{\partial t} + \nabla \cdot [(\rho e + \frac{1}{2}\|\mathbf{v}\|^2)\mathbf{v} - (\mathbf{T} + \mathbf{T}_{\mathbf{M}}) \cdot \mathbf{v} + \mathbf{h}] = 0 \qquad \Sigma_{tot} = \rho e + \frac{1}{2}\rho\|\mathbf{u}\|^2 + \|\mathbf{B}\|^2/2\mu_0$$

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

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

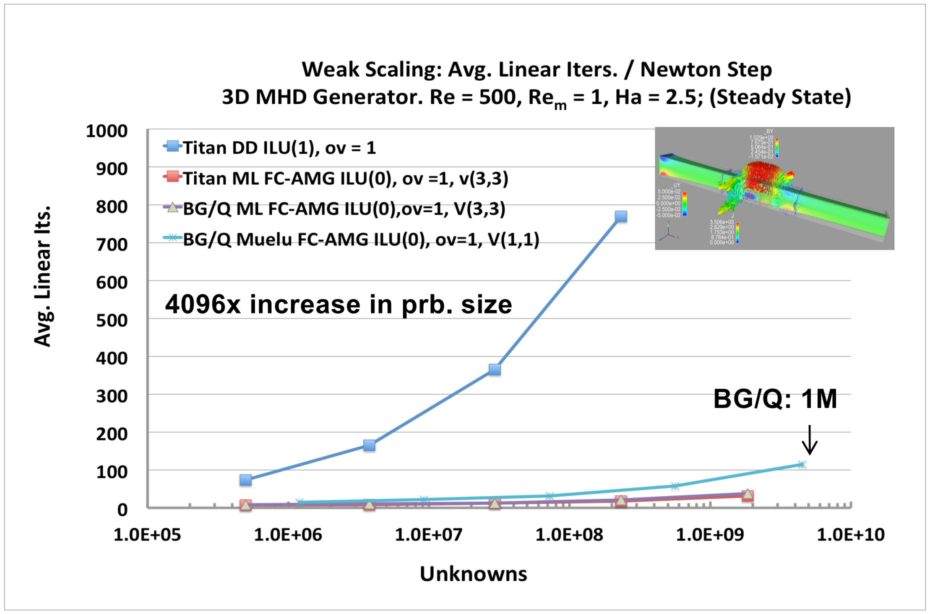
All nodal H(grad) elements using VMS stabilized weak form for the (U,P) and (B,$\psi$) saddle point problems.

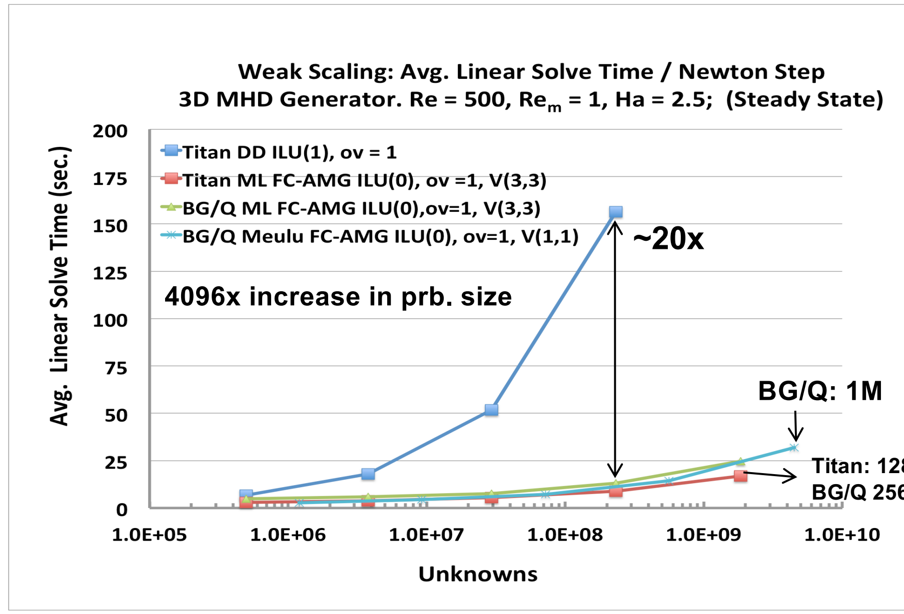
$$\begin{bmatrix} F_m & B^T & Z & 0 \\ B & C_P & 0 & 0 \\ Y & 0 & F_B & B^T \\ 0 & 0 & B & C_\psi \end{bmatrix}$$

- Divergence free involution enforced as constraint with a Lagrange multiplier (Elliptic, parabolic, hyperbolic) [Dedner et. al. 2002; Elliptic: Codina et. al. 2006, 2011, JS et. al. 2010, 2016]
  - Only weakly divergence free in FE implementation (stabilization of B - $\psi$ coupling )
- Can show relationship with projection (e.g. Brackbill and Barnes 1980), and elliptic divergence cleaning (Dedner et. al, 2002) [JS et. al. 2016].
- Issue for using $C^0$ FE for domains with re-entrant corners / soln singularities [Costabel et. al. 2000, 2002, Codina, 2011, Badia et. al. 2014]

# Large-scale Weak Scaling Studies for Cray XK7 AND BG/Q; VMS 3D FE MHD

**u P B r (similar discretizations for all variables, fully-coupled H(grad) AMG)**



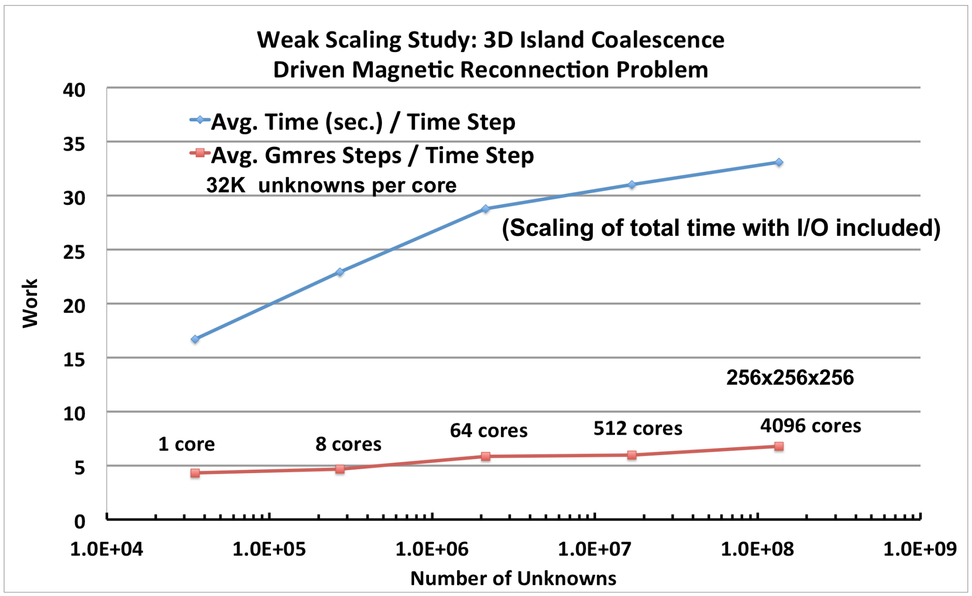

## Largest fully-coupled NK-AMG unstructured FE MHD solves demonstrated to date:

**MHD (steady) weak scaling studies to** **256K Cray XK7, 1M BG/Q**
**Largest demonstration computation MHD (steady):** **13B DoF, 1.625B elem, on 128K cores**
**Poisson sub-block solvers:** **4.1B DoF, 4.1B elem, on 1.6M cores BG/Q**

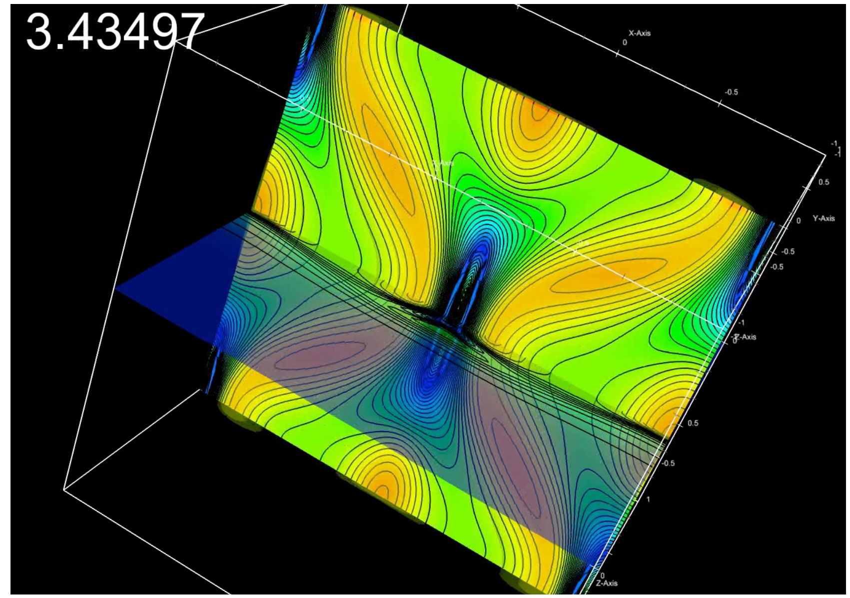
Lin, JS, Hu, Pawlowski, Cyr, Performance of Fully-coupled Algebraic Multigrid Preconditioners for Large-scale VMS Resistive MHD, J. Comp. and Applied Math, 344 (2018) 782–793

## Weak Scaling for VMS 3D Island Coalescence Problem: Driven Magnetic Reconnection [$S = 10^3$, $dt = 0.1$]

[u] [P] [B] [r] (similar discretizations for all variables, fully-coupled H(grad) AMG)




JS, Pawlowski, Cyr, Tuminaro, Chacon, Weber, Scalable Implicit Incompressible Resistive MHD with Stabilized FE and Fully-coupled Newton-Krylov-AMG, CMAME 304, 1–25, 2016




$S = 10^4$

Scaling with Lundquist No. (Re as well).

| 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)**

**Mesh: 128x128x128, dt = 0.0333.**

# Approximate Block Factorization / Physics-based Preconditioning

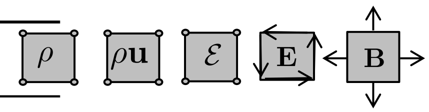
- Applies to mixed interpolation (FE), staggered (FV), physics compatible discretization approaches using segregated unknown blocking

- Applies to systems where coupled AMG is difficult or might fail (e.g. Hyperbolic systems with strong off diagonal physics coupling)

- Enables specialized optimal AMG, e.g. H(grad), H(curl) for disparate discretizations.

# Illustration of Time-scales and an IMEX Partition for Multi-fluid Plasma System Model

Ionization/recombination [diagonal (s)/off diagonal (s,t)]




**Density**

$$\partial_t \rho_s + \nabla\cdot(\rho_s \mathbf{u}_s) = -\rho_s n_e (I_s + R_s) + m_s n_e (n_{s-1} I_{s-1} + n_{s+1} R_{s+1})$$

Cyclotron frequency

**Momentum**

$$\partial_t(\rho_s \mathbf{u}_s) + \nabla\cdot(\rho_s \mathbf{u}_s \otimes \mathbf{u}_s + p_s \underline{\mathbf{I}} + \underline{\Pi}_s) = q_s n_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) + \sum_{t \neq s} \alpha_{s;t} \rho_s \rho_t (\mathbf{u}_t - \mathbf{u}_s)$$

$$-\rho_s \mathbf{u}_s n_e (I_s + R_s) + \frac{m_s}{m_{s-1}} n_e \rho_{s-1} \mathbf{u}_{s-1} I_{s-1} + (n_e \rho_{s+1} \mathbf{u}_{s+1} + n_{s+1} \rho_e \mathbf{u}_e) R_{s+1}$$

Collisional

**Energy**

$$\partial_t \mathcal{E}_s + \nabla\cdot[(\mathcal{E}_s + p_s)\mathbf{u}_s + \mathbf{u}_s \cdot \underline{\Pi}_s + \mathbf{h}_s] = q_s n_s \mathbf{u}_s \cdot \mathbf{E} + \sum_t \ldots (T_t - T_s) + m_t (\mathbf{u}_t - \mathbf{u}_s)^2]$$

$$-\mathcal{E}_s n_e (I_s + R_s) + \frac{m_s}{m_{s-1}} n_e \mathcal{E}_{s-1} I_{s-1} + (n_e \mathcal{E}_{s+1} + n_{s+1} \mathcal{E}_e) R_{s+1}$$

Strong off diagonal coupling for plasma oscillation

**Charge and Current**

$$q = \sum_s q_s n_s \qquad \mathbf{J} = \sum_s q_s n_s \mathbf{u}_s$$

**Maxwell's Equations**

$$\frac{1}{c^2}\partial_t \mathbf{E} - \nabla \times \mathbf{B} + \mu_0 \mathbf{J} = \mathbf{0} \qquad \nabla\cdot\mathbf{E} = \frac{q}{\epsilon_0}$$

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = \mathbf{0} \qquad \nabla\cdot\mathbf{B} = 0$$

Light wave off diagonal coupling

**IMEX: Time Integration**

$$\mathrm{M}\dot{\mathrm{U}} + \mathbf{F} + \mathbf{G} = 0$$

Explicit Hydrodynamics

Implicit EM, EM sources, sources for species interactions

Other work on multifluid plasma formulations, solution algorithms:

See e.g.
Abgral et. al.;
Barth;
Kumar et. al.;
Laguna et. al.;
Rossmanith et. al.;
Shumlak et. al.;
B. Srinivasan et. al.;

## Illustrate Physics-based and Approximate Block Factorizations with Simple Example

## Strongly Coupled Off-diagonal Physics & Disparate Discretizations (e.g. structure-preserving)

$$\frac{\partial u}{\partial t} = \frac{\partial v}{\partial x}\ , \quad \frac{\partial v}{\partial t} = \frac{\partial u}{\partial x}$$

Fully-continuous Wave System Analysis:

$$\frac{\partial u}{\partial t} = \frac{\partial v}{\partial x}\ , \quad \frac{\partial v}{\partial t} = \frac{\partial u}{\partial x}$$

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 v}{\partial t \partial x} = \frac{\partial^2 v}{\partial x \partial t} = \frac{\partial^2 u}{\partial x^2}$$

Discrete Sys.: E.g. 2nd order FD (illustration)

$$(I - \beta \Delta t^2 \mathcal{L}_{xx}) u^{n+1} = \mathcal{F}^n$$

Fully-discrete:

Approximate Block Factorizations & Schur-complements:

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

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

The Schur complement is then

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

Recall: This is motivating how we develop preconditioners, not for developing solvers. The NK method still seeks the solution to the original nonlinear/linear system residual!

[w/ L. Chacon (LANL) ]

Physics-based and Approximate Block Factorizations:

Strongly Coupled Off- Diagonal Physics & Disparate Discretizations (e.g. structure-preserving)

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

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

Result:

1) Stiff (large-magnitude) off-diagonal hyperbolic type operators (blocks) are now combined onto diagonal Schur-complement operator (block) of preconditioned system.

2) Partitioning of coupled physics into sub-systems enables exisiting *SCALABLE* AMG optimized for the correct structure preserving spaces e.g. H(grad), H(curl), H(div) to be used.
(e.g. **Teko block-preconditioning using Trilinos ML/Muelu**; **FieldSplit in PetSc with Hyper**)

Still Requires:
3) Effective sparse Schur complement approximations to preserve strong cross-coupling of physics and critical stiff unresolved time-scales, and be designed for efficient solution by iterative methods.

[w/ L. Chacon (LANL) ]

# Extending the Simple Example

A coupled convection diffusion problem with periodic BCs

and u=sin(2πx), v=cos(2πx)

$$\left(\frac{\partial}{\partial t} + \begin{bmatrix} a & c \\ c & a \end{bmatrix} \frac{\partial}{\partial x} - d\frac{\partial^2}{\partial x^2}\right) \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Three time-scales of interest

- $\tau_d=h^2/d$ – Diffusive time scale
- $\tau_a=h/a$ – Advection time scale (we assume a=1)
- $\tau_c=h/c$ – Coupled wave time scale

$$CFL_d = \frac{d\Delta t}{h^2}, CFL_a = \frac{a\Delta t}{h}, CFL_c = \frac{c\Delta t}{h}$$

CFL < 1 roughly the explicit stability limit varies with temporal / spatial discretization

# Block Preconditioning and Time-Scales (e.g. FD discretization coupled convection/diffusion/first-order wave coupled system)

$$\begin{pmatrix} \frac{1}{\Delta t}I + dD + aC & cC \\ cC & \frac{1}{\Delta t}I + dD + aC \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} R_u \\ R_v \end{pmatrix}$$

$$\mathcal{P}^*_{SC} = \begin{pmatrix} \frac{1}{\Delta t}I + dD + aC & cC \\ 0 & S \end{pmatrix}$$

$$S = \frac{1}{\Delta t}I + dD + aC - c^2C\left(\frac{1}{\Delta t}I + dD + aC\right)^{-1}C$$

$$\mathcal{P}_J = \begin{pmatrix} \frac{1}{\Delta t}I + dD + aC & 0 \\ 0 & \frac{1}{\Delta t}I + dD + aC \end{pmatrix} \quad \mathcal{P}_{GS} = \begin{pmatrix} \frac{1}{\Delta t}I + dD + aC & cC \\ 0 & \frac{1}{\Delta t}I + dD + aC \end{pmatrix}$$

*Only the upper diagonal of the block LU factorization is used in the Schur-complement as in Murphy, Golub, Wathen SISC 2000 -> 2 iterations in GMRES for exact inversion of sub-block solver and Schur complement.

Block Preconditioning and Time-Scales (e.g. FD discretization Implicit coupled convection/diffusion/first-order wave coupled system)

AVG. outer iterations in the dof based block factorization linear solver

| $CFL_c$ | $10^{-2}$ | $10^{-1}$ | $10^{0}$ | $10^{1}$ | $10^{2}$ |
|---|---|---|---|---|---|
| GS | 2 | 3 | 67 | 231 | 414 |
| J | 3 | 5 | 125 | 465 | 500 |
| SC* | 2 | 2 | 2 | 2 | 2 |

$$CFL_a = 1, CFL_d = 1$$

| $CFL_c$ | $10^{-2}$ | $10^{-1}$ | $10^{0}$ | $10^{1}$ | $10^{2}$ |
|---|---|---|---|---|---|
| GS | 2 | 3 | 5 | 13 | 30 |
| J | 3 | 4 | 9 | 26 | 78 |
| SC* | 2 | 2 | 2 | 2 | 2 |

$$CFL_a = 1, CFL_d = 10^2$$

**Schur complement is important when unresolved coupling time-scale is fast**

**Jacobi and GS are effective when coupling is "less important"; Block diagonal dominance, M-matrices, one directional coupling, etc. (see e.g. Axelsson, Neytcheva, NLAA (2013), Elsner, Mehrmann Num. Math (91), Y. Saad, Iterative Meth. Book 2003)**

*Only the upper diagonal of the block LU factorization is used and exact computation/inversion of operators for illustrative purposes. The result of 2 outer iterations follows from the result in Murphy, Golub, Wathen SISC 2000

# Incomplete References for Scalable Block Preconditioning of MHD / Maxwell Systems


**Physics-Based MHD and XMHD**

- Knoll and Chacon et. al. “JFNK methods for accurate time integration of stiff-wave systems”, SISC 2005
- Chacon “Scalable parallel implicit solvers for 3D MHD”, J. of Physics, Conf. Series, 2008
- Chacon “An optimal, parallel, fully implicit NK solver for three-dimensional visco-resistive MHD, PoP 2008
- L. Chacon and A. Stanier, “A scalable, fully implicit alg. for the reduced two-field low-β extended MHD model,” J. Comput. Phys., 2016.

**Approximate Block Factorization & Schur-complements MHD**

- Cyr, JS, Tuminaro, Pawlowski, Chacon. “A new approx. block factorization precond. for 2D .. reduced resistive MHD”, SISC 2013
- Phillips, Elman, Cyr, JS, Pawlowski “A block precond. for an exact penalty formulation for stationary MHD”, SISC 2014
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- Cyr, JS, Tuminaro, “Teko an abstract block prec. capability with concrete example app. to Navier-Stokes and resistive MHD, SISC, 2016
- Wathen, Grief, Schotzau, Preconditioners for Mixed Finite Element Discretizations of Incompressible MHD Equations, SISC 2017
- Li, Ni, Zheng, A Charge-Conservative Finite Element Method for Inductionless MHD Equations. Part II: A Robust Solver, SISC 2019;

**Block Preconditioners for Maxwell**

- Greif and Schotzau. "Precond. for the discretized time-harmonic Maxwell equations in mixed form," Numer. Lin. Alg. Appl. 2007.
- Wu, Huang, and Li. "Block triangular preconditioner for static Maxwell equations," J. Comput. Appl. Math. 2011
- Wu, Huang, Li. "Modified block precond. for discretized time- harmonic Maxwell .. in mixed form," J. Comp. Appl. Math. 2013.
- Adler, Petkov, and Zikatanov. "Numerical approximation of asymptotically disappearing solutions of Maxwell’s eqns," SISC 2013.
- Phillips, JS, Cyr, “Scalable Precond. for Structure Preserving Discretizations of Maxwell Equations in First Order Form”, SISC 2018

**Norm Equivalence Methods**

- Mardal and Winther “Preconditioning discretizations of systems of partial differential equations”. NLAA, 2011
- Ma, Hu, Hu, Xu. "Robust preconditioners for incompressible MHD Models," JCP 2016.
- Hu, Ma, Xu. “Stable finite element methods preserving div B = 0 exactly for MHD models”, Numerische Mathematik 2017

**Step back to CFD and incompressible flow for a moment to**

**Introduce block approximate factorization (physics-based) preconditioners**

# Multi-Physics and mixed discretizations: Block Preconditioning

**An alternative to fully-coupled AMG: Segregate system into physical fields (unknowns, dof)**

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \nabla^2 \mathbf{u} + \nabla p = f$$

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

**Discretization and linearization leads to block linear system**

$$\begin{bmatrix} F & B^T \\ B & C \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}$$

Build preconditioners by manipulating block linear system

Recall:
1) C = 0 for Stable Mixed Q2/Q1 Taylor-Hood type discretizations of this saddle point problem (Ladyzhenskaya–Babuška–Brezzi (LBB), inf-sup stable for Stokes)

2) Variational Multiscale (VMS) stabilized methods (Hughes et. al.) introduce stabilizing weak form operators for coercive formulations (C essentially a scaled Laplacian type operator)

## Brief Overview of Block Preconditioning Methods for Navier-Stokes:

| Discrete N-S | Exact LDU Factorization | Approx. LDU |
|---|---|---|
| $\begin{bmatrix} F & B^T \\ \hat{B} & C \end{bmatrix}$ | $\begin{bmatrix} I & 0 \\ \hat{B}F^{-1} & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & S \end{bmatrix} \begin{bmatrix} I & F^{-1}B^T \\ 0 & I \end{bmatrix}$ <br> $S = C - \hat{B}F^{-1}B^T$ | $\begin{bmatrix} I & 0 \\ \hat{B}\mathcal{F}_l^{-1} & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & S \end{bmatrix} \begin{bmatrix} I & \mathcal{F}_u^{-1}B^T \\ 0 & I \end{bmatrix}$ |

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

(Taxonomy of Block Preconditioners, Elman, Howle, JS, Shuttleworth, Tuminaro, JCP 2008)

**E.g. Incompressible Navier-Stokes**
**Stable Q2 - Velocity, and Q1 Pressure (Taylor Hood)**

$$\begin{bmatrix} F & B^T \\ \hat{B} & 0 \end{bmatrix}$$

**Lower diagonal of saddle point problem has zero entry. – No block *Jacobi or Guass-Siedel***

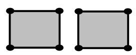
**With block preconditioning can use optimal AMG type methods on sub-problems.**

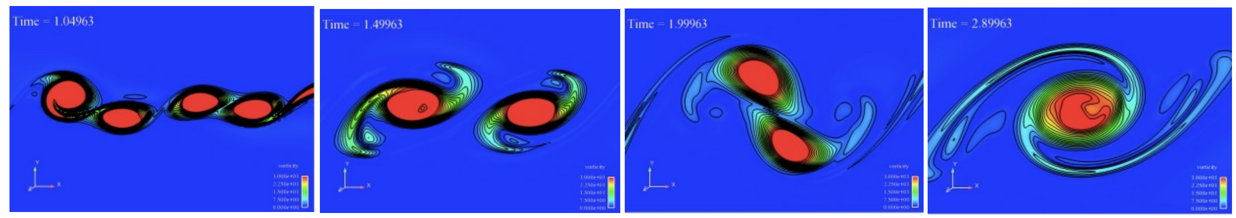
**Momentum transient convection-diffusion:** $F \Delta u = r_u$

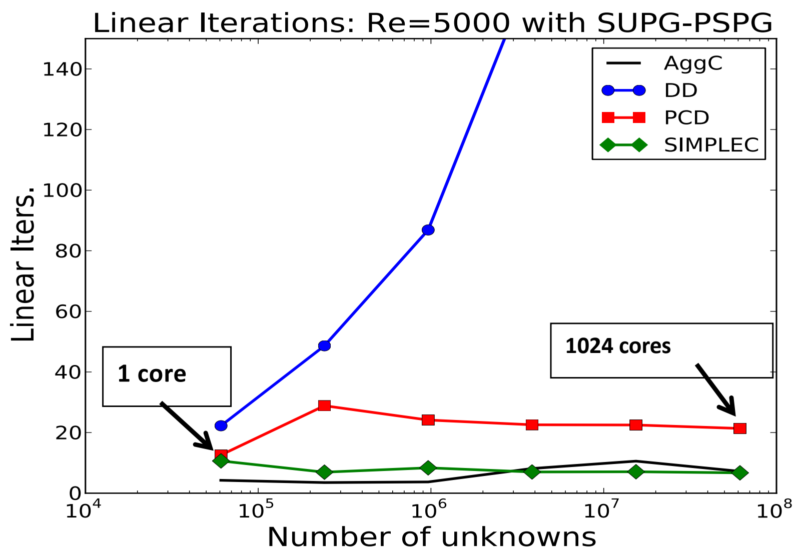
**Pressure – Poisson type (e.g. PCD):** $A_p \Delta p = -F_p r_p$

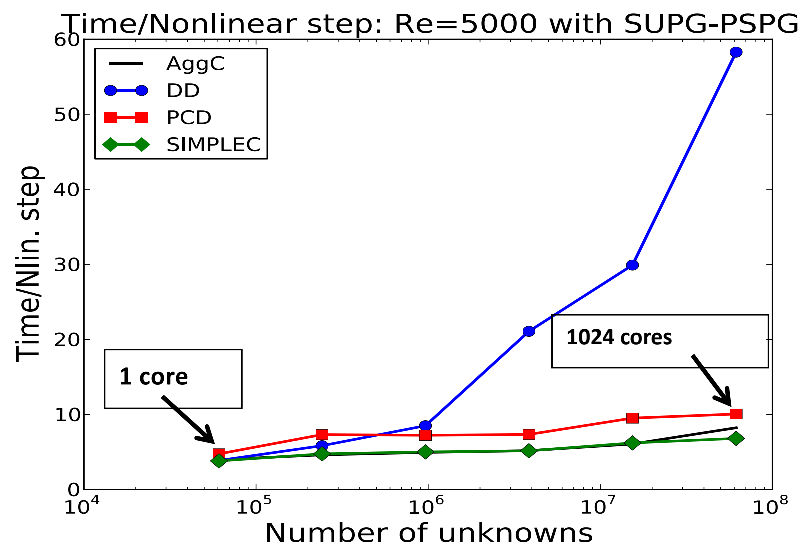
**Kay, Loghin, Wathan, Silvester, Elman (1999 - 2006);**
**Benzi, Golub, Liesen, 2005**
**Elman, Howle, JS, Shuttleworth, Tuminaro (2003,2008)**

# Transient Kelvin-Helmholtz Shear Layer Instability Incompressible Navier-Stokes VMS FE




**Kelvin Helmholtz: Re=5000, Weak scaling at $CFL_p = \infty$ ; $CFL_u$=2.5**

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

## Now Return to MHD

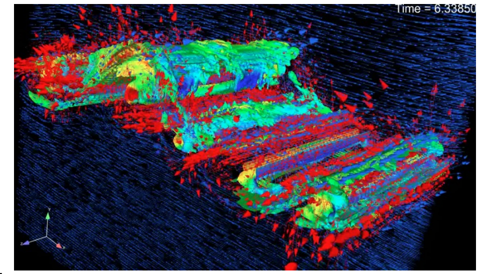
## Block approximate factorization (physics-based) preconditioners

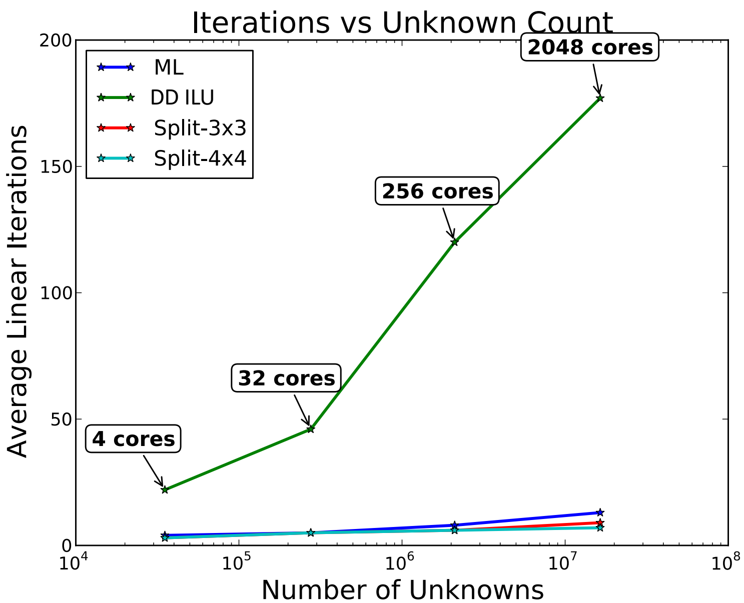
## ABF Precond. strongly couples Alfven wave operators and reduces to 3 - 2x2 blocks

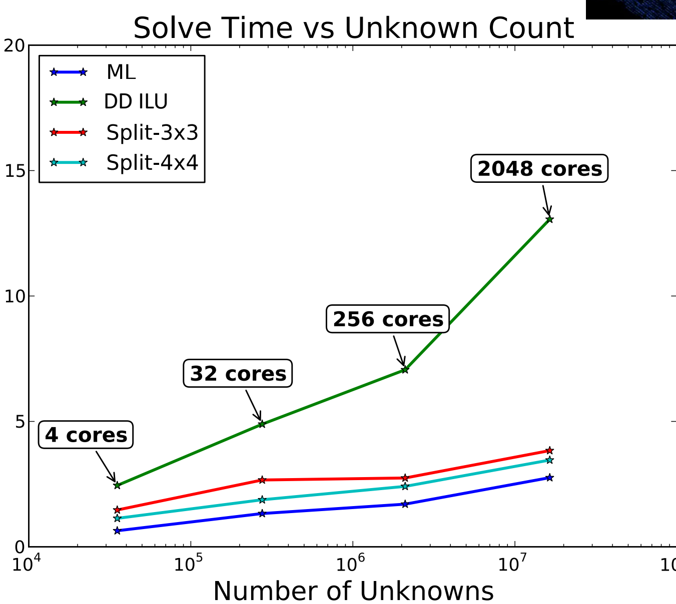
$$\begin{bmatrix} F_m & B^T & Z & 0 \\ B & C_P & 0 & 0 \\ Y & 0 & F_B & B^T \\ 0 & 0 & B & C_\psi \end{bmatrix} \approx \begin{bmatrix} F_m & 0 & Z & 0 \\ 0 & I & 0 & 0 \\ Y & 0 & F_B & I \\ 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} F_m{}^{-1} & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & F_B{}^{-1} & 0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

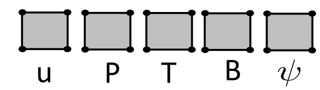
- Order-of-magnitude of structural error terms indicates small perturbation of initial system, $O(\Delta t)$ .
- Analysis of eigenstructure of related 3x3 system (u,p, [B,$\psi$]), and numerical studies, indicated encouraging bound on eigenvalue spectrum. Results confirmed with numerical tests.
- Reduction to 3 - 2x2 block systems that can be approximated by Schur complement approaches from CFD
  - 2 - Saddle point type 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 $P = F_B - Y\hat{F}_m^{-1}Z$
    Bounds Alfven wave coupling with isotropic wave operator and speed $V_A = \frac{\mathbf{B}}{\sqrt{\rho\mu_0}}$ .

# 3D Hydromagnetic Kelivn-Helholtz Instability
# Approximate Block Preconditioning VMS FE
# [Re $=10^4$, Rem$=10^4$, $M_A = 3$; $CFL_{p,\psi} = \infty$; $CFL_u$ ~0.125],




**Fully coupled Algebraic**

**ML:** Uncoupled AMG with repartitioning

**DD:** Additive Schwarz Domain Decomposition

**FC-AMG – ILU(0), V(3,3);**

**3x3, 4x4 use SIMPLEC approx. and V(3,3) with Gauss-Seidel smoothers**

## Now Consider Structure Preserving Discretizations (e.g. DeRham Sequence [Nodal, Edge, Face, Vol.])

$$
\begin{array}{ccccccc}
H^1 & \xrightarrow{\nabla} & H(curl) & \xrightarrow{\nabla\times} & H(div) & \xrightarrow{\nabla\cdot} & L^2 \\
\downarrow I & & \downarrow I & & \downarrow I & & \downarrow I \\
H^{-1} & \xleftarrow[-\nabla\cdot]{} & H(curl)^* & \xleftarrow[\nabla\times]{} & H(div)^* & \xleftarrow[-\nabla]{} & L^2
\end{array}
$$

$$
\begin{array}{ccccccc}
nodes_1 & \xrightarrow{\hat{G} = Q_E^{-1} G} & edges & \xrightarrow{\hat{K} = Q_B^{-1} K} & faces & \xrightarrow{\hat{D} = Q_\phi^{-1} D} & nodes_0 \\
\downarrow Q_\rho & & \downarrow Q_E & & \downarrow Q_B & & \downarrow Q_\phi \\
nodes_1^* & \xleftarrow[\hat{G}^t = G^t Q_E^{-1}]{} & edges^* & \xleftarrow[\hat{K}^t = K^t Q_B^{-1}]{} & faces^* & \xleftarrow[\hat{D}^t = D^t Q_\phi^{-1}]{} & nodes_0^*
\end{array}
$$

**Block approximate factorization (physics-based) preconditioners used to segregate disparate discretizations into sub-systems that can be iteratively solved by optimal AMG methods in the correct spaces**

## Magnetic Vector-Potential MHD Formulation: structure-preserving ( $\mathbf{B} = \nabla \times \mathbf{A}\ ; \nabla \cdot \mathbf{B} = 0$ )

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

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

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

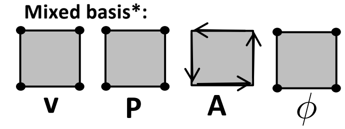
$$R_P = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

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

$$\mathbf{R_A} = \sigma \frac{\partial \mathbf{A}}{\partial t} + \nabla \times \frac{1}{\mu}\nabla \times \mathbf{A} - \sigma \mathbf{v} \times \nabla \times \mathbf{A} + \sigma \nabla \phi = \mathbf{0}; \qquad \mathbf{B} = \nabla \times \mathbf{A}$$

$$R_\phi = \nabla \cdot \sigma \nabla \phi = 0$$

**Mixed basis*:**




Nodal H(grad) and Edge H(curl) Elements [Intrepid]

- **Divergence free involution for B enforced to machine precision by structure-preserving edge-elements**
- **Mixed basis, Q1/Q1 VMS FE Navier-Stokes, A-edge, Q1 Lagrange Multiplier**

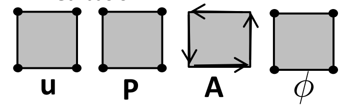
Follows from $\vec{E} = -\frac{\partial \vec{A}}{\partial t} - \nabla \phi\ ;\ \ \mathbf{E} = -\mathbf{u} \times \mathbf{B} + \ \eta \mathbf{J};\ \ \mathbf{J} = \frac{1}{\mu_0}\nabla \times \mathbf{B};\ \mathbf{B} = \nabla \times \mathbf{A}$

## Magnetic Vector-Potential Form.: Hydromagnetic Kelvin-Helmholtz Problem (fixed CFL)

**Structure of Block Preconditioner: Critical 3x3 Block Sys.**

**Operator-Split into 2 – 2x2 Sys. with Sparse Schur Complement Approximations**

Mixed basis*:



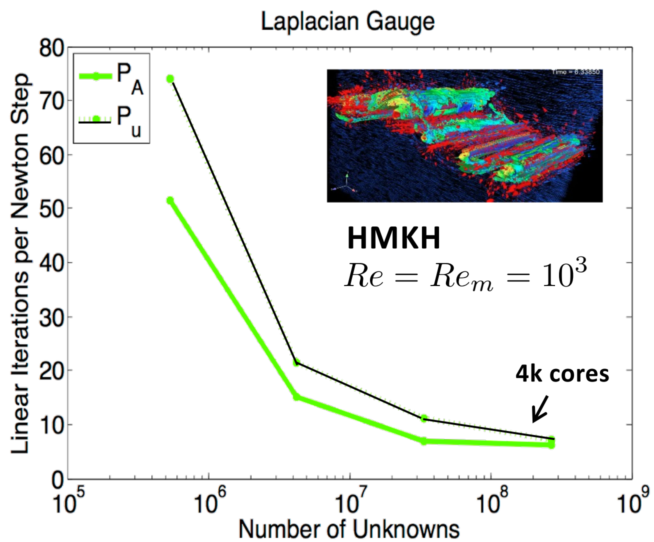

$$\mathcal{A}_{GSG} = \left( \begin{array}{ccc|c} F & B^t & Z & 0 \\ B & C & 0 & 0 \\ Y & 0 & G & D^t \\ \hline 0 & 0 & 0 & L \end{array} \right) \qquad \mathcal{P}_{\mathbf{A}} = \begin{pmatrix} F & 0 & Z \\ 0 & I & 0 \\ Y & 0 & G \end{pmatrix} \begin{pmatrix} F^{-1} & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix} \begin{pmatrix} F & B^t & 0 \\ B & C & 0 \\ 0 & 0 & I \end{pmatrix}$$

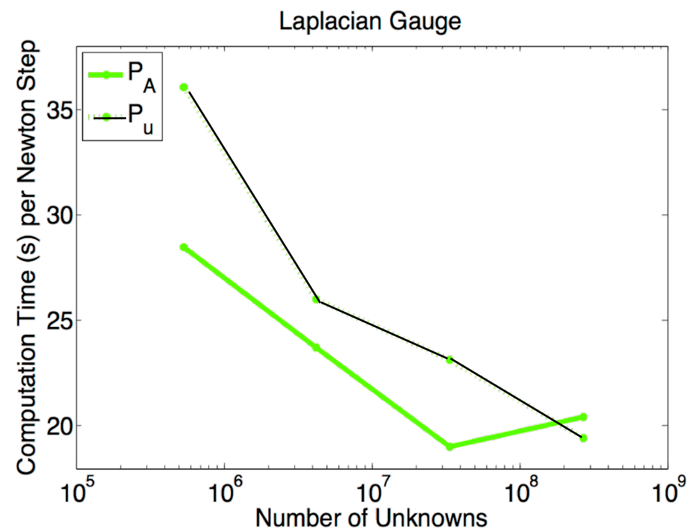
$$\hat{S}_{\mathbf{A}} = G - Y\hat{F}^{-1}Z \quad \text{(SIMPLEC, Alfven wave)}$$

$$\hat{S}_P = C - B\hat{F}^{-1}B^t \quad \text{(PCD)}$$

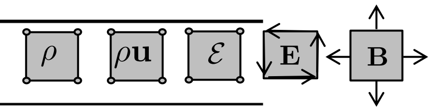
**Segregation into**

- **H(grad) system AMG for velocity**
- **H(curl) AMG for magnetic vector potential (SIMPLEC approx.)**
- **Scalar H(grad) AMG for pressure (PCD commutator)**



# 5 Moment Multi-fluid EM Plasma System Model



| | |
|---|---|
| Density | $\partial_t \rho_s + \nabla\cdot\left(\rho_s \mathbf{u}_s\right) = -\rho_s n_e \left(I_s + R_s\right) + m_s n_e \left(n_{s-1} I_{s-1} + n_{s+1} R_{s+1}\right)$ |
| Momentum | $\partial_t \left(\rho_s \mathbf{u}_s\right) + \nabla\cdot\left(\rho_s \mathbf{u}_s \otimes \mathbf{u}_s + p_s \underline{\mathbf{I}} + \underline{\boldsymbol{\Pi}}_s\right) = q_s n_s \left(\mathbf{E} + \mathbf{u}_s \times \mathbf{B}\right) + \sum_{t\neq s} \alpha_{s;t} \rho_s \rho_t \left(\mathbf{u}_t - \mathbf{u}_s\right)$ $-\rho_s \mathbf{u}_s n_e \left(I_s + R_s\right) + \frac{m_s}{m_{s-1}} n_e \rho_{s-1} \mathbf{u}_{s-1} I_{s-1} + \left(n_e \rho_{s+1} \mathbf{u}_{s+1} + n_{s+1} \rho_e \mathbf{u}_e\right) R_{s+1}$ |
| Energy | $\partial_t \mathcal{E}_s + \nabla\cdot\left[\left(\mathcal{E}_s + p_s\right)\mathbf{u}_s + \mathbf{u}_s \cdot \underline{\boldsymbol{\Pi}}_s + \mathbf{h}_s\right] = q_s n_s \mathbf{u}_s \cdot \mathbf{E} + \sum_{t\neq s} \frac{\alpha_{s;t}\rho_s\rho_t}{m_s + m_t}\left[A_{s;t} k_{\mathrm{B}} \left(T_t - T_s\right) + m_t \left(\mathbf{u}_t - \mathbf{u}_s\right)^2\right]$ $-\mathcal{E}_s n_e \left(I_s + R_s\right) + \frac{m_s}{m_{s-1}} n_e \mathcal{E}_{s-1} I_{s-1} + \left(n_e \mathcal{E}_{s+1} + n_{s+1} \mathcal{E}_e\right) R_{s+1}$ |
| Charge and Current | $q = \sum_s q_s n_s$ $\qquad \mathbf{J} = \sum_s q_s n_s \mathbf{u}_s$ |
| Maxwell's Equations | $\frac{1}{c^2}\partial_t \mathbf{E} - \nabla\times\mathbf{B} + \mu_0 \mathbf{J} = \mathbf{0}$ $\qquad \nabla\cdot\mathbf{E} = \frac{q}{\epsilon_0}$ <br> $\partial_t \mathbf{B} + \nabla\times\mathbf{E} = \mathbf{0}$ $\qquad \nabla\cdot\mathbf{B} = 0$ |

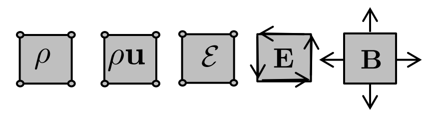
Other work on multifluid plasma formulations, solution algorithms:

See e.g.
Abgral et. al.;
Barth;
Kumar et. al.;
Laguna et. al.;
Rossmanith et. al.;
Shumlak et. al.;
B. Srinivasan et. al.;

## Scalable Physics-based Preconditioners for Physics-compatible Discretizations

$$
\left[\begin{array}{cccccc|c|c}
\mathbf{D}_{\rho_i} & \mathbf{K}^{\rho_i}_{\rho_i u_i} & 0 & \mathbf{Q}^{\rho_i}_{\rho_e} & 0 & 0 & 0 & 0 \\
\mathbf{D}^{\rho_i u_i}_{\rho_i} & \mathbf{D}_{\rho_i u_i} & 0 & \mathbf{Q}^{\rho_i u_i}_{\rho_e} & \mathbf{Q}^{\rho_i u_i}_{\rho_e u_e} & 0 & \mathbf{Q}^{\rho_i u_i}_{E} & \mathbf{Q}^{\rho_i u_i}_{B} \\
\mathbf{D}^{\mathcal{E}_i}_{\rho_i} & \mathbf{D}^{\mathcal{E}_i}_{\rho_i u_i} & \mathbf{D}_{\mathcal{E}_i} & \mathbf{Q}^{\mathcal{E}_i}_{\rho_e} & \mathbf{Q}^{\mathcal{E}_i}_{\rho_e u_e} & \mathbf{Q}^{\mathcal{E}_i}_{\mathcal{E}_e} & \mathbf{Q}^{\mathcal{E}_i}_{E} & 0 \\
\mathbf{Q}^{\rho_e}_{\rho_i} & 0 & 0 & \mathbf{D}_{\rho_\mathbf{e}} & \mathbf{K}^{\rho_e}_{\rho_e u_e} & 0 & 0 & 0 \\
\mathbf{Q}^{\rho_e u_e}_{\rho_i} & \mathbf{Q}^{\rho_e u_e}_{\rho_i u_i} & 0 & \mathbf{D}^{\rho_e u_e}_{\rho_e} & \mathbf{D}_{\rho_e u_e} & 0 & \mathbf{Q}^{\rho_e u_e}_{E} & \mathbf{Q}^{\rho_e u_e}_{B} \\
\mathbf{Q}^{\mathcal{E}_e}_{\rho_i} & \mathbf{Q}^{\mathcal{E}_e}_{\rho_i u_i} & \mathbf{Q}^{\mathcal{E}_e}_{\mathcal{E}_i} & \mathbf{D}^{\mathcal{E}_e}_{\rho_e} & \mathbf{D}^{\mathcal{E}_e}_{\rho_e u_e} & \mathbf{D}_{\mathcal{E}_e} & \mathbf{Q}^{\mathcal{E}_e}_{E} & 0 \\
\hline
0 & \mathbf{Q}^{E}_{\rho_i u_i} & 0 & 0 & \mathbf{Q}^{E}_{\rho_e u_e} & 0 & \mathbf{Q}_E & \mathbf{K}^{E}_{B} \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & \mathbf{K}^{B}_{E} & \mathbf{Q}_B
\end{array}\right]
\left[\begin{array}{c}
\rho_i \\ \rho_i \mathbf{u}_i \\ \mathcal{E}_i \\ \rho_e \\ \rho_e \mathbf{u}_e \\ \mathcal{E}_e \\ \hline \mathbf{E} \\ \hline \mathbf{B}
\end{array}\right]
$$

**Ion/electron plasma**
**~16 Coupled**
**Nonlinear PDEs**




**Group the hydrodynamic variables together (similar H(grad) discretization)**

$$\mathbf{F} = (\rho_i, \rho_i \mathbf{u}_i, \mathcal{E}_i, \rho_e, \rho_e \mathbf{u}_e, \mathcal{E}_e)$$

**Resulting 3x3 block system**

$$
\begin{bmatrix}
\mathbf{D}_F & \mathbf{Q}^F_E & \mathbf{Q}^F_B \\
\mathbf{Q}^E_F & \mathbf{Q}_E & \mathbf{K}^E_B \\
0 & \mathbf{K}^B_E & \mathbf{Q}_B
\end{bmatrix}
\begin{bmatrix}
\mathbf{F} \\ \mathbf{E} \\ \mathbf{B}
\end{bmatrix}
$$

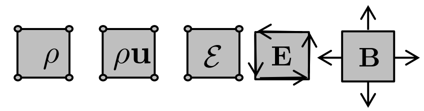
**Reordered 3x3**

$$
\begin{bmatrix}
\mathbf{Q}_B & \mathbf{K}^B_E & 0 \\
\mathbf{K}^E_B & \mathbf{Q}_E & \mathbf{Q}^E_F \\
\mathbf{Q}^F_B & \mathbf{Q}^F_E & \mathbf{D}_F
\end{bmatrix}
\begin{bmatrix}
\mathbf{B} \\ \mathbf{E} \\ \mathbf{F}
\end{bmatrix}
$$

## ***Physics-based/ABF Approach Enables Optimal AMG Sub-block Solvers***

$$\begin{bmatrix} \mathbf{Q}_B & \mathbf{K}_E^B & 0 \\ 0 & \hat{\mathcal{D}}_E & \mathbf{Q}_F^E \\ 0 & 0 & \hat{\mathbf{S}}_F \end{bmatrix} \begin{bmatrix} \mathbf{B} \\ \mathbf{E} \\ \mathbf{F} \end{bmatrix}$$

**16 Coupled Nonlinear PDEs**




$$\hat{\mathbf{S}}_F = \mathbf{D}_F - \mathcal{K}_E^F \tilde{\tilde{\mathcal{D}}}_E^{-1} Q_F^E$$

**CFD type system**
**node-based coupled**
**ML: H(grad) AMG**
**(SIMPLEC: Schur-compl.)**

$$\hat{\mathcal{D}}_E = \mathbf{Q}_E + \mathbf{K}_B^E \bar{\mathbf{Q}}_B^{-1} \mathbf{K}_E^B$$

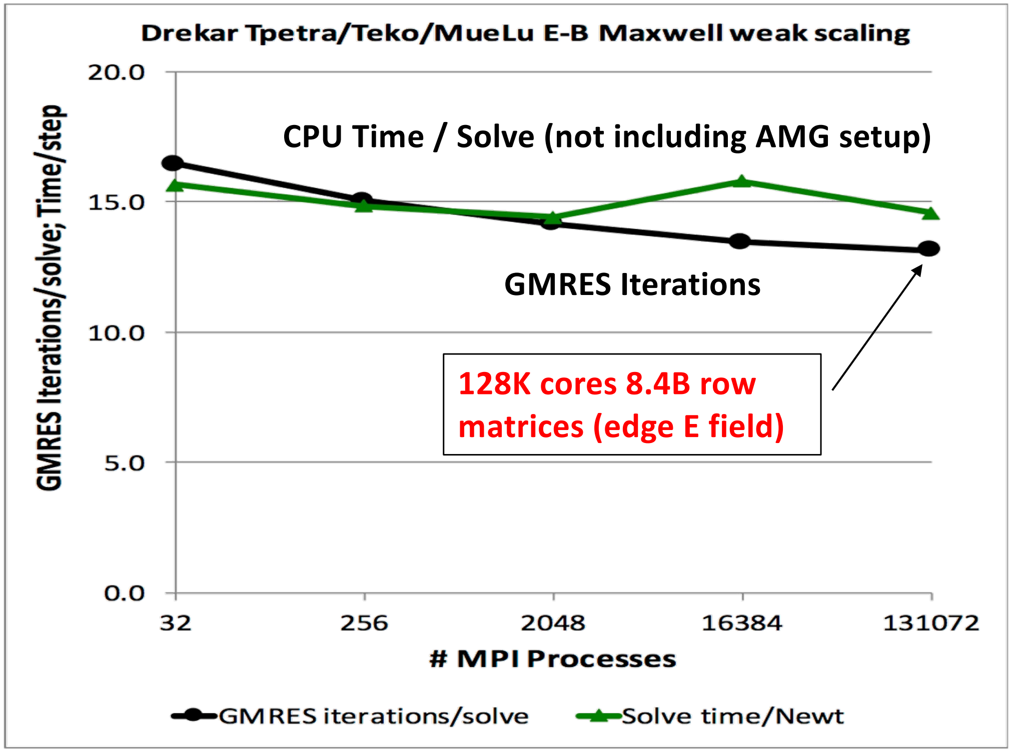
**Compare to:** $\dfrac{\partial^2 \mathbf{E}}{\partial t^2} + \dfrac{1}{\sigma \mu_0} \nabla \times \nabla \times \mathbf{E} = \mathbf{0}$

**Electric field system**
**Edge-based curl-curl type**
**ML: H(grad) AMG with grad-div stab.**
**or H(curl) AMG (ML-refMaxwell, or Hyper-AMS)**

$$\mathbf{B} = -\bar{\mathbf{Q}}_B^{-1} \mathbf{K}_E^B \; \mathbf{E}$$

**Face-based simple**
**mass matrix Inversion.**
**V-cycle Gauss-Seidel**

## Weak Scaling for 3D Free-space Electro Magnetic Pulse with Block Maxwell Eq. Preconditioners on Trinity




$$\mathcal{D}^E = \mathbf{Q}_E - \mathbf{K}_B^E \bar{\mathbf{Q}}_B^{-1} \mathbf{K}_E^B$$

**Maxwell subsystem: electric field**
**Edge-based curl-curl type system**
**with grad-div stabilization for AMG.**

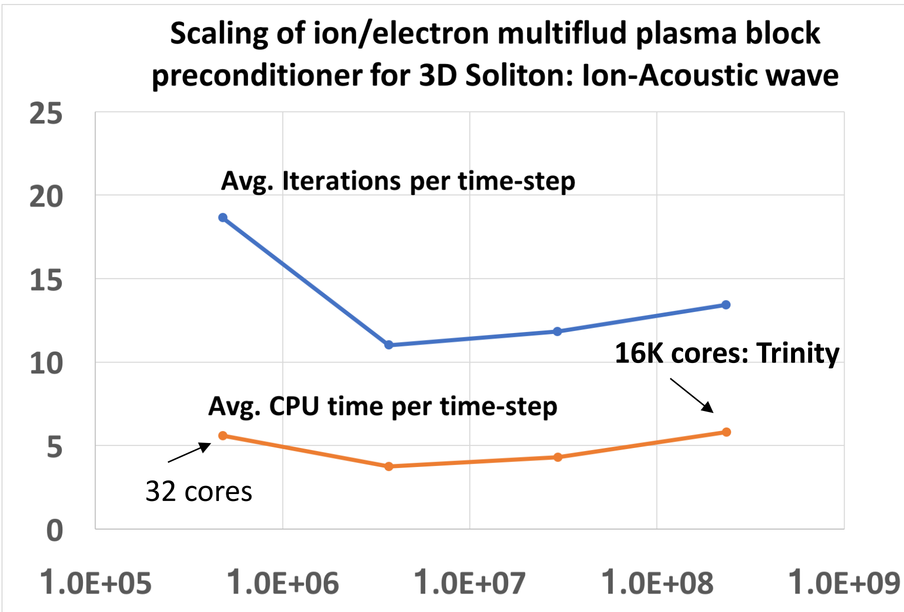
**Good scaling on block solves (at least for solve; setup needs improvement)**

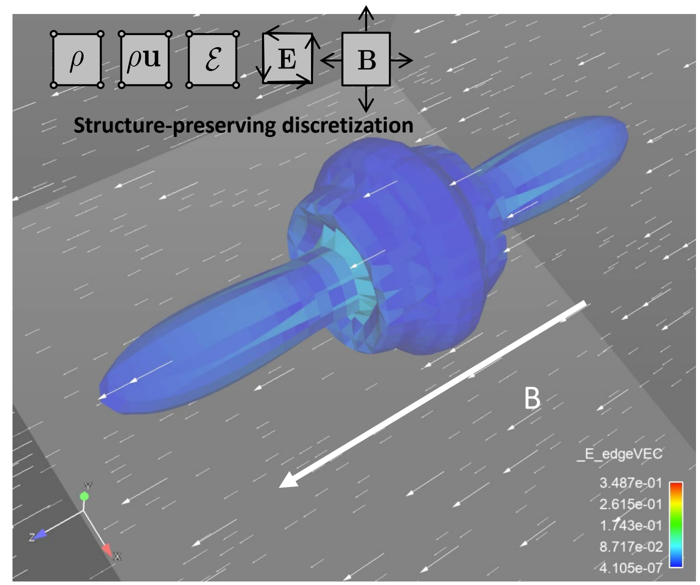
**Max $CFL_{EM}$ ~200, demonstrated to $CFL_c > 10^4$ on many applications**

GS smoother with H(grad) AMG

Max $CFL_c$ ~ 200

# Demonstration of scalable physics-based preconditioners / solvers for multifluid (ion-electron) EM plasmas: 3D Gaussian high pressure initial condition for isentropic ion-acoustic wave propagation




Iso-surface of ion density colored by electric field magnitude

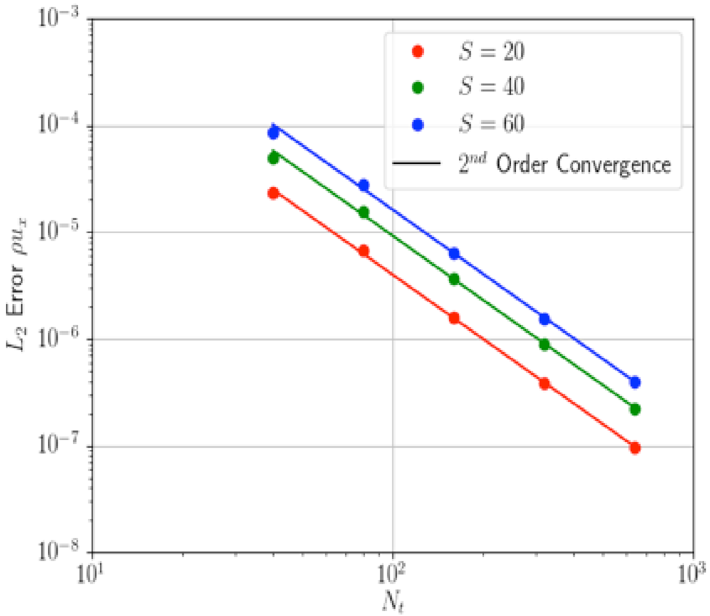
1) SimpleC for E,B contribution to fluid Schur-complement
2) System H(grad) AMG 1 V-cycle DD-ILU smoother for Euler sub-system.
3) H(grad) AMG 1 V-cycle for Grad-div stabilized curl-curl system & DD-LU smoother
4) H(grad) AMG 1 V-cycle for B field mass matrix & Gauss-Seidel smoother

Isentropic flow $\frac{P}{P_0} = (\frac{\rho}{\rho_0})^\gamma$

$$\mu = \frac{m_i}{m_e} = 25$$

# Robustness and Accuracy: Asymptotic IMEX Solution of Full Multifluid EM Plasma Model in MHD Limit (Visco-Resistive Alfven Wave)

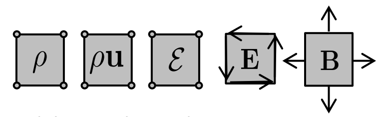
*Implicit L-stable and IMEX SSP/L-stable time integration and block preconditioners enable solution of multifluid EM plasma model in the asymptotic resistive MHD limit.*




Accuracy in MHD limit (IMEX)

| Plasma Scales for S = 60 | | |
|---|---|---|
| | Electrons | Ions |
| $\omega_p \Delta t$ | $10^7$ - $10^9$ | $10^6$ - $10^7$ |
| $\omega_c \Delta t$ | $10^6$ - $10^7$ | $10^3$ - $10^4$ |
| $\nu_{\alpha\beta} \Delta t$ | $10^{10}$ - $10^{11}$ | $10^7$ - $10^8$ |
| $\nu_S \Delta t/\Delta x$ | $10^{-2}$ | $10^{-4}$ |
| $u \Delta t/\Delta x$ | $10^{-4}$ | $10^{-4}$ |
| $\mu \Delta t/\rho \Delta x^2$ | $10^{-1}$ - $10^1$ | $10^{-2}$ - $10^0$ |
| $c \Delta t/\Delta x$ | $10^2$ | |

IMEX terms: implicit/explicit




Nodal FE Hydro and Structure-preserving discretization for EM

Implicitly overstepping stiff modes, not controlling accuracy, can make an intractable explicit computation – tractable with IMEX methods.

Overstepping fast time scales is both stable and accurate. The inclusion of a resistive operator adds dissipation to the electron dynamics on top of the L-stable time integrator.


S. T. Miller, E. C. Cyr, JS, R. M. J. Kramer, E. G. Phillips, S. Conde, R. P. Pawlowski, IMEX and exact sequence discretization of the multi-fluid plasma model. In press for JCP

# 2 Tokamak Related Preliminary Examples

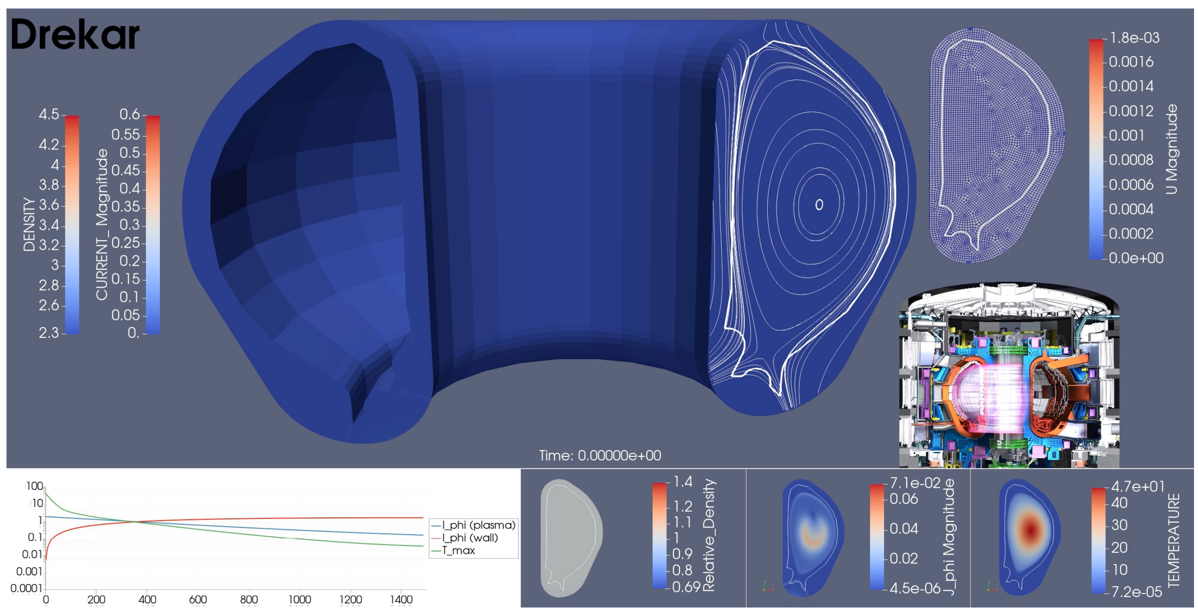
**Computational Goals of Tokamak Disruption Simulation (TDS) Center SciDAC-4 Partnership (DOE OFES/ASCR)**

**Develop and evaluate advanced hierarchy of plasma physics models and scalable solution methods to understand disruption physics and explore mitigation strategies to avoid damage to the reactor.**

- ❑ **Attempt is to achieve temperature of ~100M deg K (6x Sun temp.),**
- ❑ **Energy confinement times O(1-10) min. are desired.**
- ❑ **Plasma instabilities/disruptions can cause break of confinement, huge plasma thermal energy loss, and discharge very large electrical currents (~20MA) into structure.**
- ❑ **ITER can sustain only a limited number of disruptions, O(1 – 5) significant instabilities.**

Proof-of-principle

Vertical displacement event (VDE) disruption simulation in ITER plasma and wall region.



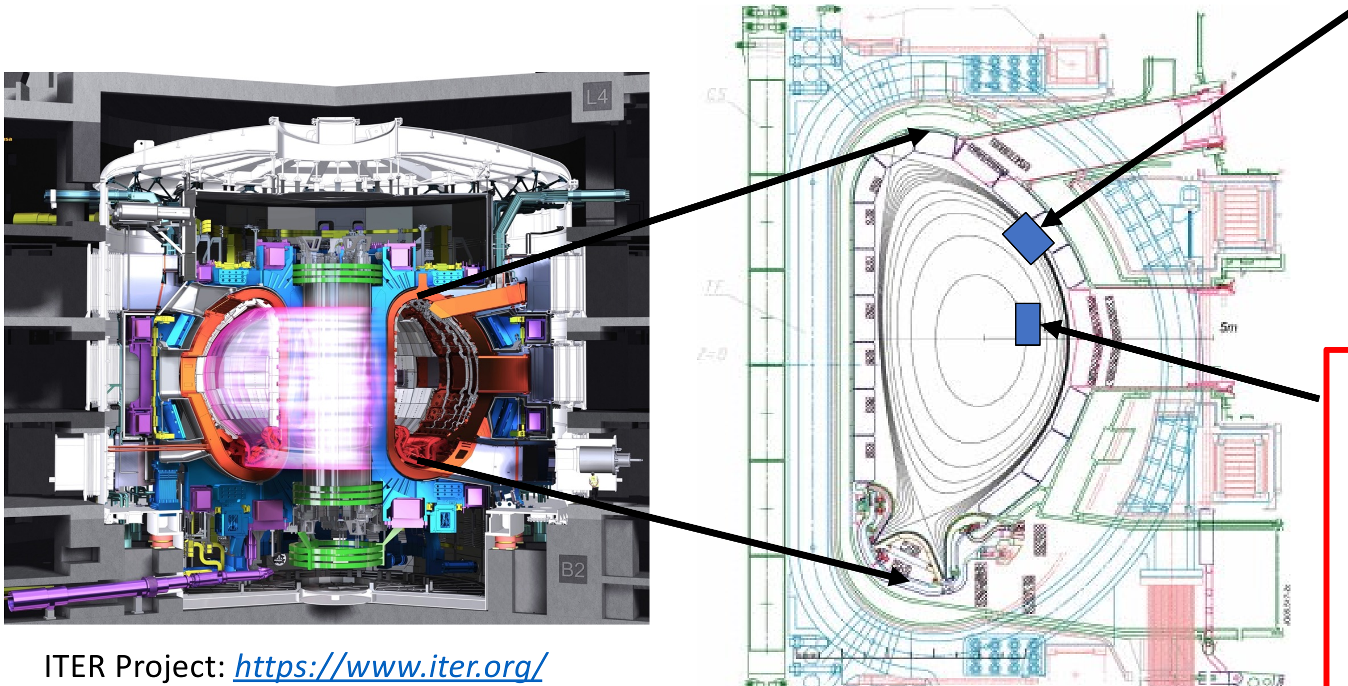
## An Approximate Block Factorization of 3x3 Jacobin system leads to two 2x2 systems and allows more efficient larger Alfven wave CFL simulations (e.g. plasma only region)

$$\begin{bmatrix} \mathbf{F_B} & \mathcal{B}_\mathbf{B}{}^T & \mathbf{Y}_{\text{nst}} \\ \mathcal{B}_\mathbf{B} & \mathbf{L_r} & \mathbf{C}_{\text{nst}} \\ \mathbf{Z} & & \mathbf{F}_{\text{nst}} \end{bmatrix} \approx \begin{bmatrix} \mathbf{F_B} & & \mathbf{Y}_{\text{nst}} \\ & \mathbf{I} & \\ \mathbf{Z} & & \mathbf{F}_{\text{nst}} \end{bmatrix} \begin{bmatrix} \mathbf{F_B}{}^{-1} & & \\ & \mathbf{I} & \mathbf{C}_{\text{nst}} \\ & & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{F_B} & \mathcal{B}_\mathbf{B}{}^T & \\ \mathcal{B}_\mathbf{B} & \mathbf{L_r} & \\ & & \mathbf{I} \end{bmatrix}$$

| $\text{CFL}_a^{max}$ | Num. Timestep | Linear Its. per non-Lin It. | Setup Time | Solve Time | Total Time |
|---|---|---|---|---|---|
| 50 | 1764 | 25.48 | 25250.70 | 16628.80 | 41879.50 |
| 100 | 908 | 29.16 | 13283.60 | 9835.80 | 23119.40 |
| 200 | 490 | 34.27 | 7367.84 | 6293.74 | 13661.58 |
| 400 | 288 | 42.86 | 4594.03 | 4838.48 | 9432.51 |
| 600 | 222 | 49.33 | 3680.76 | 4435.00 | 8115.76 |
| 800 | 196 | 84.73 | 3310.57 | 6864.51 | 10175.08 |
| 1000 | 186 | 136.23 | 3169.22 | 10972.20 | 14141.42 |
| 1600 | 180 | 138.63 | 3190.51 | 11202.20 | 14392.71 |

- ILUT with threshold=0.1 for $S_{nst}$
- Enforce max $\text{CFL}_\mathbf{u} \leq 1$
- Lundquist number $S = 3 \times 10^3$

***Disruption is a prompt termination of a plasma confinement in a tokamak and can be a showstopper for ITER. Mitigate to control thermal and current quench evolution.***




ITER Project: https://www.iter.org/

DOE Advanced Scientific Computing Research (ASCR) / Office of Fusion Energy (OFES)
SciDAC Partnership: Tokamak Disruption Simulation (TDS) Project

**Preliminary Models of Gas Injection for Disruption Mitigation**

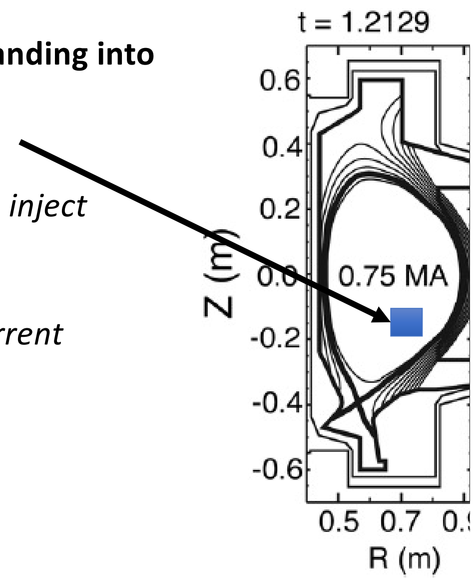
Dynamics of Neutral Gas Jet Injection at an angle wrt B Field

- Hydrodynamics of jet
- Collisional effects
- Ionization/recombination
    - E field interactions for charged species
    - Interactions with B field for charged species

Gas Injection Assumed Distribution at time t= 0 for Neutral Gas Core Inside Separatrix

- Hydrodynamics of neutral core expansion
- Collisional effects
- Ionization/recombination
    - E field interactions for charged species
    - In 2D,3D interactions with B field for charged species

**Preliminary 1D Gas Injection Simulations of Higher Z Neutral Gas (He, Ne, Ar ) Cores Expanding into a 100ev Deuterium (D+,e-) Plasma**




- *To attempt to control the loss of plasma internal energy (thermal quench) one idea is to inject neutral impurities to enhance radiation loss.*

- *To mitigate the effect of runaway electrons potentially impacting the wall (electrical current quench), an idea is to inject neutrals to enhance dissipation of high-energy electrons.*

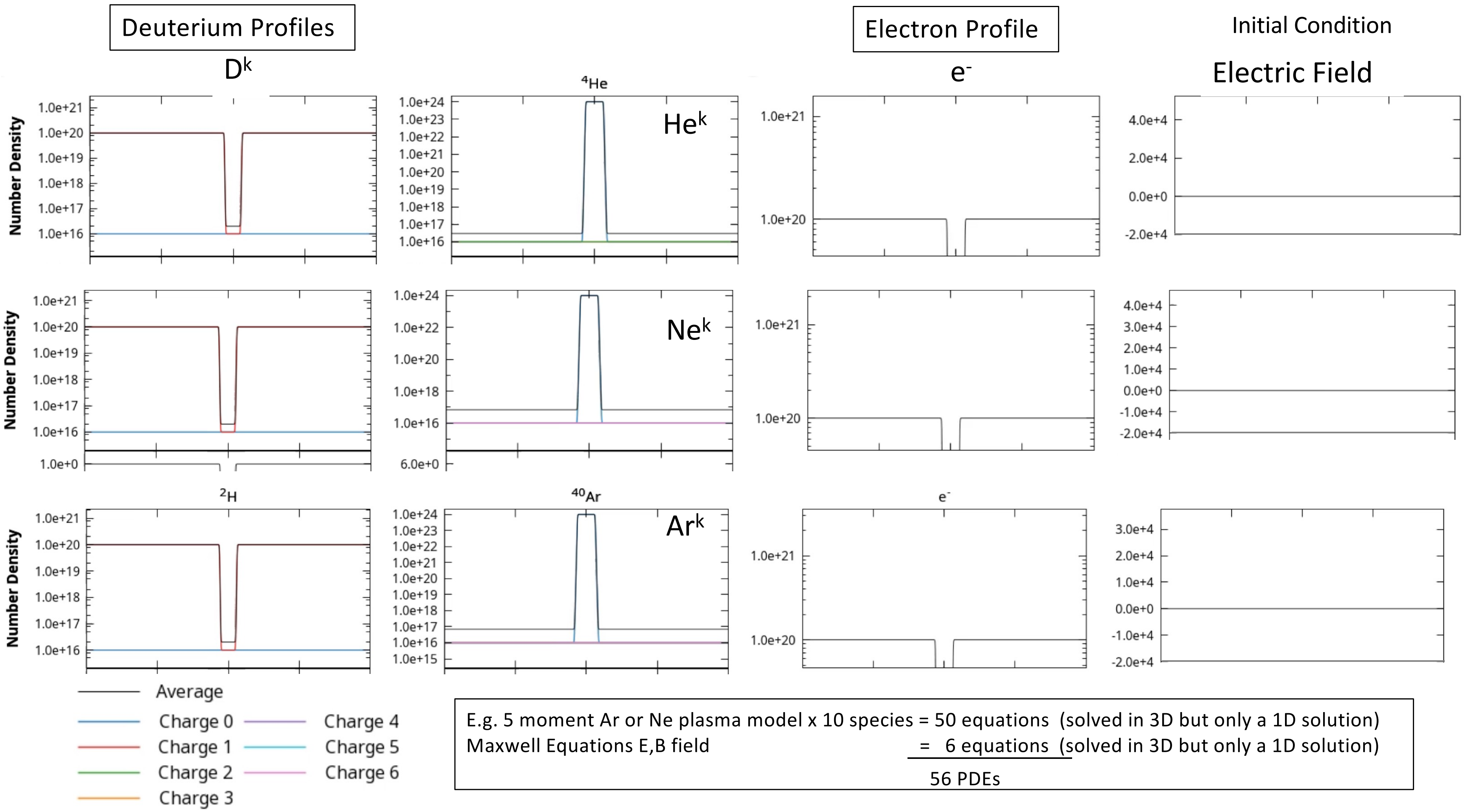
<u>Problem outline: Representative of the core plasma</u>

- Initial ~fully ionized Deuterium plasma at n = $10^{20}$, T = 100ev (~1M degrees K)

- Neutral Argon ($Ar^0$) core introduced at n = $10^{24}$ , T = $10^{-1}$ev (~1000 degrees K)

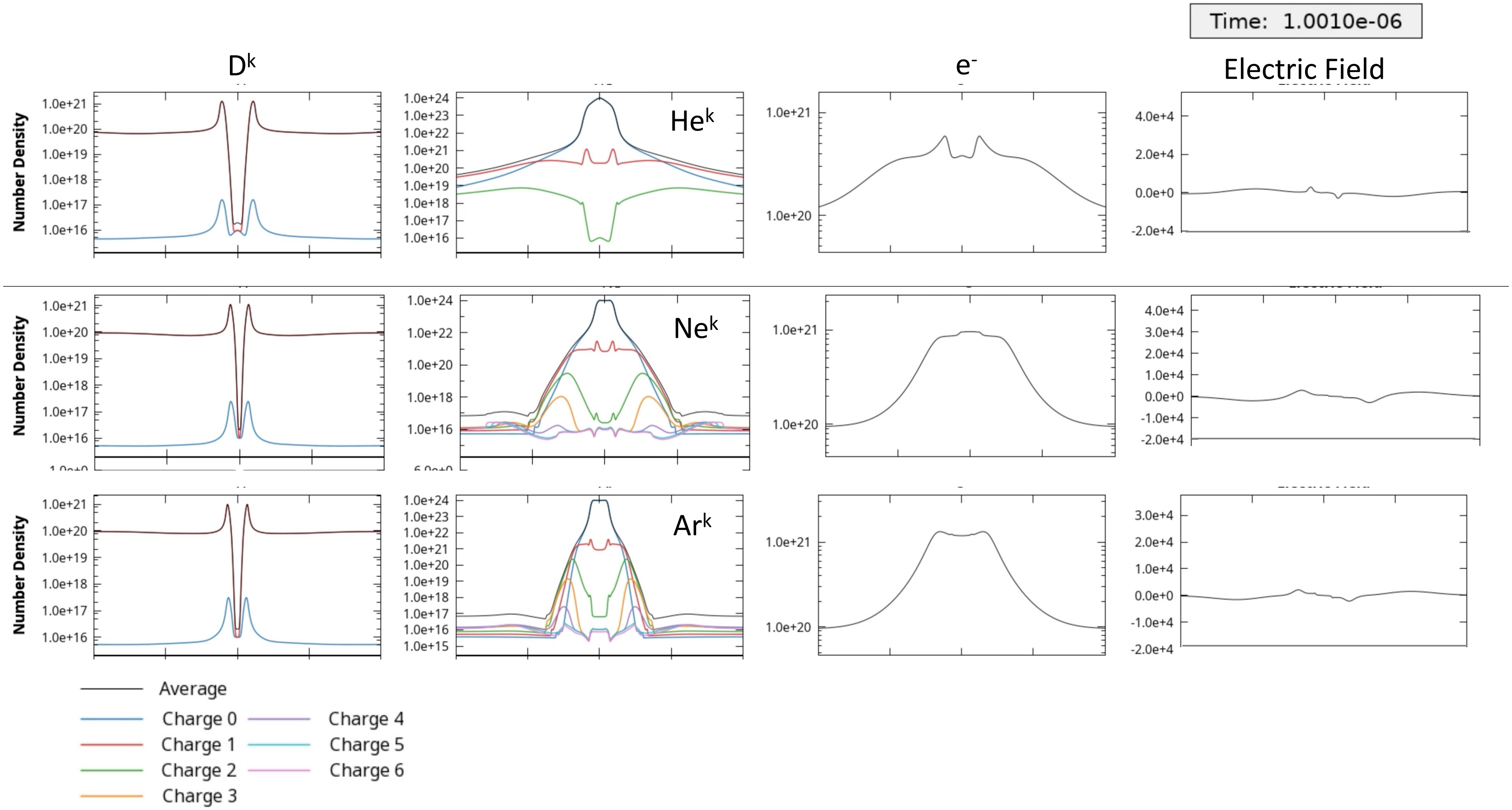
- Parallel B – field is ignorable (due to geometry in 1D so B does not modify transport)

- Domain in x is [0.3m,0.3m]; mesh is 4096 x 1 x 1 elements

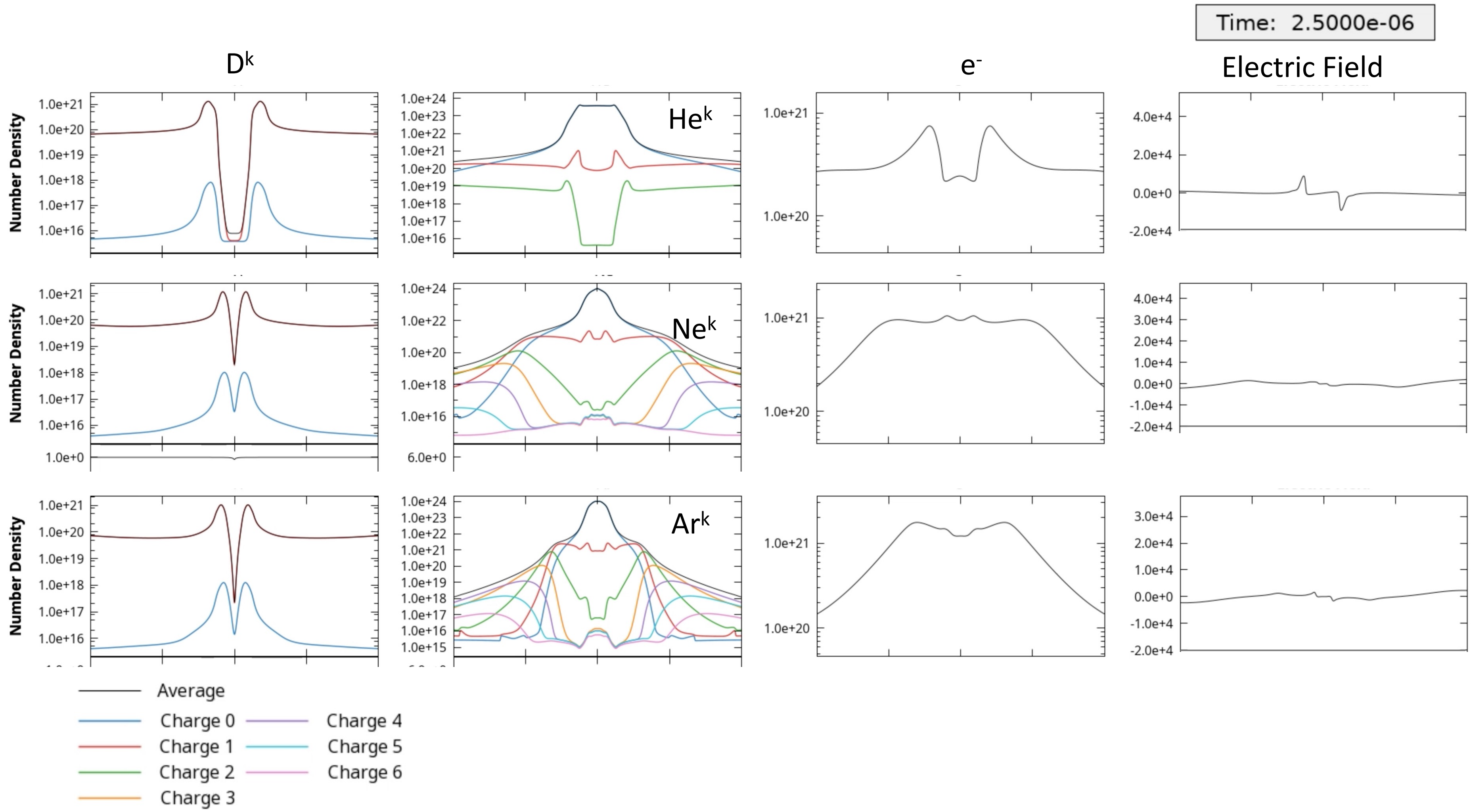



E.g. 5 moment Ar or Ne plasma model x 10 species = 50 equations (solved in 3D but only a 1D solution)
Maxwell Equations E,B field = 6 equations (solved in 3D but only a 1D solution)

56 PDEs

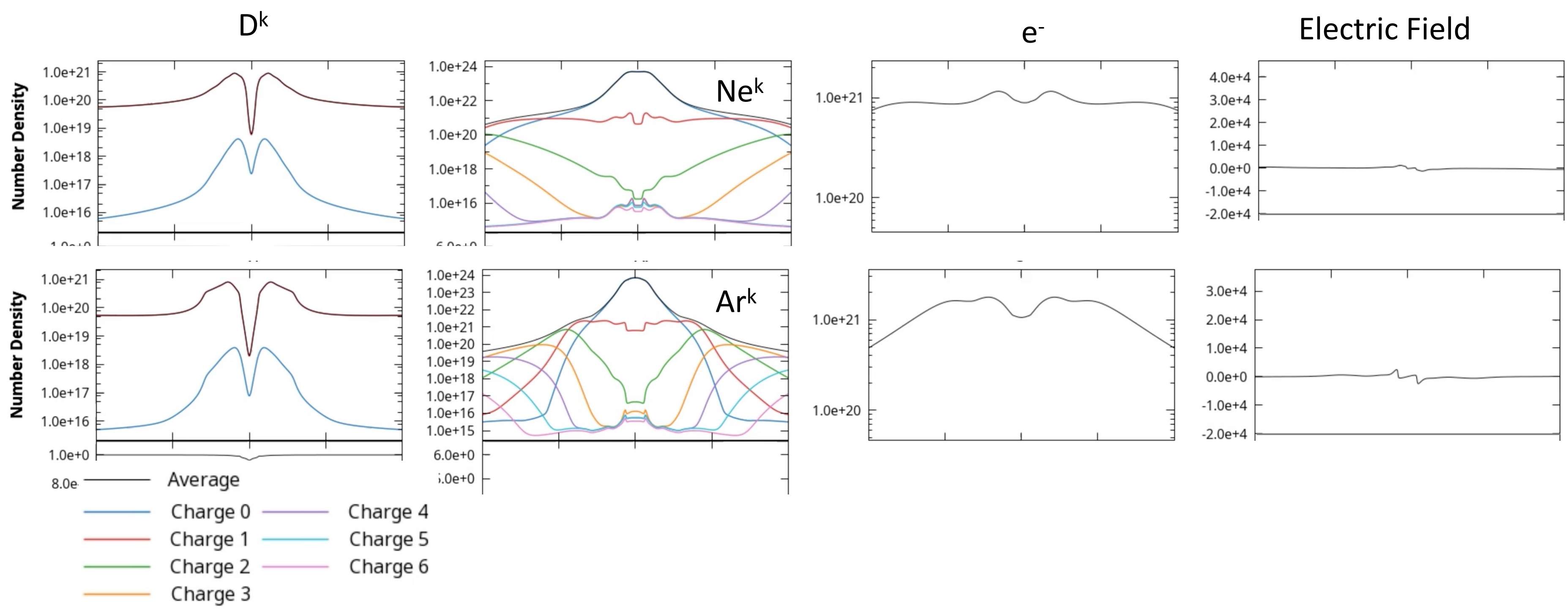


Time: 1.0010e-06
Dk
e-
Electric Field
Hek
Nek
Ark
Number Density
1.0e+21
1.0e+20
1.0e+19
1.0e+18
1.0e+17
1.0e+16
1.0e+24
1.0e+23
1.0e+22
1.0e+15
4.0e+4
3.0e+4
2.0e+4
1.0e+4
0.0e+0
-1.0e+4
-2.0e+4
Average
Charge 0
Charge 1
Charge 2
Charge 3
Charge 4
Charge 5
Charge 6



Time: 2.5000e-06
D^k
He^k
Ne^k
Ar^k
e^-
Electric Field
Number Density
1.0e+21
1.0e+20
1.0e+19
1.0e+18
1.0e+17
1.0e+16
1.0e+24
1.0e+23
1.0e+22
1.0e+15
1.0e+0
6.0e+0
4.0e+4
3.0e+4
2.0e+4
1.0e+4
0.0e+0
-1.0e+4
-2.0e+4
Average
Charge 0
Charge 1
Charge 2
Charge 3
Charge 4
Charge 5
Charge 6

Time: 5.0000e-06



## Conclusions

- **Robustness, efficiency / scalability of fully-implicit /IMEX parallel NK - AMG solvers is very good.**
- **Physics-based block decomposition and approximate Schur complement preconditioners must have effective approximation of dominant off-diagonal coupling and time-scales in MHD/multifluid plasmas represented. Can provide scalable solution of complex multiphysics plasma models.**
- **Iterative solvers and (nonlinear/linear ) convergence criteria for multiphysics systems is challenging!**
- **General mathematical libraries and components (e.g. Trilinos) are very valuable for enabling:**
  - **Flexible development of implicit formulations of multiphysics systems (e.g. MHD, multifluid)**
  - **Exploration of advanced physics/mathematical models and PDE spatial discretizations**
  - **Dev. of complex physics-based / approximate Schur complement block preconditioners**
- **Adoption of well defined, and functionally separated, solution method kernels to promote robustness and help in assessment when time-step failure, convergence problems occur.**
  - **IMEX time-integration, Nonlinear solvers, Linear solvers, Scalable block and AMG preconditioning**

The End.