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Scalable Block Preconditioning Methods for Solution of Implicit / IMEX Finite Element Continuum Plasma Physics Models

John N. Shadid

Computational Mathematics Department
Sandia National Laboratories

**Department of Mathematics and Statistics*
University of New Mexico

Collaborators:

Roger Pawlowski, Edward Phillips, Paul Lin, Eric Cyr, Ray Tuminaro, Sidafa Conde, Sibu Mabuza

Sandia National Laboratories

Luis Chacon

Los Alamos National Lab

Fusion Energy Sciences

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Outline

- General Scientific and Mathematical/Computational Motivation
- Very Brief Description of Resistive MHD and Multifluid EM Plasma Models
- Overview of Numerical Solution Methods
- Scalable Solution of
  - Stabilized FE Resistive MHD (Fully-coupled system AMG)
  - Structure Preserving MHD (Approximate Block Factorization & AMG sub-block solvers)
  - Multifluid EM Plasmas (ion/electron)
- Very Preliminary Results for Reconnection and Tokamak Related Simulations

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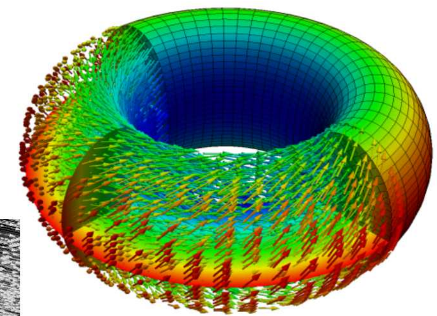
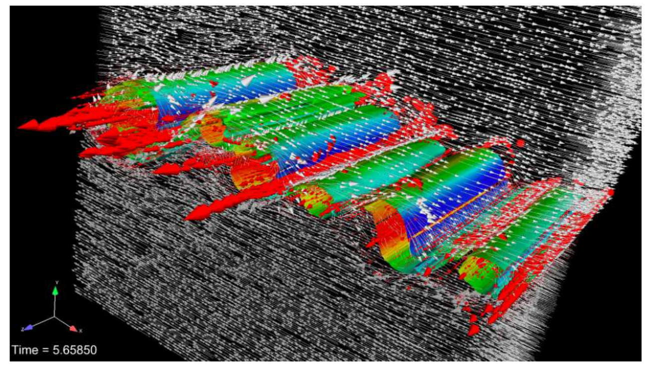
Motivation: Science/Technology



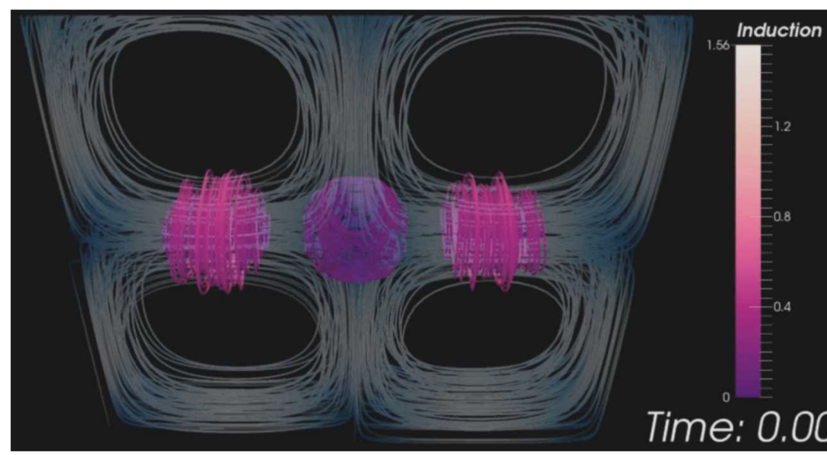
MHD tokamak equilibrium (Soloveev)

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

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



Hydromagnetic Kelvin-Helmholtz Instability



MHD Taylor-Green Vortex with Sondak (Harvard), Oberai (USC)

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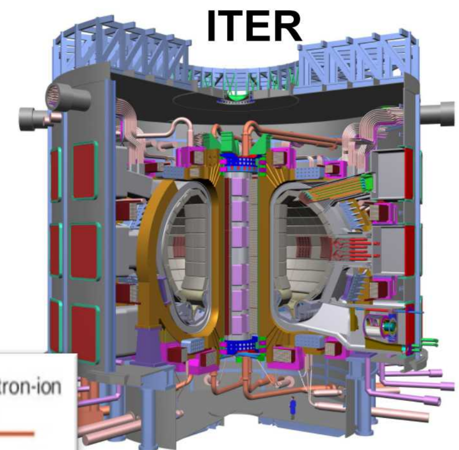
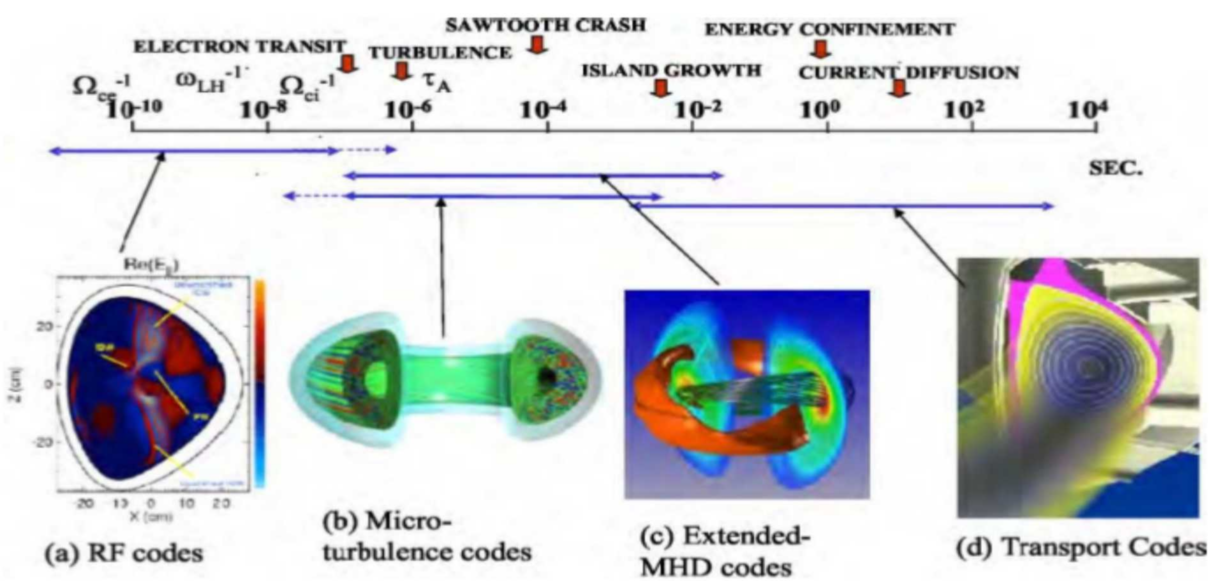
Tokamak Magnetic Confinement Fusion (MCF): Understanding and controlling instabilities/disruptions in plasma confinement is critical.

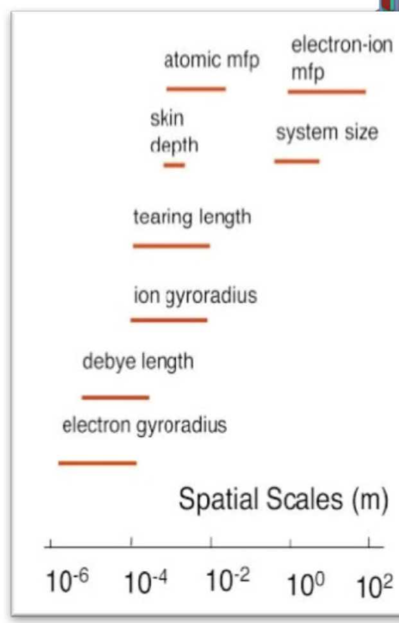


Goal for Fusion Device:

- **Attempt is to achieve temperature of ~100M deg K (6x Sun temp.) ,**
- **Energy confinement times O(1 – 10) min is desired.**

MCF Devices 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

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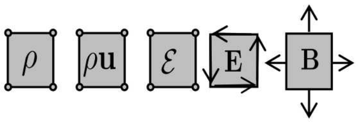
Our Mathematical Approach - develop:

- **Stable, higher-order accurate implicit/IMEX formulations for multiple-time-scale systems**

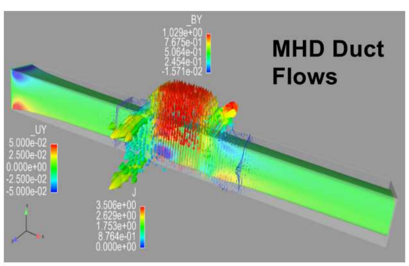
- **Stable and accurate unstructured FE spatial discretizations. Options enforcing key mathematical properties (e.g. structure preserving forms: div B = 0; positivity ρ , P; DMP)**

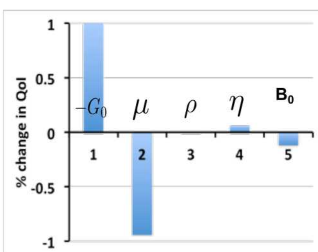


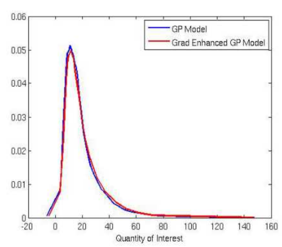
- **Robust, efficient fully-coupled nonlinear/linear iterative solution based on Newton-Krylov methods**

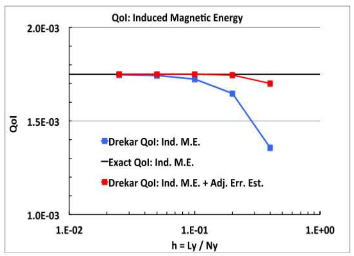
- **Scalable and efficient multiphysics preconditioners utilizing physics-based and approximate block factorization/Schur complement preconditioners with multi-level (AMG) sub-block solvers**

=> Also enables beyond forward simulation & integrated UQ (adjoints - error estimates, sensitivities; surrogate modeling (E.g. GP), …)









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A Few Examples of Relevant Continuum / PDE-based Models for

- Resistive MHD,
- Multifluid Plasmas,

and Associated Solution Methods

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

Resistive MHD Model in Residual Notation

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

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

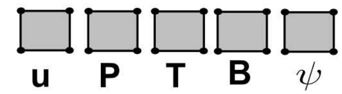
$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot [\rho \mathbf{v} \otimes \mathbf{v} - (\mathbf{T} + \mathbf{T}_M)] + 2\rho\Omega \times \mathbf{v} - \rho \mathbf{g} = \mathbf{0}$$

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

$$\frac{\partial \Sigma_{tot}}{\partial t} + \nabla \cdot \left[(\rho e + \frac{1}{2}\rho\|\mathbf{u}\|^2)\mathbf{u} + \frac{\mathbf{E} \times \mathbf{B}}{\mu_0} + \mathbf{T} \cdot \mathbf{u} + \mathbf{q}\right] = 0 \qquad \Sigma_{tot} = \rho e + \frac{1}{2}\rho\|\mathbf{u}\|^2 + \|\mathbf{B}\|^2/2\mu_0$$

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

$$\frac{1}{c_h}\frac{\partial \psi}{\partial t} + \frac{1}{c_p}\psi + \nabla \cdot \mathbf{B} = 0$$

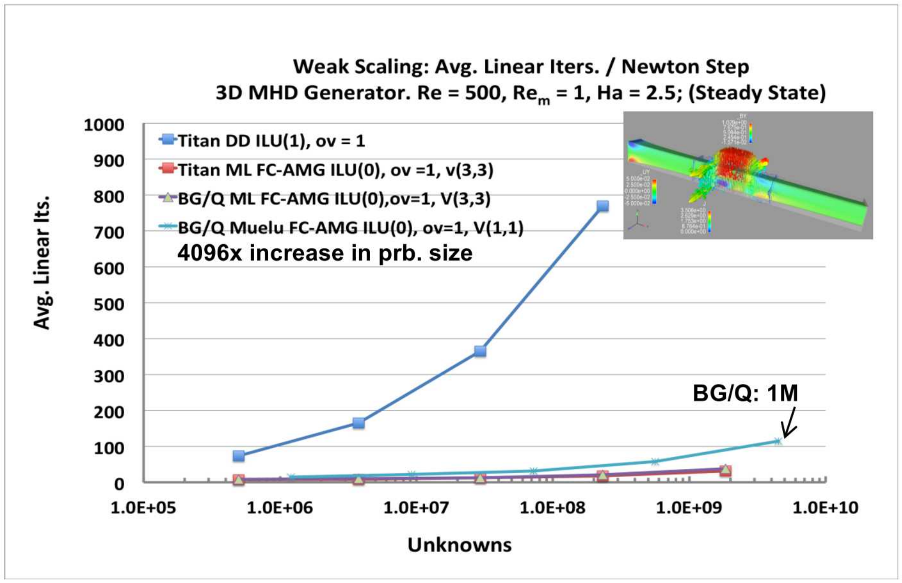


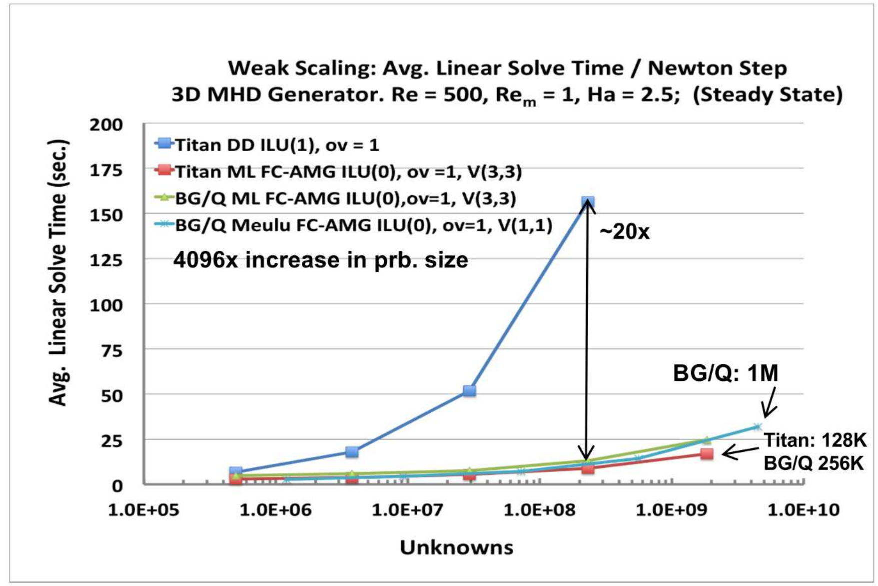
All nodal H(grad) elements using stabilized weak from

- 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 -ψ 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 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)





<u>Largest fully-coupled unstructured FE MHD solves demonstrated to date:</u>

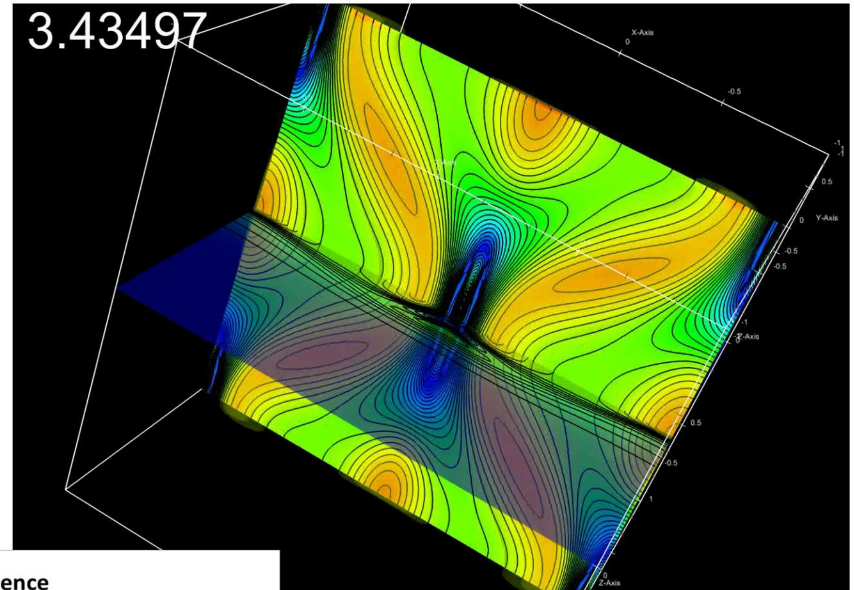
MHD (steady) weak scaling studies to 128K Cray XK7, 1M BG/Q

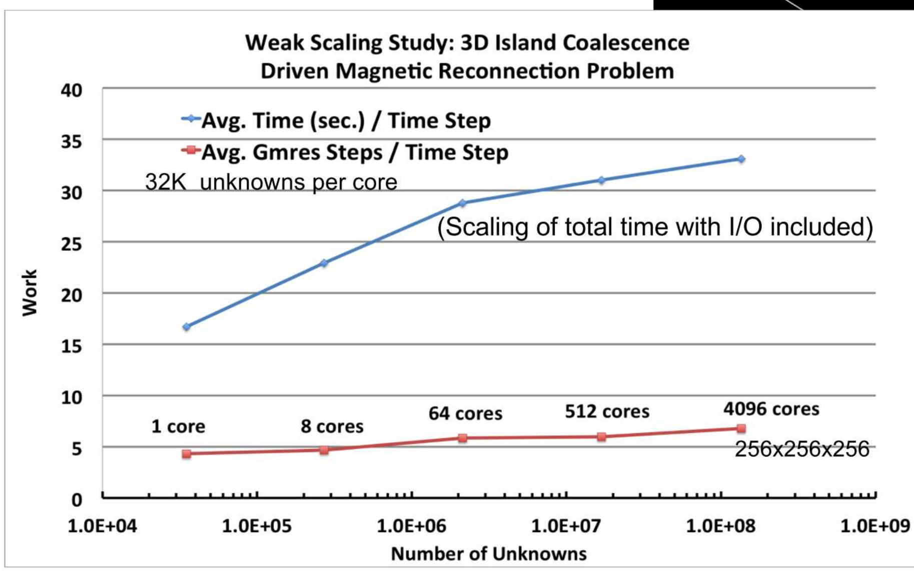
Large demonstration computations

- **MHD (steady): 13B DoF, 1.625B elem, on 128K cores**
- **CFD (Transient): 40B DoF, 10.0B elem, on 128K cores**

Poisson sub-block solvers: 4.1B DoF, 4.1B elem, on 1.6M cores

Scaling for VMS 3D Island Coalescence Problem: Driven Magnetic Reconnection [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.

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

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

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

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

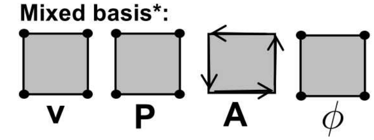
$$\mathbf{R_A} = \sigma \frac{\partial \mathbf{A}}{\partial t} + \nabla \times \frac{1}{\mu} \nabla \times \mathbf{A} - \sigma \mathbf{v} \times \nabla \times \mathbf{A} + \sigma \nabla \phi = \mathbf{0}; \qquad \mathbf{B} = \nabla \times \mathbf{A}$$

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

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

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

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**

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

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

- **Mixed basis, Q1/Q1 VMS FE Navier-Stokes, A-edge, Q1 Lagrange Multiplier**

Multi-fluid 5-Moment Plasma System Model (Structure-preserving)

Density	$\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a) = \sum_{b \neq a} (n_a \rho_b \bar{\nu}^{+}_{ab} - n_b \rho_a \bar{\nu}^{-}_{ab})$
Momentum	$\frac{\partial (\rho_a \mathbf{u}_a)}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a \otimes \mathbf{u}_a + p_a I + \Pi_a) = q_a n_a (\mathbf{E} + \mathbf{u}_a \times \mathbf{B})$ $- \sum_{b \neq a} [\rho_a (\mathbf{u}_a - \mathbf{u}_b) n_b \bar{\nu}^{M}_{ab} + \rho_b \mathbf{u}_b n_a \bar{\nu}^{+}_{ab} - \rho_a \mathbf{u}_a n_b \bar{\nu}^{-}_{ab}]$
Energy	$\frac{\partial \varepsilon_a}{\partial t} + \nabla \cdot ((\varepsilon_a + p_a) \mathbf{u}_a + \Pi_a \cdot \mathbf{u}_a + \mathbf{h}_a) = q_a n_a \mathbf{u}_a \cdot \mathbf{E} + Q^{src}$ $- \sum_{b \neq a} \left[(T_a - T_b) k \bar{\nu}^{E}_{ab} - \rho_a \mathbf{u}_a \cdot (\mathbf{u}_a - \mathbf{u}_b) n_b \bar{\nu}^{M}_{ab} \right.$
Charge and Current Density	$q = \sum_k q_k n_k \qquad \mathbf{J} = \sum_k q_k n_k \mathbf{u}_k$
Maxwell's Equations	$\frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} + \mu_0 \mathbf{J} = \mathbf{0} \qquad \nabla \cdot \mathbf{E} = \frac{q}{\epsilon_0}$ $\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0} \qquad \nabla \cdot \mathbf{B} = 0$

Cyclotron Frequency

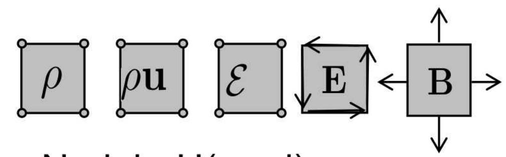
Strong off diagonal coupling for plasma oscillation

Light wave

IMEX: Time Integration $\mathbf{M}\dot{\mathbf{U}} + \mathbf{F} + \mathbf{G} = 0$

Explicit Hydrodynamics

Implicit EM, EM sources, sources for species $(\rho_a, \rho_a \mathbf{u}_a, \epsilon_a)$ interactions



Nodal - H(grad),
Edge - H(curl)
Face - H(div)
Elements
[Intrepid]

Other work on mulitfluid formulations, solution algorithms:

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

Physics-based and Approximate Block Factorizations:

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

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

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

[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 *SCALABLE* AMG optimized for the correct spaces e.g. H(grad), H(curl) to be used. (e.g. **Teko block-preconditioning using 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)]

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 algorithm for the reduced two-field low-β extended MHD model,” J. Comput. Phys., vol. 326, pp. 763–772, 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
- Phillips, JS, Cyr, Elman, Pawlowski. "Block Preconditioners for Stable Mixed Nodal and Edge Finite Element Representations of Incompressible Resistive MHD," SISC 2016.
- Cyr, JS, Tuminaro, “Teko an abstract block preconditioning capability with concrete example applications to Navier-Stokes and resistive MHD, SISC, 2016
- Wathen, Grief, Schotzau, Preconditioners for Mixed Finite Element Discretizations of Incompressible MHD Equations, SISC 2017

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.

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

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

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

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

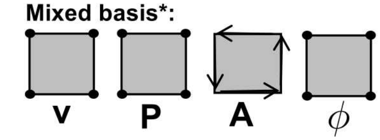
$$\mathbf{R}_{\mathbf{A}} = \sigma \frac{\partial \mathbf{A}}{\partial t} + \nabla \times \frac{1}{\mu} \nabla \times \mathbf{A} - \sigma \mathbf{v} \times \nabla \times \mathbf{A} + \sigma \nabla \phi = \mathbf{0}; \quad \mathbf{B} = \nabla \times \mathbf{A}$$

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

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

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

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**

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

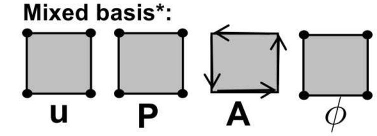
$$\begin{array}{ccccccc}
nodes_1 & \xrightarrow{\hat{G} = Q_E^{-1}G} & edges & \xrightarrow{\hat{K} = Q_B^{-1}K} & faces & \xrightarrow{\hat{D} = Q_\phi^{-1}D} & nodes_0 \\
\downarrow Q_\rho & & \downarrow Q_E & & \downarrow Q_B & & \downarrow Q_\phi \\
nodes_1^* & \xleftarrow{\hat{G}^t = G^t Q_E^{-1}}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

- **Mixed basis, Q1/Q1 VMS FE Navier-Stokes, A-edge, Q1 Lagrange Multiplier**

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

Structure of Block Preconditioner: Critical 3x3 Block Sys.
Split into 2 – 2x2 Sys. with Sparse Schur Complement Approximations

Mixed basis*:

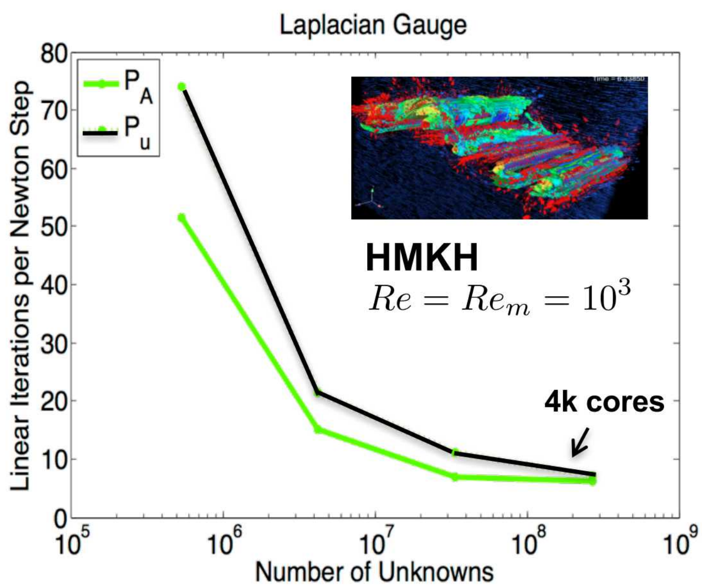


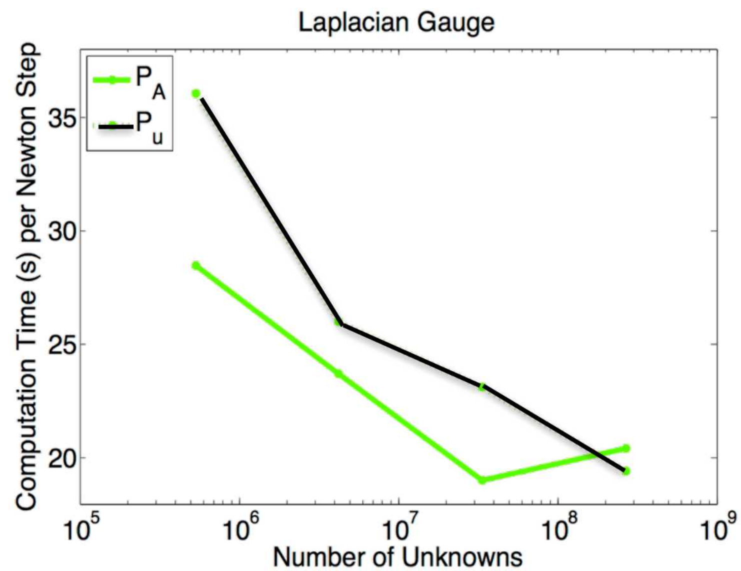
$$\mathcal{A}_{GSG} = \left(\begin{array}{ccc|c} F & B^t & Z & 0 \\ B & C & 0 & 0 \\ Y & 0 & G & D^t \\ \hline 0 & 0 & 0 & L \end{array}\right) \qquad \mathcal{P}_{\mathbf{A}} = \begin{pmatrix} F & 0 & Z \\ 0 & I & 0 \\ Y & 0 & G \end{pmatrix} \begin{pmatrix} F^{-1} & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I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

$$\hat{S}_{\mathbf{A}} = G - Y\hat{F}^{-1}Z \qquad \hat{S}_P = C - B\hat{F}^{-1}B^t$$

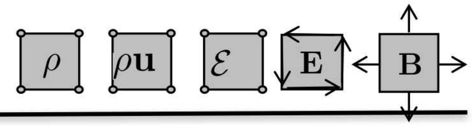
Segregation into

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





Multi-fluid 5-Moment Plasma System Models



Density	$\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a) = \sum_{b \neq a} (n_a \rho_b \bar{\nu}_{ab}^{+} - n_b \rho_a \bar{\nu}_{ab}^{-})$
Momentum	$\frac{\partial (\rho_a \mathbf{u}_a)}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a \otimes \mathbf{u}_a + p_a I + \Pi_a) = q_a n_a (\mathbf{E} + \mathbf{u}_a \times \mathbf{B})$ $- \sum_{b \neq a} [\rho_a (\mathbf{u}_a - \mathbf{u}_b) n_b \bar{\nu}_{ab}^{M} + \rho_b \mathbf{u}_b n_a \bar{\nu}_{ab}^{+} - \rho_a \mathbf{u}_a n_b \bar{\nu}_{ab}^{-}]$
Energy	$\frac{\partial \varepsilon_a}{\partial t} + \nabla \cdot ((\varepsilon_a + p_a) \mathbf{u}_a + \Pi_a \cdot \mathbf{u}_a + \mathbf{h}_a) = q_a n_a \mathbf{u}_a \cdot \mathbf{E} + Q_a^{src}$ $- \sum_{b \neq a} \left[(T_a - T_b) k \bar{\nu}_{ab}^{E} - \rho_a \mathbf{u}_a \cdot (\mathbf{u}_a - \mathbf{u}_b) n_b \bar{\nu}_{ab}^{M} - n_a \bar{\nu}_{ab}^{+} \varepsilon_b + n_b \bar{\nu}_{ab}^{-} \varepsilon_a \right]$
Charge and Current Density	$q = \sum_k q_k n_k \qquad \mathbf{J} = \sum_k q_k n_k \mathbf{u}_k$
Maxwell's Equations	$\frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} + \mu_0 \mathbf{J} = \mathbf{0} \qquad \nabla \cdot \mathbf{E} = \frac{q}{\epsilon_0}$ $\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0} \qquad \nabla \cdot \mathbf{B} = 0$

Miller, Cyr, JS, Kramer, Phillips, Conde, Pawlowski, IMEX and exact sequence discretization of the multi-fluid plasma model. submitted to JCP

Phillips, JS, Cyr, Miller, Enabling Scalable Multiuid Plasma Simulations through Block Preconditioning 2019, LNCSE

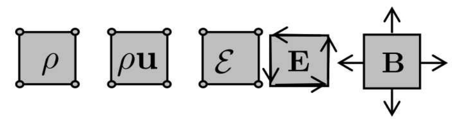
Other work on formulations, solution algorithms:

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

Scalable Physics-based Preconditioners for Physics-compatible Discretizations

$$\begin{bmatrix}
\mathbf{D}_{\rho_i} & \mathbf{K}^{\rho_i}_{\rho_i u_i} & 0 & \mathbf{Q}^{\rho_i}_{\rho_e} & 0 & 0 & 0 & 0 \\
\mathbf{D}^{\rho_i u_i}_{\rho_i} & \mathbf{D}_{\rho_i u_i} & 0 & \mathbf{Q}^{\rho_i u_i}_{\rho_e} & \mathbf{Q}^{\rho_i u_i}_{\rho_e u_e} & 0 & \mathbf{Q}^{\rho_i u_i}_{E} & \mathbf{Q}^{\rho_i u_i}_{B} \\
\mathbf{D}^{\mathcal{E}_i}_{\rho_i} & \mathbf{D}^{\mathcal{E}_i}_{\rho_i u_i} & \mathbf{D}_{\mathcal{E}_i} & \mathbf{Q}^{\mathcal{E}_i}_{\rho_e} & \mathbf{Q}^{\mathcal{E}_i}_{\rho_e u_e} & \mathbf{Q}^{\mathcal{E}_i}_{\mathcal{E}_e} & \mathbf{Q}^{\mathcal{E}_i}_{E} & 0 \\
\mathbf{Q}^{\rho_e}_{\rho_i} & 0 & 0 & \mathbf{D}_{\rho_\mathbf{e}} & \mathbf{K}^{\rho_e}_{\rho_e u_e} & 0 & 0 & 0 \\
\mathbf{Q}^{\rho_e u_e}_{\rho_i} & \mathbf{Q}^{\rho_e u_e}_{\rho_i u_i} & 0 & \mathbf{D}^{\rho_e u_e}_{\rho_e} & \mathbf{D}_{\rho_e u_e} & 0 & \mathbf{Q}^{\rho_e u_e}_{E} & \mathbf{Q}^{\rho_e u_e}_{B} \\
\mathbf{Q}^{\mathcal{E}_e}_{\rho_i} & \mathbf{Q}^{\mathcal{E}_e}_{\rho_i u_i} & \mathbf{Q}^{\mathcal{E}_e}_{\mathcal{E}_i} & \mathbf{D}^{\mathcal{E}_e}_{\rho_e} & \mathbf{D}^{\mathcal{E}_e}_{\rho_e u_e} & \mathbf{D}_{\mathcal{E}_e} & \mathbf{Q}^{\mathcal{E}_e}_{E} & 0 \\
0 & \mathbf{Q}^{E}_{\rho_i u_i} & 0 & 0 & \mathbf{Q}^{E}_{\rho_e u_e} & 0 & \mathbf{Q}_E & \mathbf{K}^{E}_{B} \\
0 & 0 & 0 & 0 & 0 & 0 & \mathbf{K}^{B}_{E} & \mathbf{Q}_B
\end{bmatrix}
\begin{bmatrix}
\rho_i \\ \rho_i \mathbf{u}_i \\ \mathcal{E}_i \\ \rho_e \\ \rho_e \mathbf{u}_e \\ \mathcal{E}_e \\ \mathbf{E} \\ \mathbf{B}
\end{bmatrix}$$

Ion/electron plasma
16 Coupled
Nonlinear PDEs



Group the hydrodynamic variables together (similar 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

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

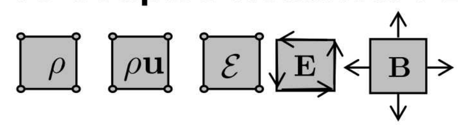
Reordered 3x3

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

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



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

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(curl) AMG with grad-div stab.
(lumped mass)

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

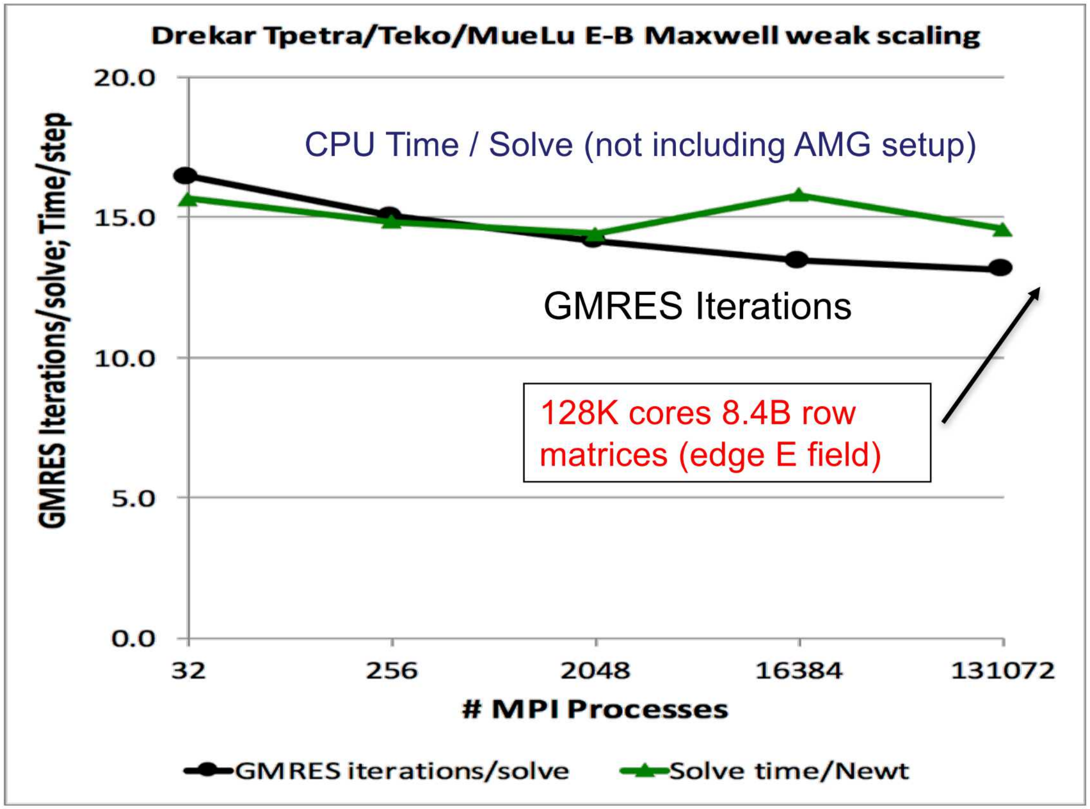
Face-based simple
mass matrix Inversion.
V-cycle Gauss-Siedel

Augmentation of Schur Complement

$$\hat{D}_E \sim \frac{1}{c^2 \Delta t} I + \Delta t \nabla \times \nabla \times$$

- Null space of curl is all gradients of scalars.
- Augmenting with $-\Delta t \nabla \nabla \cdot$ yields a vector Laplacian. Then gradients are not annihilated
- Similar strategy to augmented Lagrangian techniques (CFD: Benzi & Olshanskii; Maxwell: Wu, Huang, & Li)
- Can be regarded as adding a scaled gradient of Gauss's law $\nabla \cdot (\varepsilon \mathbf{E}) = \rho$ to Ampere's law, i.e. adding zero
- In discrete setting, augmented operator is
  $$\tilde{D}_E = \frac{1}{c^2 \Delta t} Q_{\mathbf{E}} + \Delta t K^t Q_{\mathbf{B}}^{-1} K + \Delta t G Q_\rho^{-1} G^t$$
- Removes gradients from null-space. Traditional multigrid can be used on T, even when CFL_c is large
- Of course other optimal AMG routines for curl-curl systems in e.g. ML/Muelu and Hyper can be used.

Weak Scaling for 3D 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.

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

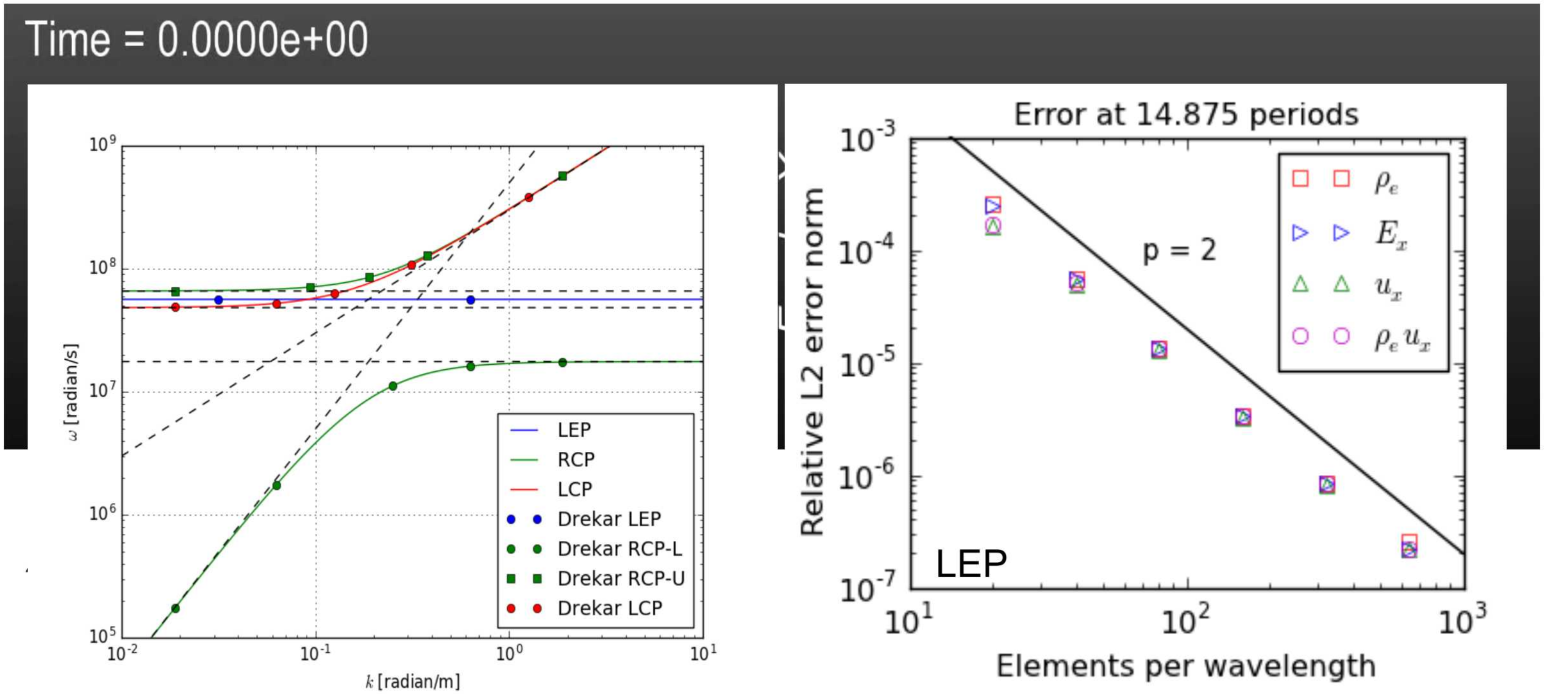
Demonstrated to $CFL_c > 10^4$

Drekar

GS smoother with H(grad) AMG

Max $CFL_c \sim 200$

Demonstration / Verification of Implicit Solution for Longitudinal Electron Plasma (LEP) Oscillation with Under-resolved TEM Waves

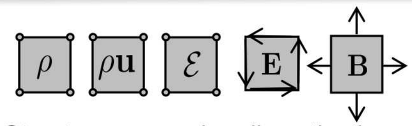


LEP: Longitudinal Electron Plasma Wave
RCP: Right Hand Circularly Polarized Wave
LCP: Left Hand Circularly Polarized Wave
(Cold plasma)

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

Initial Weak Scaling for Longitudinal Electron / Ion Plasma Oscillation and Under-resolved TEM Wave Results (Full Maxwell – two-fluid)

$$\Delta t = 1.1 \times 10^{-11} \approx 0.023\ \tau_{\omega_{pi}} \approx 0.1\ \tau_{\omega_{pe}} \geq 3 \times 10^2\ \tau_c$$



Structure-preserving discretization

N	P	Linear its / Newton	Solve time / linear solve	$\frac{\Delta t_{imp}}{\Delta t_{exp}}$
100	1	4.18	0.2	300
200	2	4.21	0.22	600
400	4	4.27	0.23	1.2E+3
800	8	4.4	0.26	2.4E+3
1600	16	4.51	0.35	4.8E+3
3200	32	4.89	0.42	9.6E+3
6400	64	6.21	0.61	1.9e+4

$\Delta x \approx 1 \mu m$

$$\mu = \frac{m_i}{m_e} = 1836.57$$

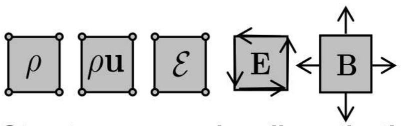
Initial weak scaling of ABF preconditioner

- Domain [0,0.01]x[0,0.0004]x[0,0.0004]; Periodic BCs in all directions
- N elements in x-direction;
- Fixed time step size for SDIRK (2,2): (not resolving TEM wave)

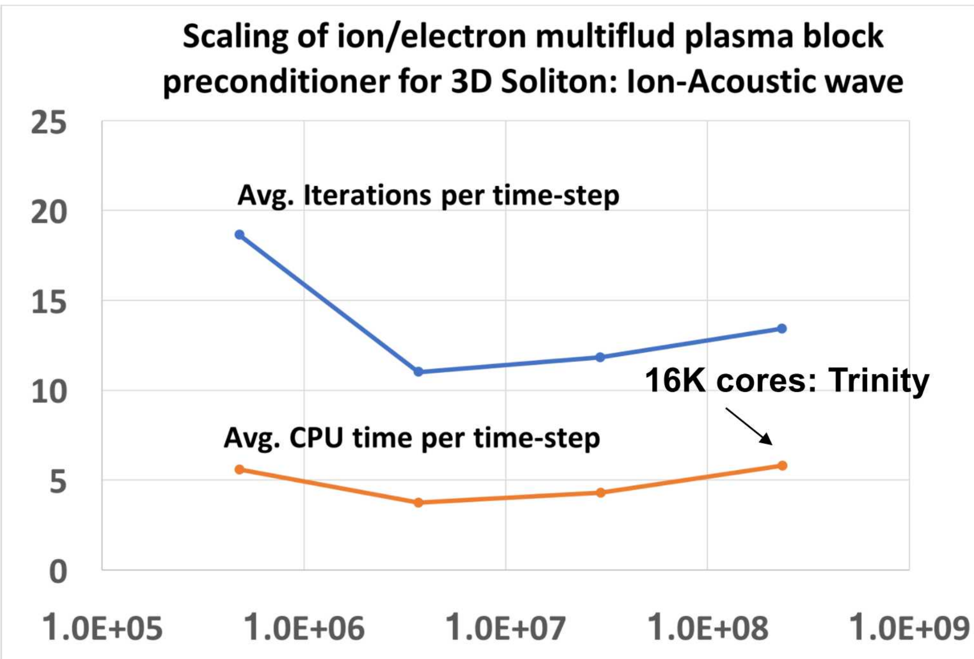
Proof of Principle

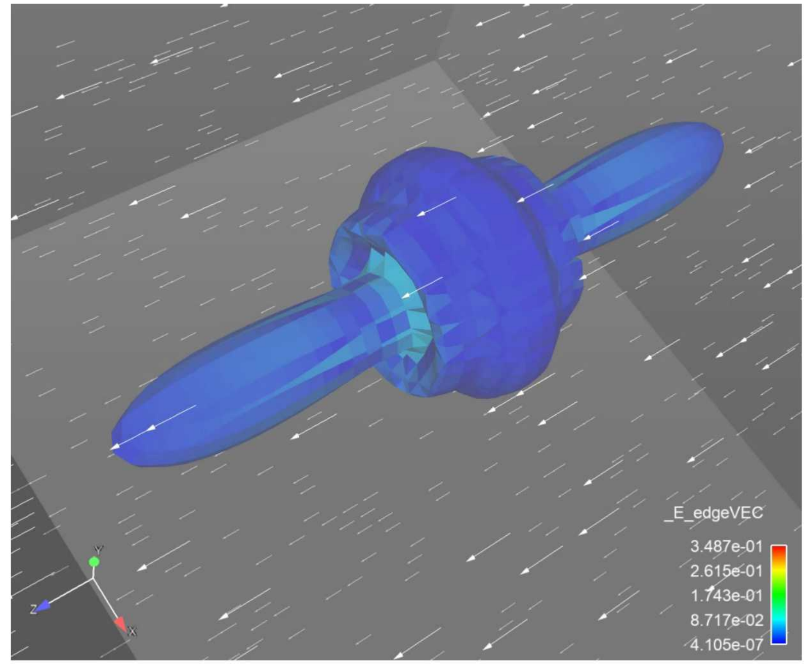
SimpleC on fluid Schur-complement
DD-ILU for Euler Eqns.
DD-LU curl-curl

3D Gaussian Density/Pressure Perturbation as initial condition
Isentropic ion-acoustic wave



Structure-preserving discretization





Iso-surface of ion density colored by electric field magnitude

Isentropic flow

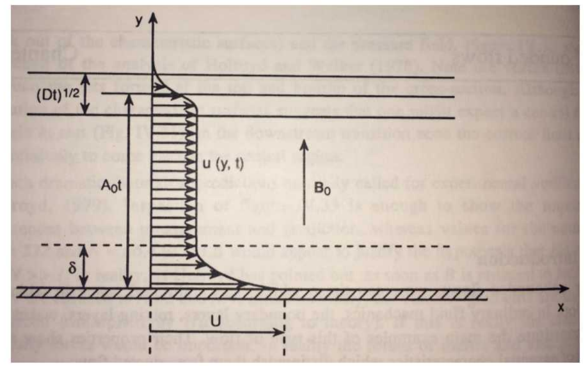
$$\rho_\alpha = m_\alpha \left(1 + e^{-10||\vec{x}-\vec{x}_0||^2}\right)$$

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

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

Resistive Alfven wave problem

- Solution is derived from resistive/viscous MHD which **ignores Hall effects**:
  - Hall parameter $\mathrm{H} = \frac{\omega_{ce}}{\nu_{ei}} = \frac{\eta\, B}{n_e e} \ll 1$
  - Reducing Hall effects in magnetized multi-fluid model is tricky - requires large collision frequency
- Problem used for verifying resistive, Lorentz force, and viscous operators:
  - Impulse shear due to a moving wall drives a **Hartmann layer**
  - Hartmann layer shear excites **Alfven wave** traveling along magnetic field
  - Alfven wave front diffuses due to momentum and magnetic diffusivity
  - Profile depends on the effective **Lundquist number** $\mathrm{S} = \frac{L\, v_A}{\lambda}$



R. Moreau, Magnetohydrodynamics, 1990

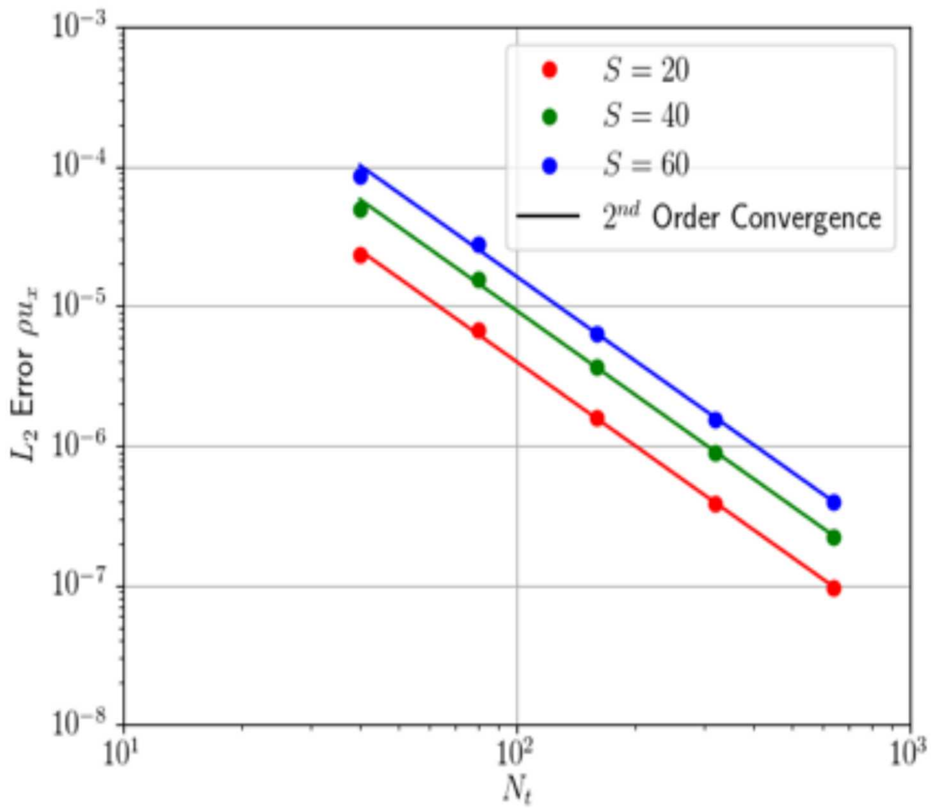
$$u_x = \frac{U}{4}\left(1 + \exp\left(\frac{v_A y}{\lambda}\right)\right)\mathrm{erfc}(\eta_+) + \frac{U}{4}\left(1 + \exp\left(-\frac{v_A y}{\lambda}\right)\right)\mathrm{erfc}(\eta_-)$$

$$B_x = \sqrt{\mu_0\rho}\,\frac{U}{4}\left(1 - \exp\left(\frac{v_A y}{\lambda}\right)\right)\mathrm{erfc}(\eta_+) - \sqrt{\mu_0\rho}\,\frac{U}{4}\left(1 - \exp\left(-\frac{v_A y}{\lambda}\right)\right)\mathrm{erfc}(\eta_-)$$

$$\eta_\pm = \frac{y \pm v_A t}{2\sqrt{\lambda t}}$$

Asymptotic Solution of Multifluid EM Plasma 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 SSP3 (3,3,2))

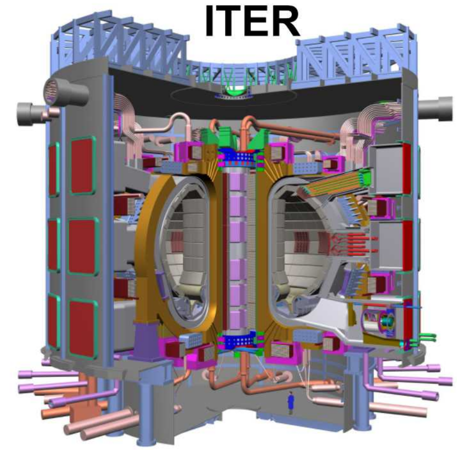
Plasma Scales for S = 60		
	Electrons	**Ions**
$\omega_p \Delta t$	10^7 - 10^9	10^6 - 10^7
$\omega_c \Delta t$	10^6 - 10^7	10^3 - 10^4
$\nu_{\alpha\beta} \Delta t$	10^{10} - 10^{11}	10^7 - 10^8
$\nu_S \Delta t / \Delta x$	10^{-2}	10^{-4}
$u \Delta t / \Delta x$	10^{-4}	10^{-4}
$\mu \Delta t / \rho \Delta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

IMEX terms: implicit/explicit

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.

A Few Preliminary Tokamak Relevant Examples for Resistive MHD and a Multifluid Plasma Model

Tokamak Magnetic Confinement Fusion (MCF): Understanding and controlling instabilities/disruptions in plasma confinement is critical.



Goal for Fusion Device:

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

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

Sandia National Laboratories

Tokamak Disruption Simulation (TDS) Center SciDAC-4 Partnership (OFES/ASCR)

Institutions: ANL, LANL, LLNL, PPPL, SNL, Columbia, UMD, UT, VT

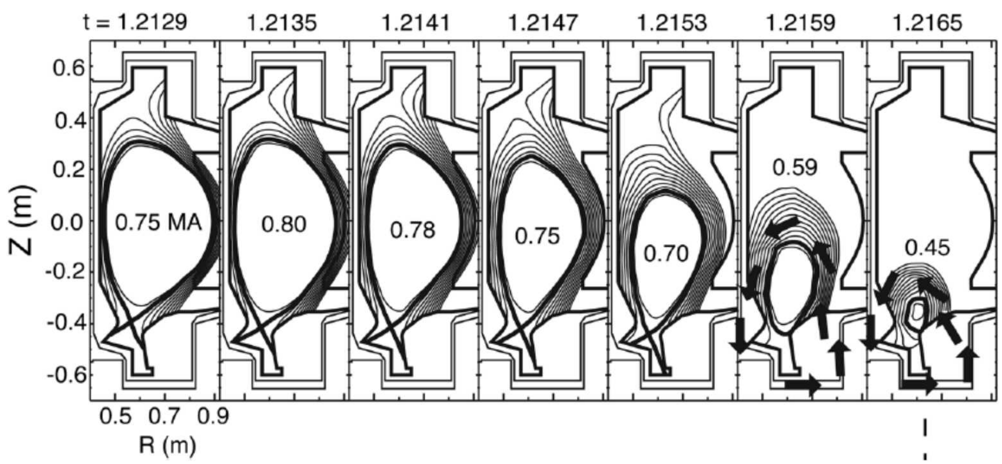
(Overall PI, OFES PI and LANL-PI, X. Tang; ASCR-PI, SNL-PI J. Shadid):

Goal for Fusion Device:

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

TDS Computational Simulation Goal

Develop and evaluate advanced hierarchy of plasma physics models and solution methods to understand disruption physics and explore mitigation strategies.



ITER Physics Expert Group on Disruptions, Nucl. Fusion 39, 2251 (1999).

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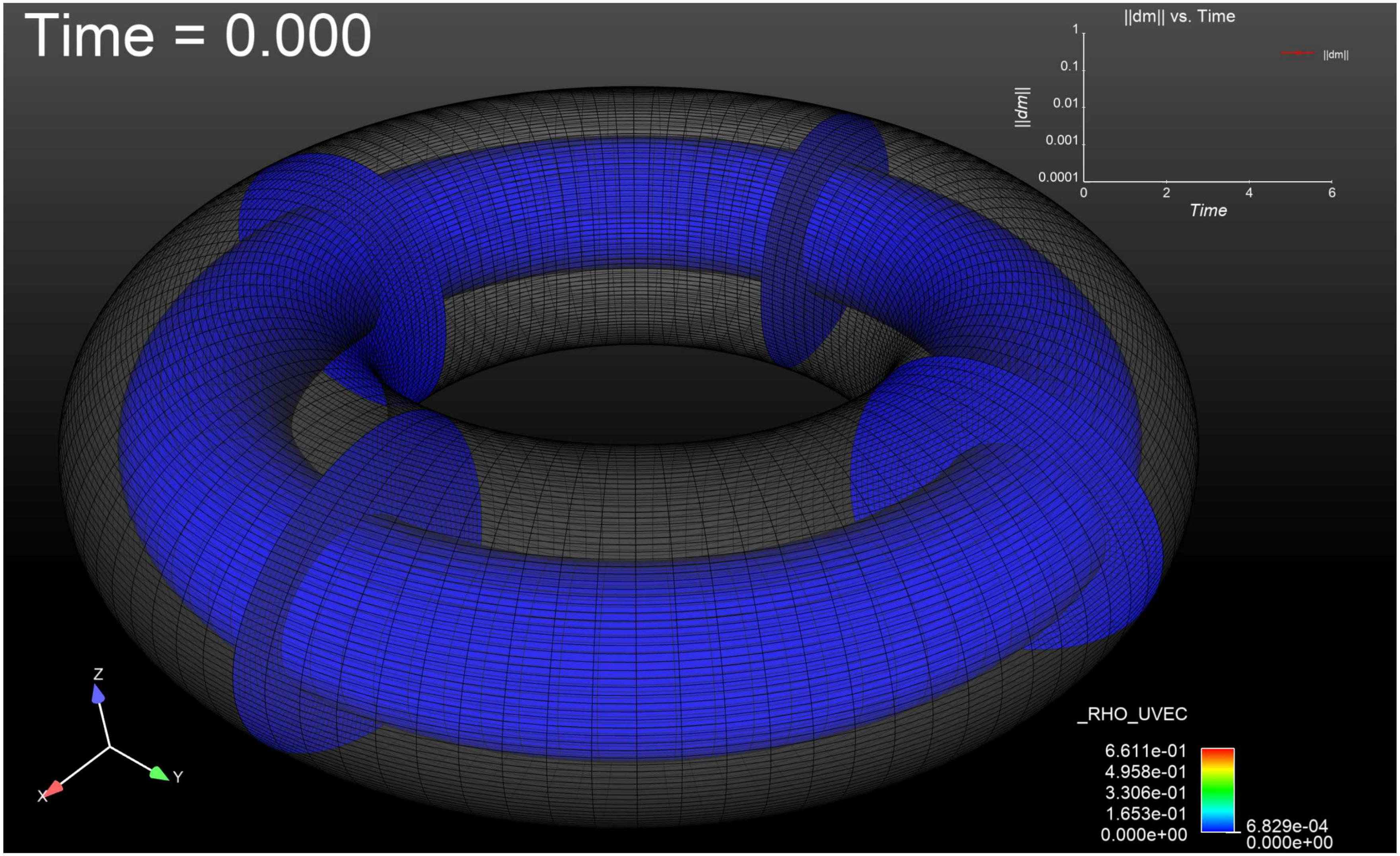
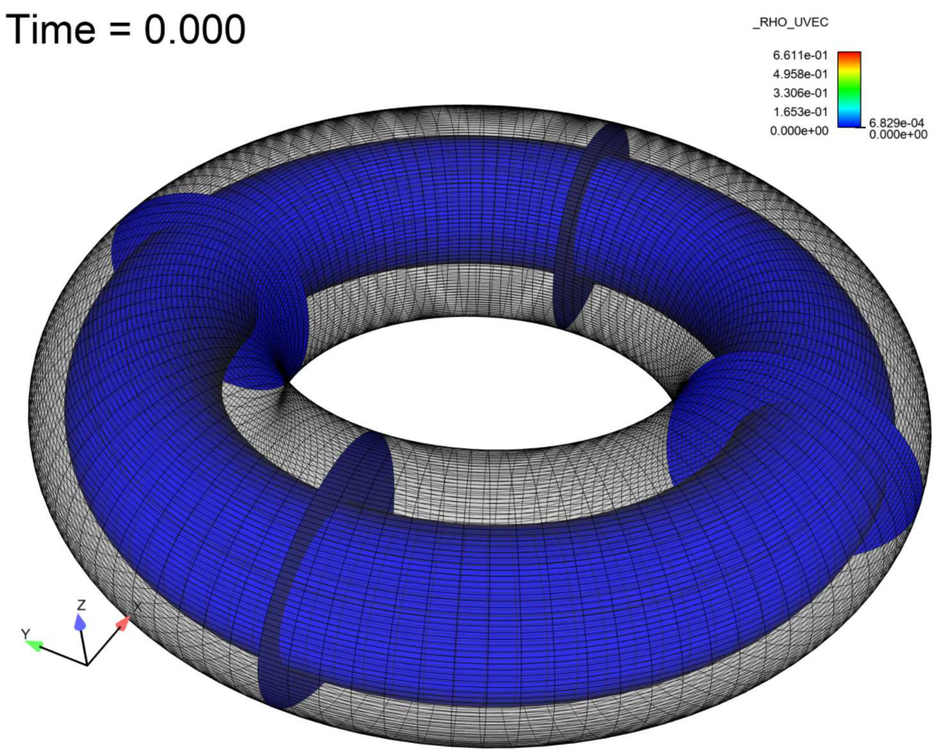
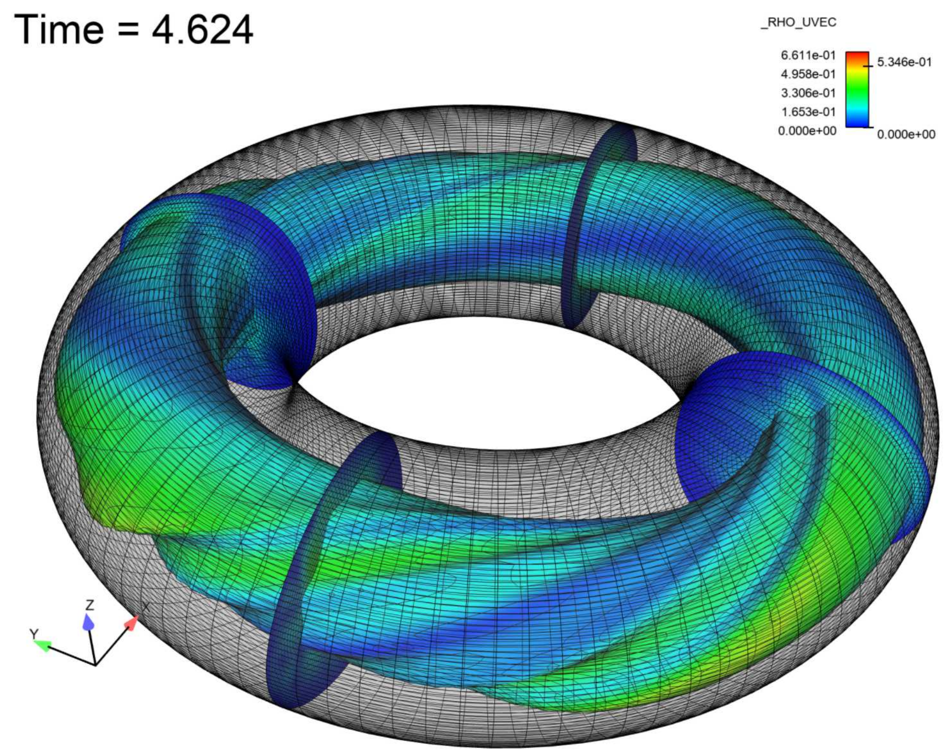
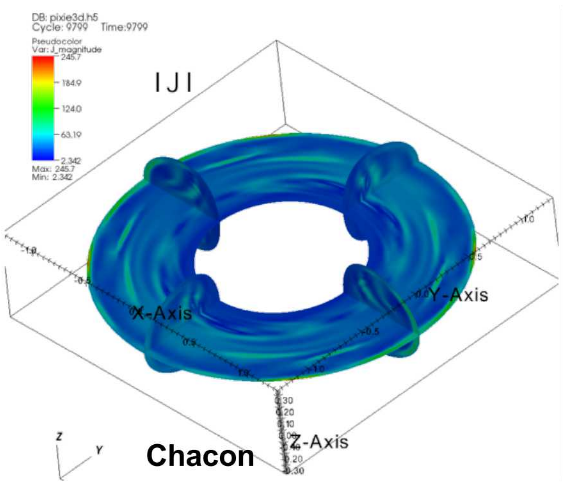

Time = 0.000
||dm|| vs. Time
1
0.1
0.01
0.001
0.0001
||dm||
0
2
4
6
Time
||dm||
Z
Y
X
_RHO_UVEC
6.611e-01
4.958e-01
3.306e-01
1.653e-01
0.000e+00
6.829e-04
0.000e+00

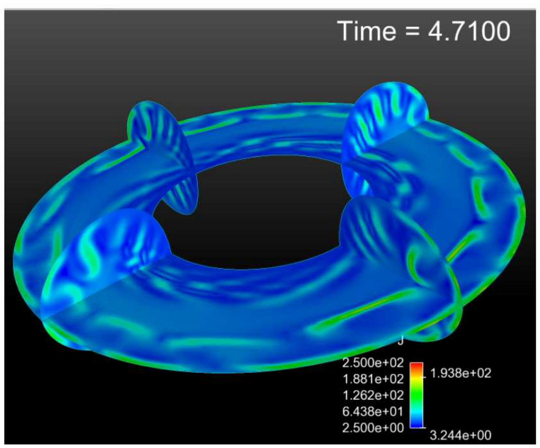
Preliminary Soloveev Nonlinear Disturbance Saturation.

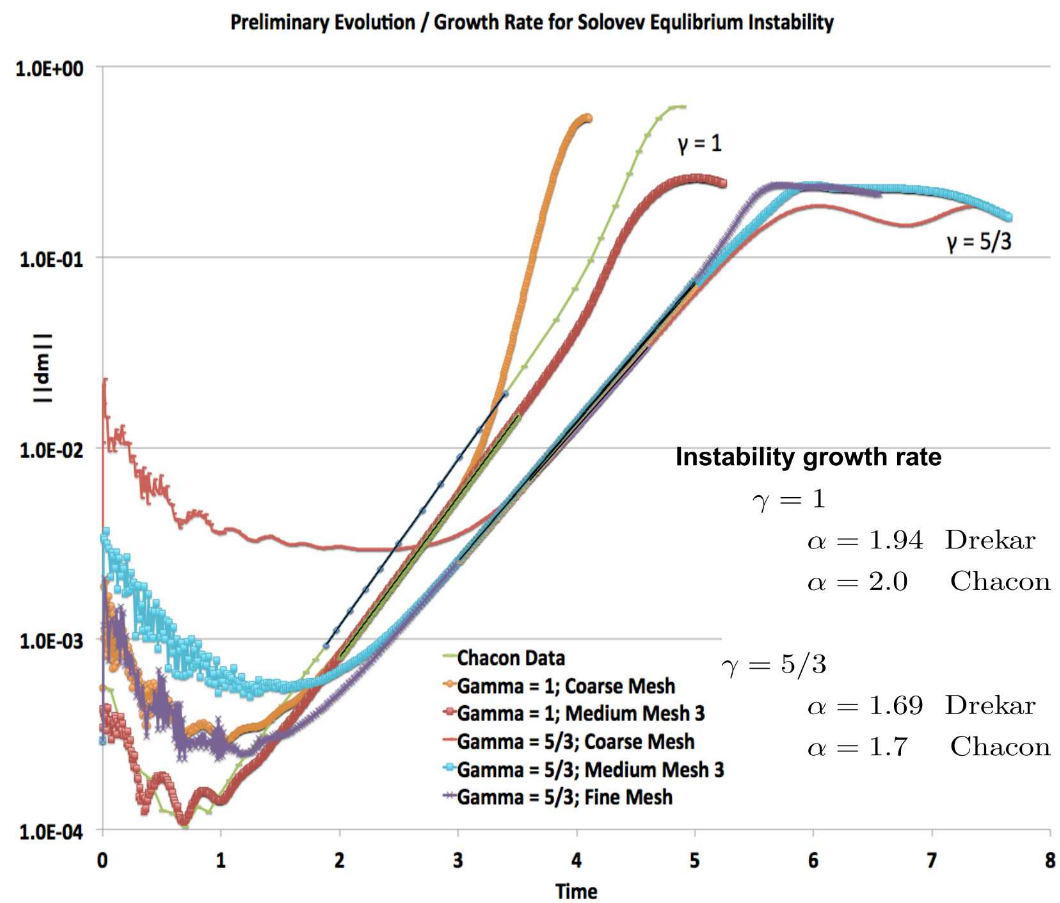




Preliminary Soloveev Equilibrium/Linear Disturbance Growth.







Instability growth rate

$\gamma = 1$

$\alpha = 1.94$ Drekar

$\alpha = 2.0$ Chacon

$\gamma = 5/3$

$\alpha = 1.69$ Drekar

$\alpha = 1.7$ Chacon

with L. Chacon (LANL)

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

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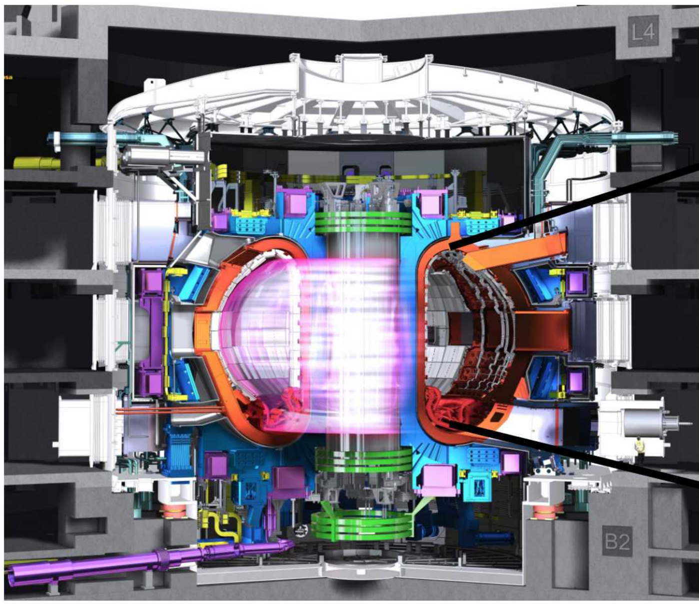
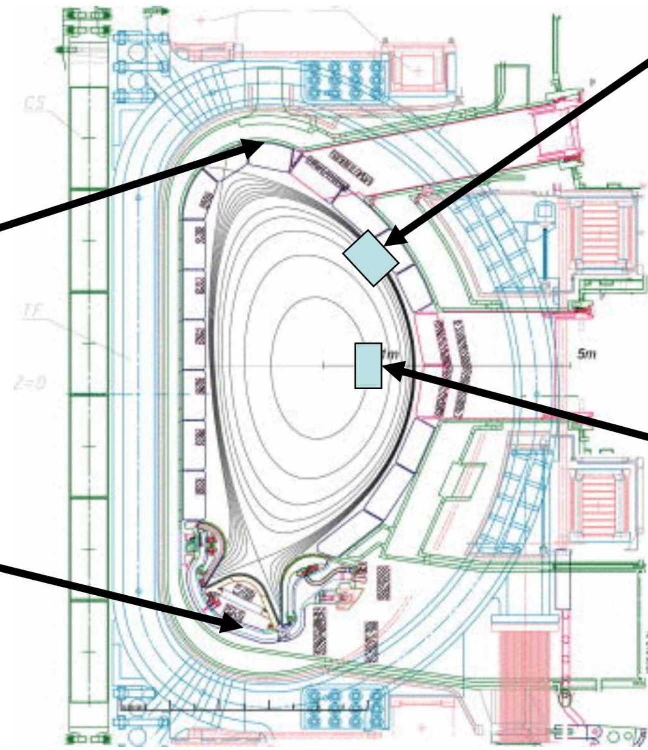
<u>Disruption is a prompt termination of a plasma confinement in a tokamak and can be a showstopper for ITER. Mitigate to control thermal and current quench evolution.</u>



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



<u>Preliminary Models of Gas Injection for Disruption Mitigation</u>

<u>Dynamics of Neutral Gas Jet Injection at an angle wrt B Field</u>

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

<u>Gas Injection Assumed Distribution at time t= 0 for Neutral Gas Core Inside Separatrix</u>

- 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

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

A Very Preliminary 1D Gas Injection Related Problem

1D High Z Neutral Gas (Ne0) Core Expansion into a 100ev Deuterium (D+,e-) Plasma

Solving Conservation of Mass, Momentum, Total Mech. Energy
(i.e. Euler sub-system with collisions / ionization / recombination and EM forces) for

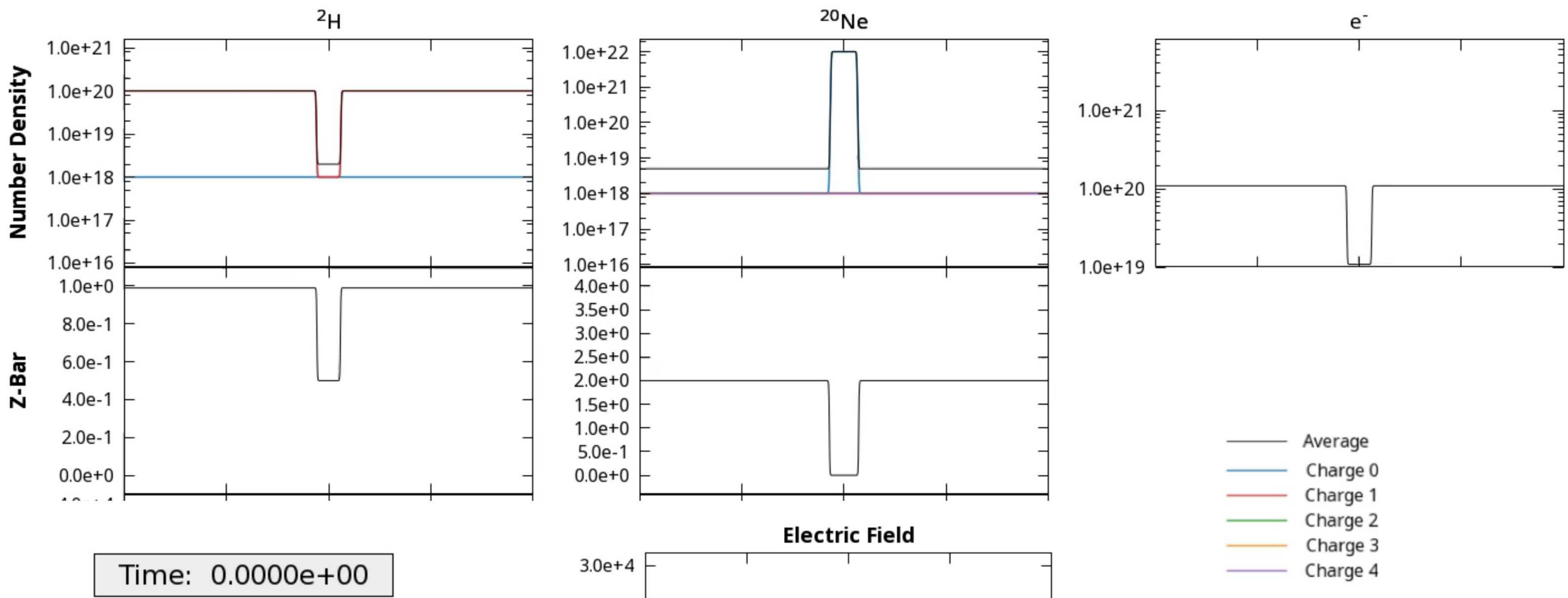
$$(D^0, D^{1+}, Ne^0, Ne^{1+}, Ne^{2+}, Ne^{3+}, Ne^{4+}, e^-)$$

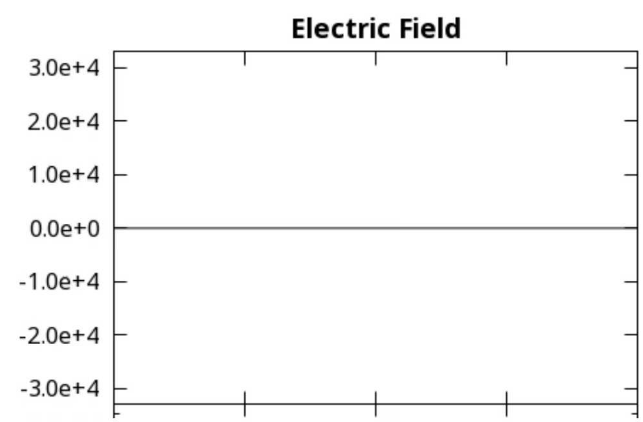
and electromagnetics for (E,B).

5 moment plasma model x 8 species	= 40 equations	(solved in 3D but only a 1D solution)
Maxwell Equations E,B field	= 6 equations	(solved in 3D but only a 1D solution)

<u>Problem outline:</u>

- Initial ~fully ionized Deuterium plasma at n = 10^{20}, T = 100ev (~1M degrees K)
- Neutral Neon (Ne^0) core introduced at n = 10^{22} , T = 10^{-1}ev (~1000 degrees K)
- Parallel B – field is ignorable (due to geometry in 1D so B does not modify transport)
- Mesh 4096x1x1 elements





Implicit iteratively limited
nodal variation (LED)
Algebraic flux correction (AFC)
Continuous Galerkin FE

Conclusions

- **Robustness, efficiency and 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.**

- **General mathematical libraries and components (e.g. Trilinos – Tempus, NOX, Aztec, ML/Meulu,Teko, Panzer, Phalanx, Intrepid, Kokkos) are very valuable for enabling:**
  - **Flexible development of implicit formulations of multiphysics systems (e.g. MHD, multifluid plasmas)**
  - **Exploration of advanced physics/mathematical models and PDE spatial discretizations**
  - **Development 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**
  - **Software abstractions also allow portability on advanced architectures**