Scalable Solution of Implicit / IMEX FE Continuum Plasma Physics Models

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NNSA National Nuclear Security Administration

CCR Center for Computing Research

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Outline

- General Scientific and Mathematical/Computational Motivation
- Brief Comments on Multiple-time-scale Plasma Systems
  - Magnetic Confinement Fusion
- 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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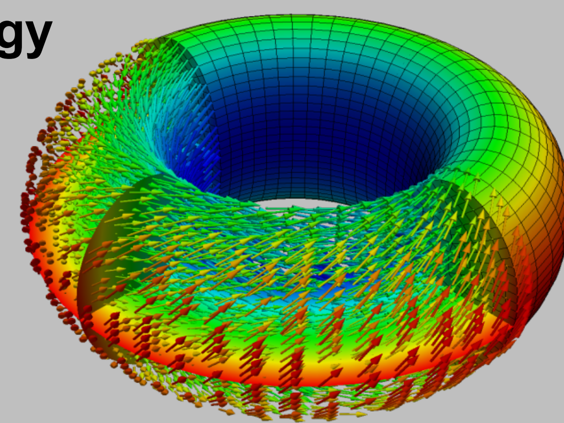
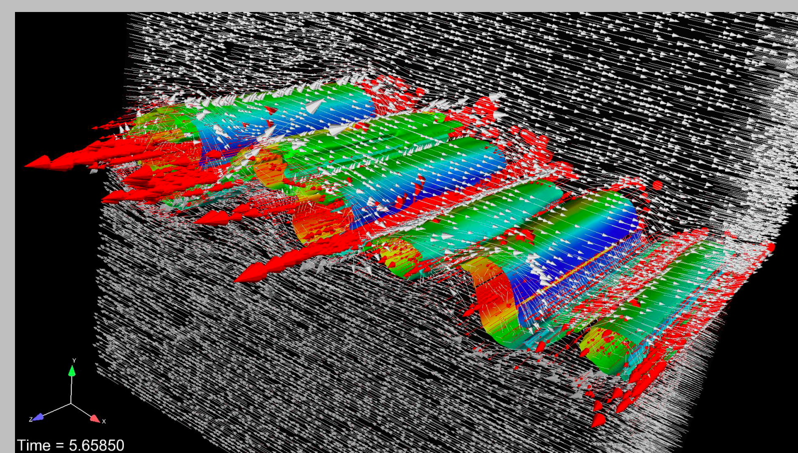
Motivation: Science/Technology



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

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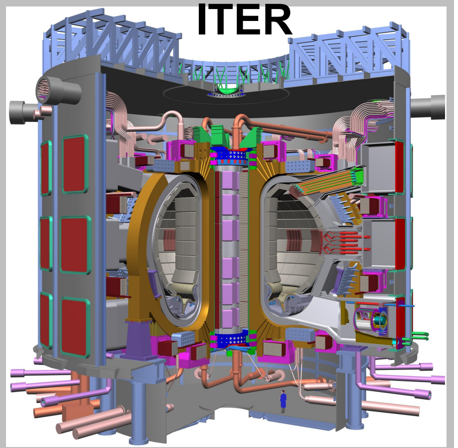
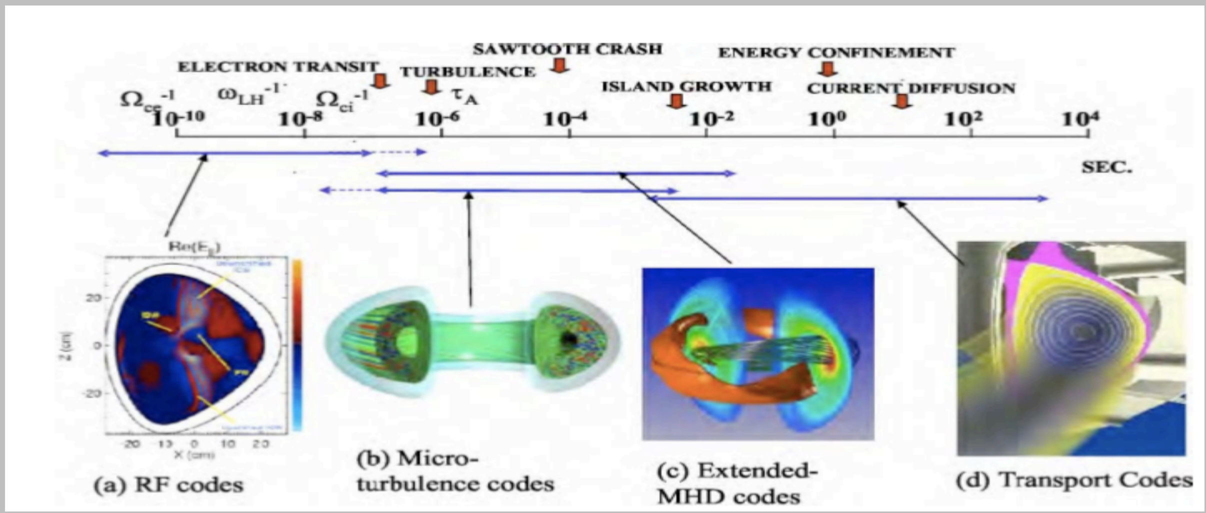
Tokamak Magnetic Confinement Fusion (MCF): Understanding and controlling instabilities/disruptions in plasma confinement is critical.

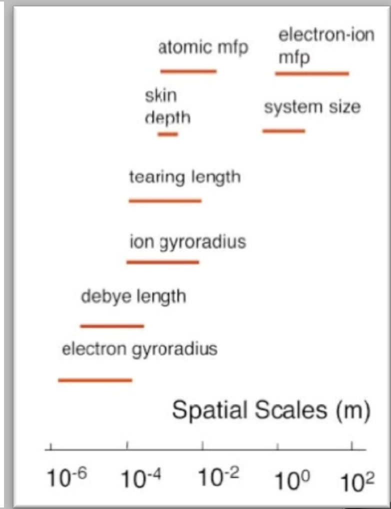


Goal for Fusion Device:

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

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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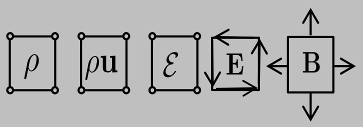
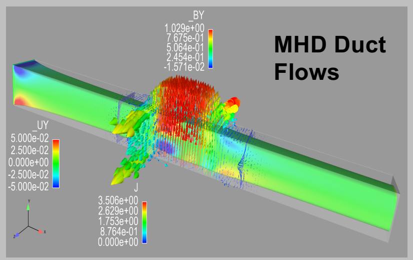
Our Mathematical Approach - develop:

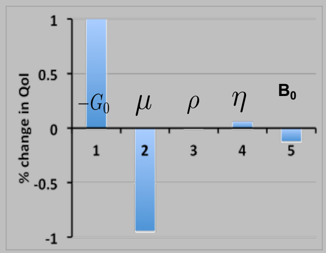
- **Stable, higher-order accurate implicit/IMEX formulations for multiple-time-scale systems**
- **Stable and accurate unstructured FE spatial discretizations. Options enforcing key mathematical properties (e.g. structure preserving forms: div B = 0; positivity ρ , P; DMP)**

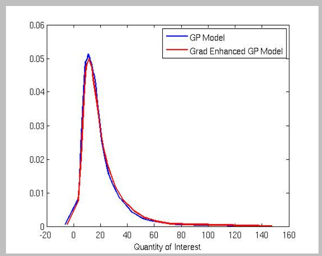


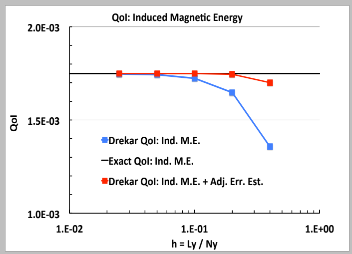
- **Robust, efficient fully-coupled nonlinear/linear iterative solution based on Newton-Krylov methods**
- **Scalable and efficient multiphysics preconditioners utilizing physics-based and approximate block factorization/Schur complement preconditioners with multi-level (AMG) sub-block solvers**

=> 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

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

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

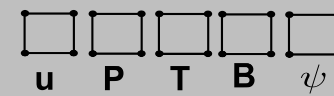
$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot [\rho \mathbf{v} \otimes \mathbf{v} - (\mathbf{T} + \mathbf{T}_M)] + 2\rho\Omega \times \mathbf{v} - \rho \mathbf{g} = \mathbf{0}$$

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

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

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

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



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]

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

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

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

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

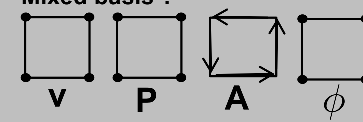
$$R_P = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

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

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

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

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**

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

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

- **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	$\frac{\partial \varepsilon_a}{\partial t} + \nabla \cdot ((\varepsilon_a + p_a) \mathbf{u}_a + \Pi_a \cdot \mathbf{u}_a + \mathbf{h}_a) = q_a n_a \mathbf{u}_a \cdot \mathbf{E} + Q^{src}_a$ $- \sum_{b \neq a} \left[(T_a - T_b) k \bar{\nu}^{E}_{ab} - \rho_a \mathbf{u}_a \cdot (\mathbf{u}_a - \mathbf{u}_b) n_b \bar{\nu}^{M}_{ab} \right.$
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

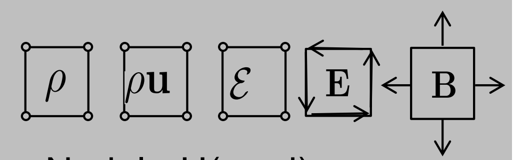
Strong off diagonal coupling for plasma oscillation

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 formulations, solution algorithms:

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

Multifluid Model: IMEX to handle multiple-time-scales

Eigen-values for 5M Euler Eqn for each species

$$\lambda_\alpha = (u_\alpha, u_\alpha \pm \sqrt{\gamma T_\alpha / m_\alpha})$$

Time-scales from Maxwell Eqn. & EM source terms

$$\tau_{EM} = \Delta x / c; \quad \tau_{\omega_{p\alpha}} = \frac{1}{\sqrt{\frac{n_\alpha q_\alpha^2}{\epsilon_0 m_\alpha}}}; \quad \tau_{\omega_{c\alpha}} = \frac{1}{\frac{q_\alpha B}{m_\alpha}}$$

Time-scales from collisions and ionization/recombination

$$\tau_{\alpha\beta}^M = \frac{1}{\nu_{\alpha\beta}^M}; \qquad \bar{\tau}_{\alpha\beta} = \frac{1}{\nu_{\alpha\beta}};$$

Implicit / Explicit (IMEX) Methods and the Implicit Sub-problem [Tempus, Rythmos]

Governing PDE Semi-discretized in Space (e.g. FV, FD, FE) written as an ODE system

$$\mathbf{u}_t + \underbrace{\mathbf{F}(\mathbf{u})}_{\text{Slow, Explicit}} + \underbrace{\mathbf{G}(\mathbf{u})}_{\text{Fast, Implicit}} = \mathbf{0}$$

IMEX Multi-stage Methods (RK-type) form a consistent set of nonlinear residuals:

$$\mathbf{u}^{(i)} = \mathbf{u}^n + \Delta t \sum_{j=1}^{i-1} \hat{a}_{ij} \mathbf{F}(\mathbf{u}^{(j)}) - \Delta t \sum_{j=1}^{i} a_{ij} \mathbf{G}(\mathbf{u}^{(j)}) \qquad \text{for } i = 1 \ldots s,$$

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \sum_{i=1}^{s} \hat{b}_i \mathbf{F}(\mathbf{u}^{(i)}) - \Delta t \sum_{i=1}^{s} b_i \mathbf{G}(\mathbf{u}^{(i)}).$$

$$\begin{array}{c|c} \hat{\mathbf{c}} & \hat{\mathbf{a}} \\ \hline & \hat{\mathbf{b}}^T \end{array} \text{ is explicit, and } \begin{array}{c|c} \mathbf{c} & \mathbf{a} \\ \hline & \mathbf{b}^T \end{array} \text{ is implicit.}$$

High-order accuracy (e.g. 2^{nd} – 5^{th}), with various stability properties have demonstrated A-, L-stability, Strong Stability Preserving (SSP), TVB, ….

See for e.g. Ascher, Ruuth and Wetton (1997), Ascher, Ruuth and Spiteri (1997), Carpenter, Kennedy, et. al (2005), Higueras et. al. (2011)

E.g. Implicit / Explicit (IMEX) Methods and the Implicit Sub-problem (contd.)

Discrete Nonlinear Sub-problem – Newton's Method, Krylov subspace linear solver (e.g. GMRES)

$$\mathcal{F}(\mathbf{u}^{(\mathbf{i})}) = \mathbf{u}^{(i)} - \mathbf{u}^{n} - \Delta t \sum_{j=1}^{i-1} \hat{a}_{ij} \mathbf{F}(\mathbf{u}^{(j)}) + \Delta t \sum_{j=1}^{i} a_{ij} \mathbf{G}(\mathbf{u}^{(j)}) = 0$$

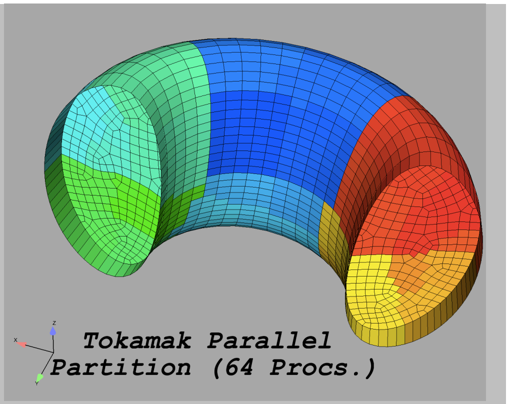
/* Find u* such that $\mathcal{F}(\mathbf{u}^{*}) = 0$ with NOX nonlinear solver, Jacobian with AD in Sacado */

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

Krylov Methods - Robust, Scalable and Efficient Parallel Preconditioners (**AztecOO,Belos**)

- Approximate Block Factorizations (**Aztec, Ifpack**)
- Physics-based Preconditioners (**Teko**)
- Multi-level solvers for systems and scalar equations (**ML, Muelu**)

Preconditioning



Three variants of preconditioning

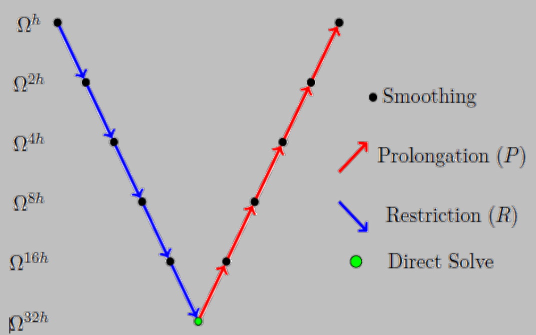
1. Domain Decomposition (AztecOO & Ifpack)

- 1 –level Additive Schwarz DD, ILU(k) Factorization on each processor w/overlap
- High parallel eff., non-optimal algorithmic scalability

2. Multilevel Methods for Systems: (ML & Muelu)

Fully-coupled Algebraic Multilevel methods

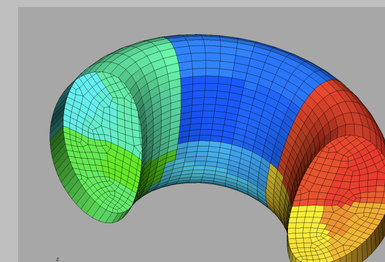
- Consistent set of DOF-ordered blocks at each node (e.g. VMS/Stabilized FE)
- Uses block non-zero structure of Jacobian
- Additive Schwarz DD ILU(k) as smoothers (Jacobi & GS possible for transients)
- Can provide optimal algorithmic scalability



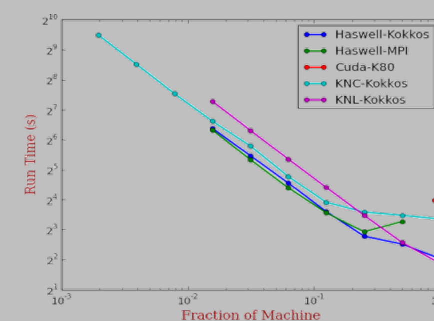
3. Approximate Block Factorization / Physics-based (Teko package)

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

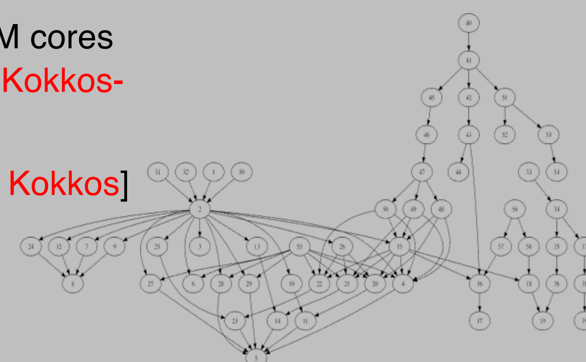
Drekar: Solution Methods / Software Infrastructure Pushing Limits of Algorithms using Component Integration



- 1^{st}-5^{th} order explicit, fully-implicit and implicit / explicit (IMEX) [Tempus, Rythmos]
- Unstructured nodal FE and physics-compatible (node, edge, face, …) methods [Drekar, Intrepid2]
- Fully coupled globalized Newton-Krylov (NK) solver (NOX)
    - Residuals are programed and automatic differentiation (AD) generates Jacobian for NK, Sensitivities, Adjoints, etc. [Sacado]
    - GMRES Krylov solvers for robustness [AztecOO, Belos]
    - Scalable preconditioners: Fully-coupled system AMG, Physics-based block preconditioners with AMG [ML, Muelu, Teko, Ifpack, Ifpack2]



- Software architecture:
    - Massively parallel R&D code:
        - MPI version demonstrated weak scaling to 1M+ cores; sub-block solvers to 1.6M cores
        - MPI+X. Employs Kokkos performance portability abstraction layer interface and Kokkos-kernels utilities for portability and move towards performance.
    - Core FE assembly capability and DAG for dependencies [Panzer, Phalanx, Intrepid2, Kokkos]
    - Solvers/Linear Alg. tools based on Trilinos packages [AztecOO/Belos, ML/Muelu, Epetra/TPetra, Teko, Ifpack, Ifpack2, ShyLu, etc.]
    - Template-based generic programming with AD of FE weak forms [Sacado]



[Drekar: Shadid, Pawlowski, Cyr, Phillips, Conde, Mabuza, Miller, Crockatt, Lin, Smith]

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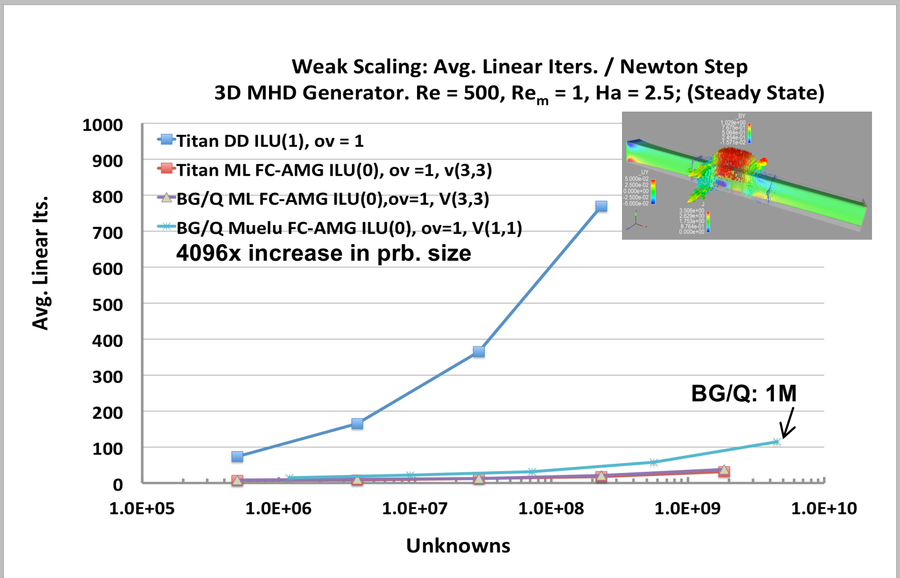
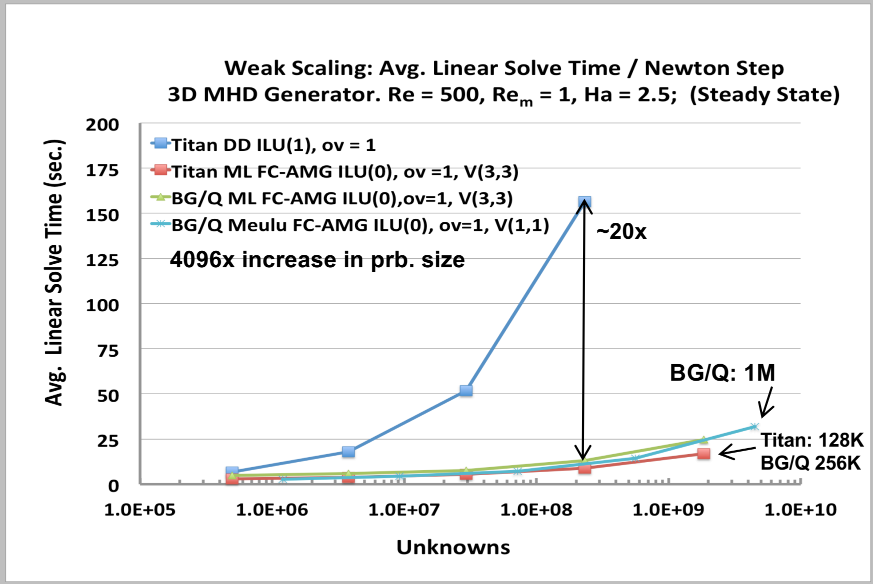
Large-scale Scaling Studies for Cray XK7 AND BG/Q; VMS 3D FE MHD

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





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

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

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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

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

[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**.)

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

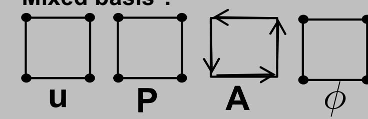
Norm Equivalence Methods

- 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 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

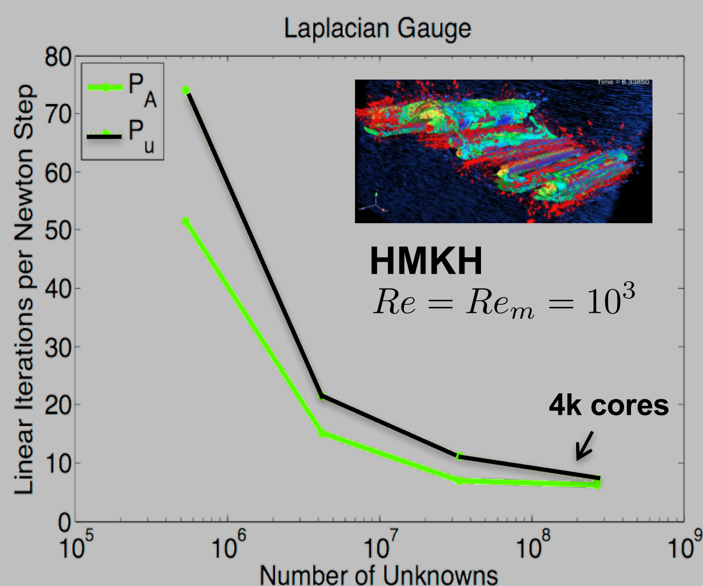
Mixed basis*:

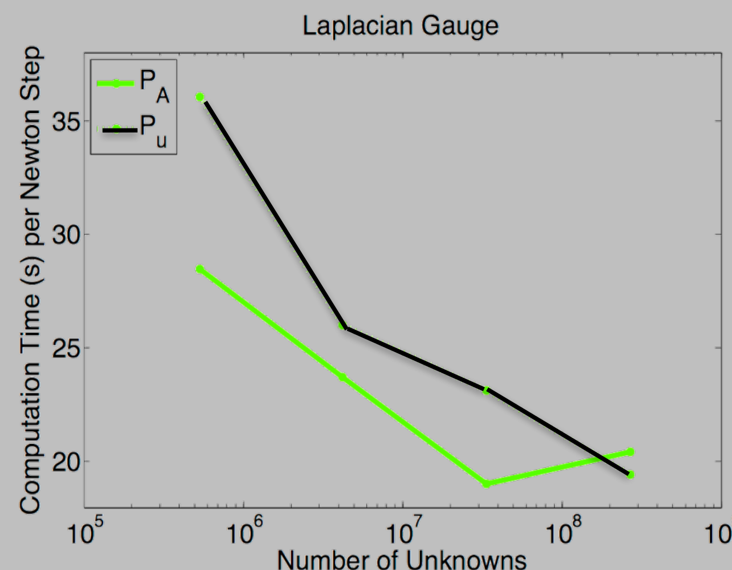


$$\mathcal{A}_{GSG} = \left(\begin{array}{ccc|c} F & B^t & Z & 0 \\ B & C & 0 & 0 \\ Y & 0 & G & D^t \\ \hline 0 & 0 & 0 & L \end{array}\right) \qquad \mathcal{P}_{\mathbf{A}} = \begin{pmatrix} F & 0 & Z \\ 0 & I & 0 \\ Y & 0 & G \end{pmatrix} \begin{pmatrix} F^{-1} & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I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

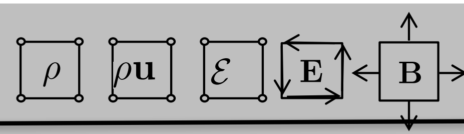
$$\hat{S}_{\mathbf{A}} = G - Y\hat{F}^{-1}Z \qquad \hat{S}_P = C - B\hat{F}^{-1}B^t$$

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	$\frac{\partial (\rho_a \mathbf{u}_a)}{\partial t} + \nabla \cdot (\rho_a \mathbf{u}_a \otimes \mathbf{u}_a + p_a I + \Pi_a) = q_a n_a (\mathbf{E} + \mathbf{u}_a \times \mathbf{B})$ $- \sum_{b \neq a} \left[\rho_a (\mathbf{u}_a - \mathbf{u}_b) n_b \bar{\nu}_{ab}^{M} + \rho_b \mathbf{u}_b n_a \bar{\nu}_{ab}^{+} - \rho_a \mathbf{u}_a n_b \bar{\nu}_{ab}^{-} \right]$
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

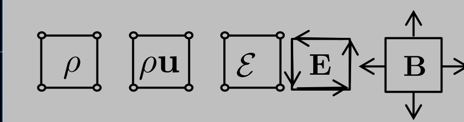
Other work on formulations, solution algorithms:

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

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

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

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

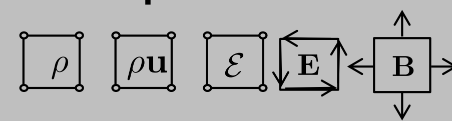
Reordered 3x3

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

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



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

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: $\frac{\partial^2 \mathbf{E}}{\partial t^2} + \frac{1}{\sigma \mu_0} \nabla \times \nabla \times \mathbf{E} = \mathbf{0}$

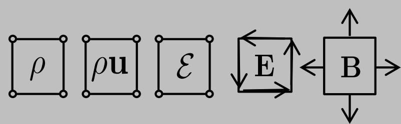
Electric field system
Edge-based curl-curl type
ML: H(curl) AMG with grad-div stab.
(lumped mass)

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

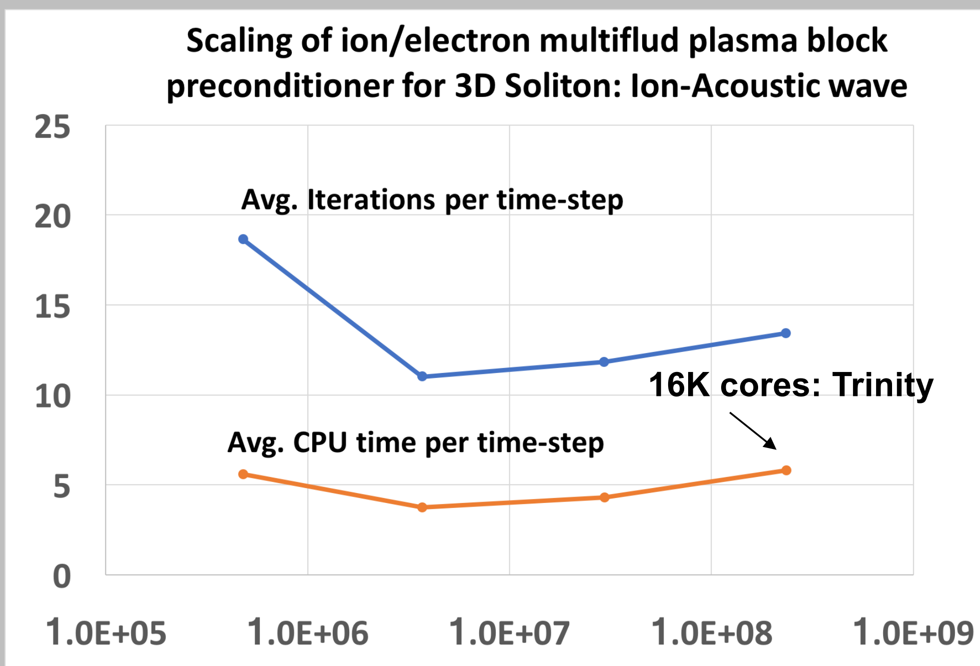
Face-based simple
mass matrix Inversion.
V-cycle Gauss-Siedel

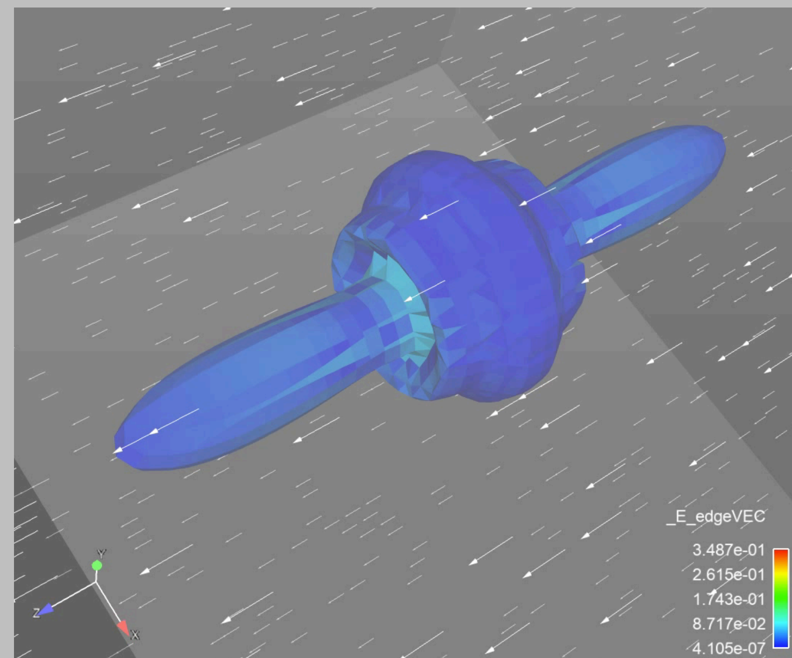
3D Gaussian Density/Pressure Perturbation as initial condition

Isentropic ion-acoustic wave



Structure-preserving discretization





Iso-surface of ion density colored by electric field magnitude

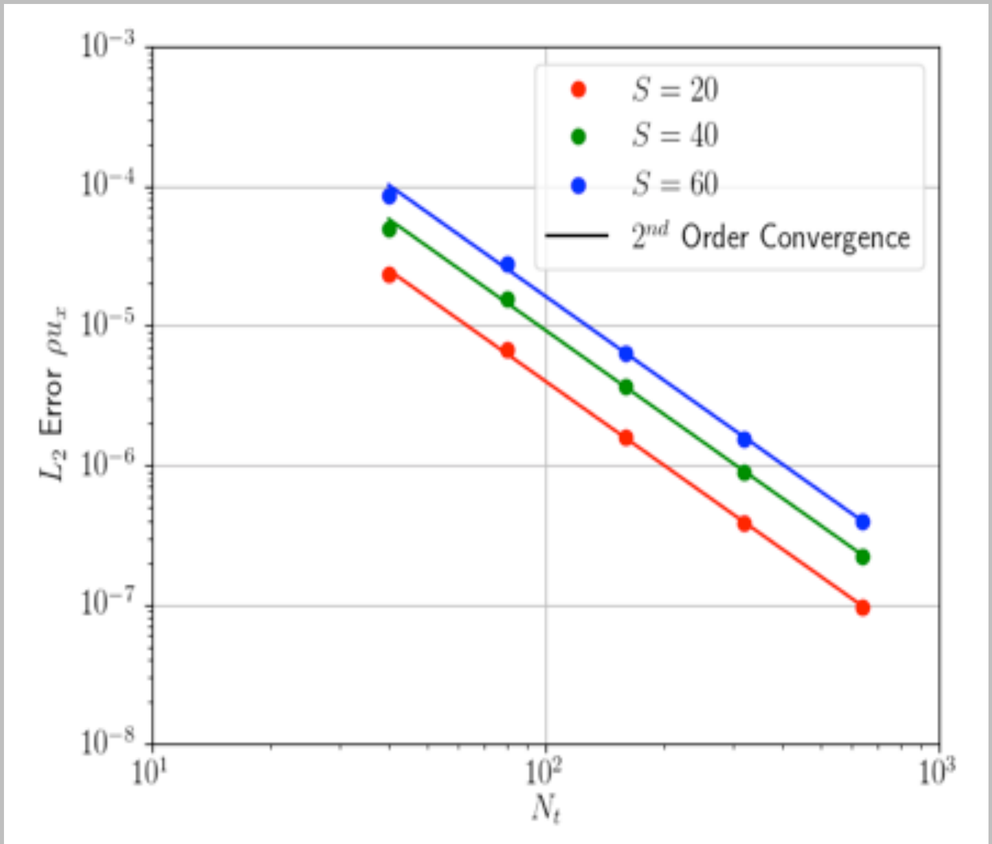
Isentropic flow

$$\frac{P}{P_0} = \left(\frac{\rho}{\rho_0}\right)^{\gamma} \qquad \rho_\alpha = m_\alpha \left(1 + e^{-10||\vec{x}-\vec{x}_0||^2}\right) \quad ||^2)$$

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

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	

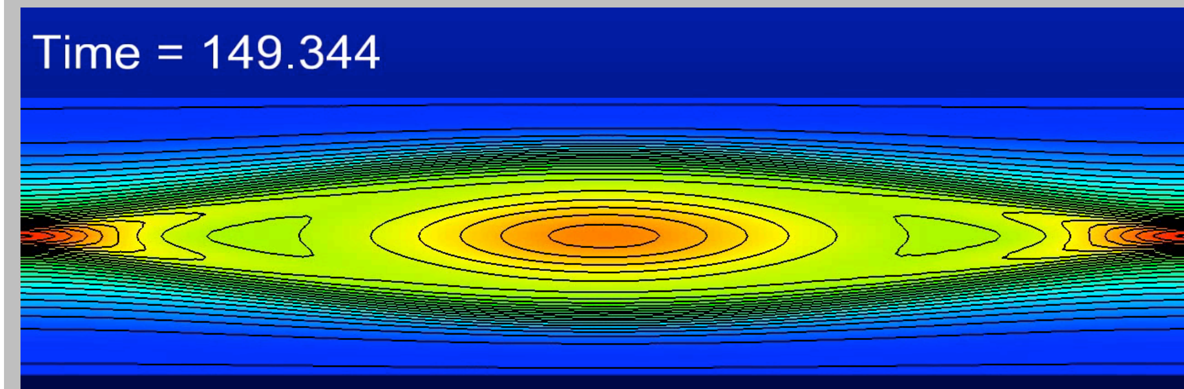
IMEX terms: implicit/explicit

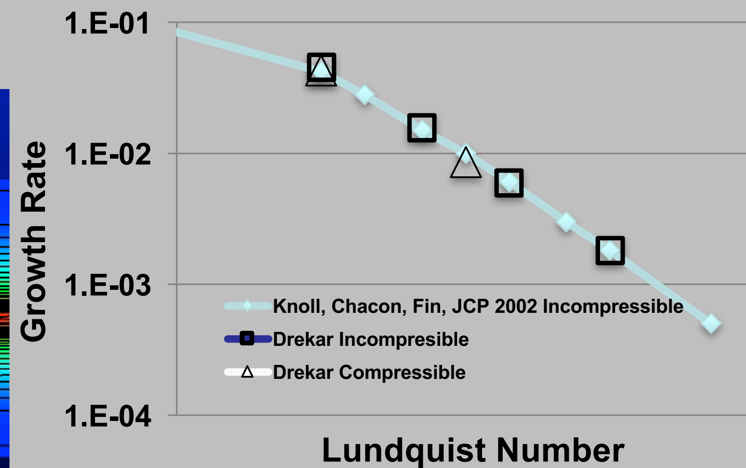
Overstepping fast time scales is both stable and accurate. The inclusion of a resistive operator adds dissipation to the electron dynamics on top of the L-stable time integrator.

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

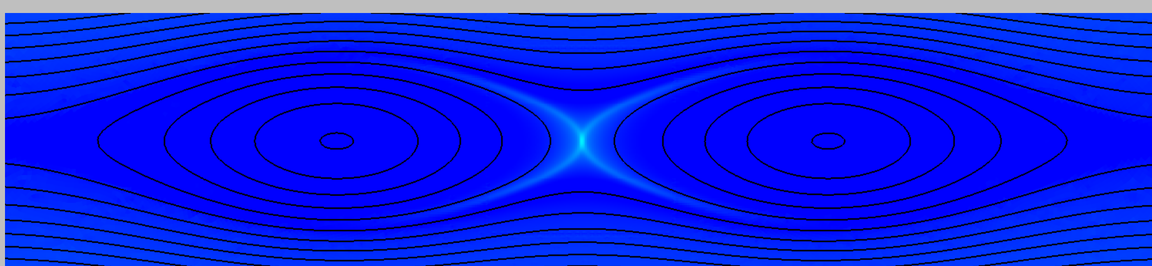
Understanding Fundamental Process and Physical Time-scales in Magnetic Reconnection

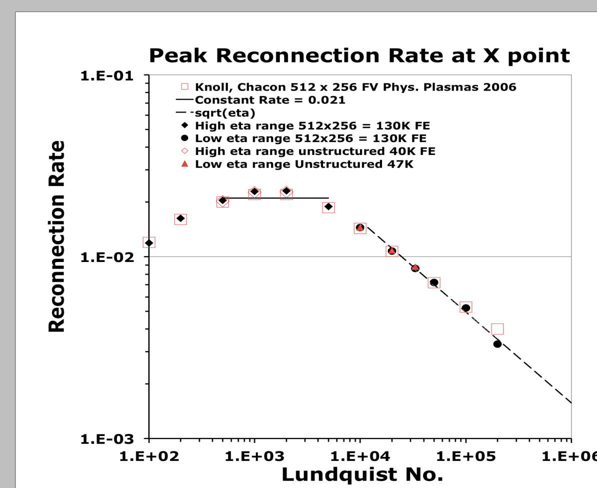
Thin Current Sheet Tearing Mode Instability



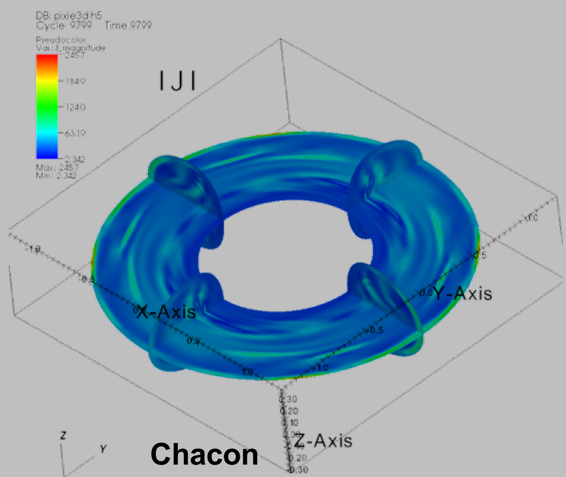


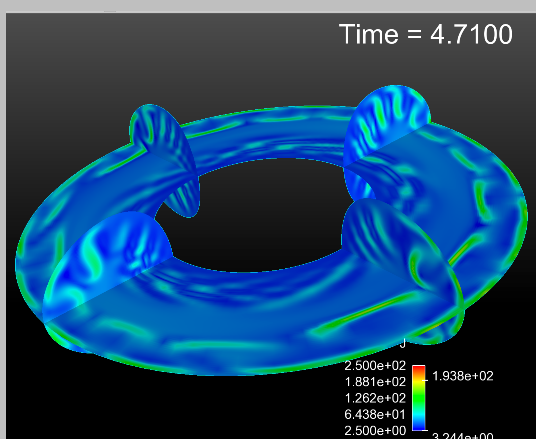
Magnetic Reconnection in Island Coalescence

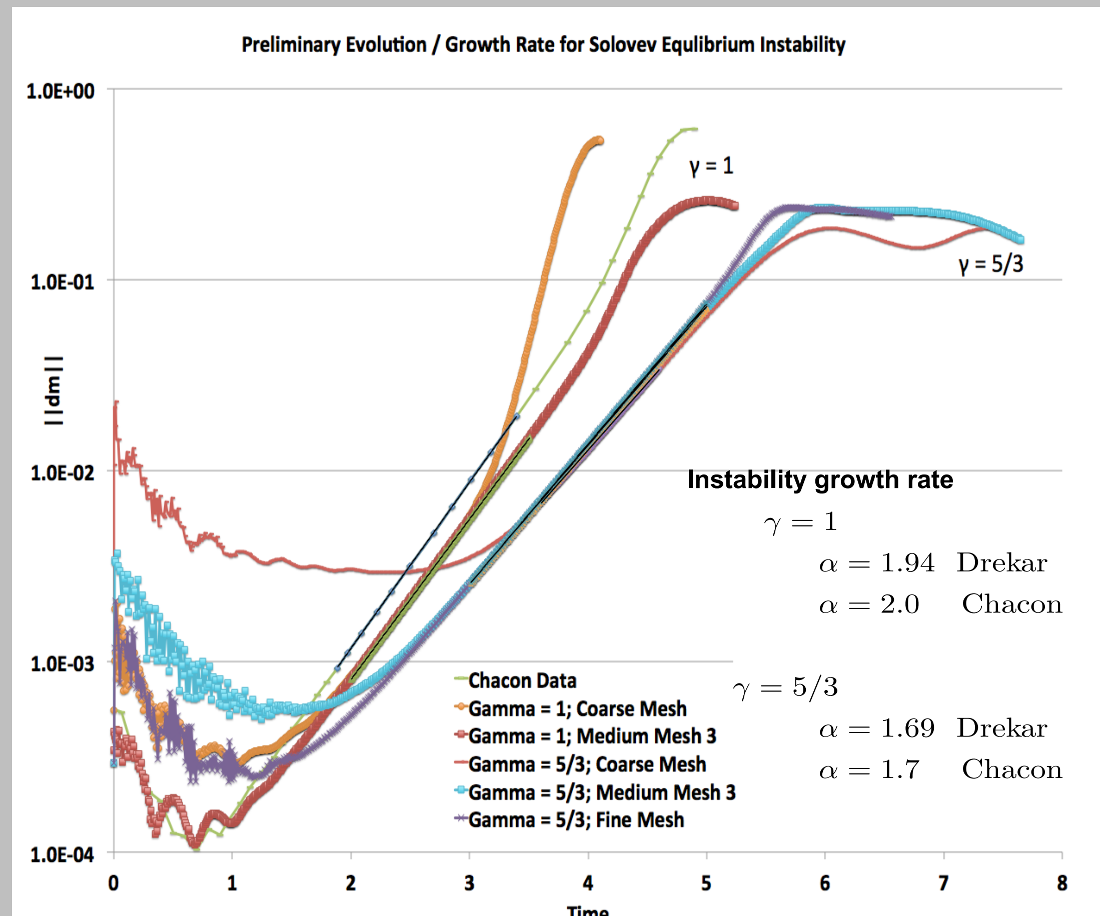




Preliminary Soloveev Equilibrium/Linear Disturbance Growth.





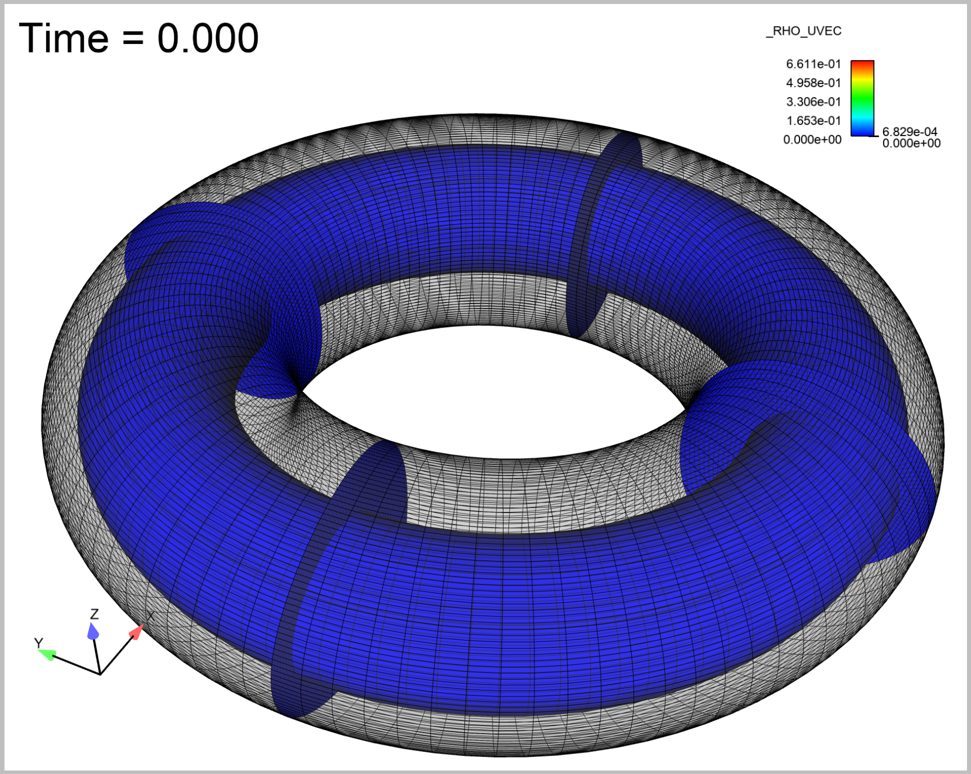


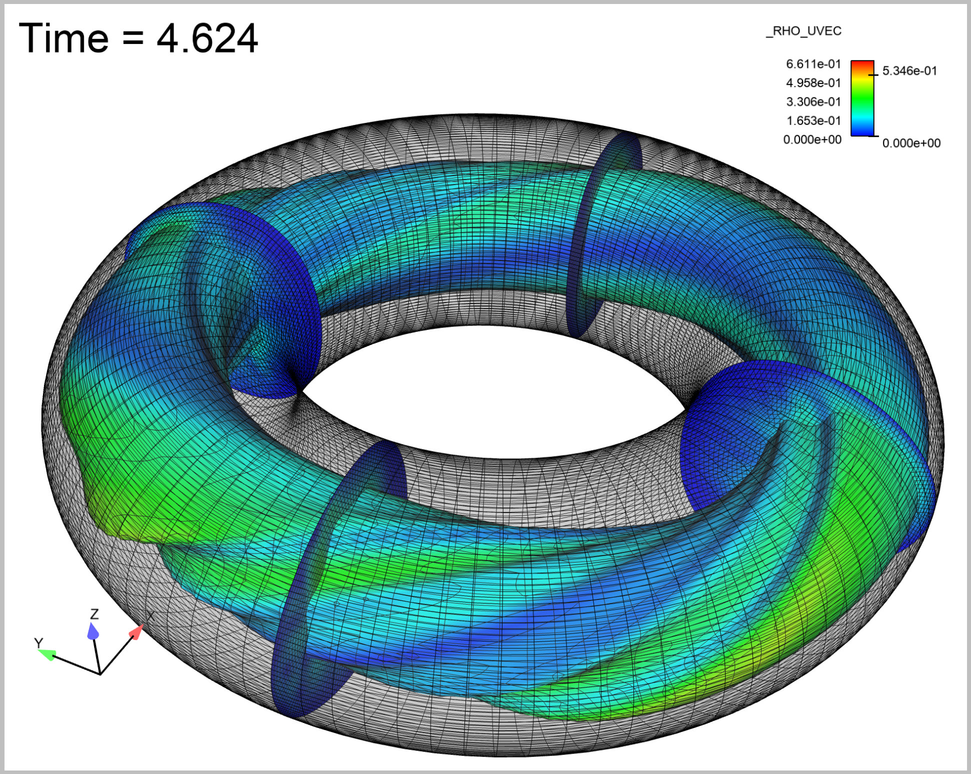
with L. Chacon (LANL)

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

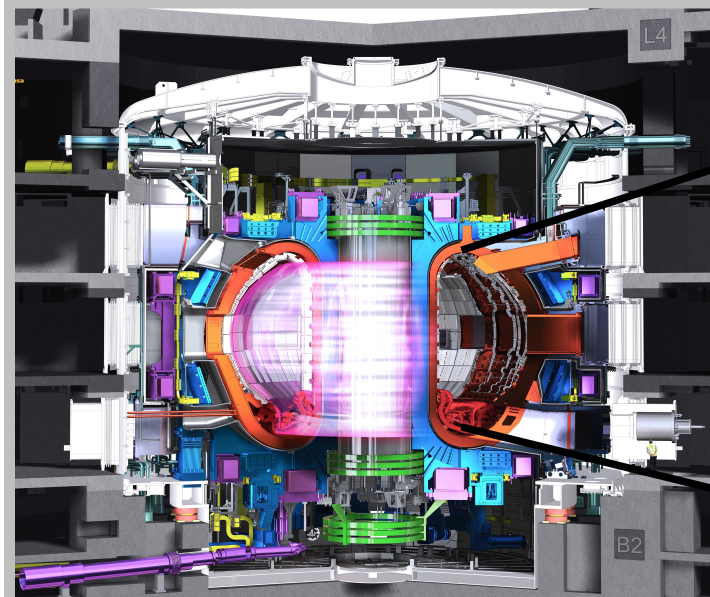
Sandia National Laboratories

Preliminary Soloveev Nonlinear Disturbance Saturation.

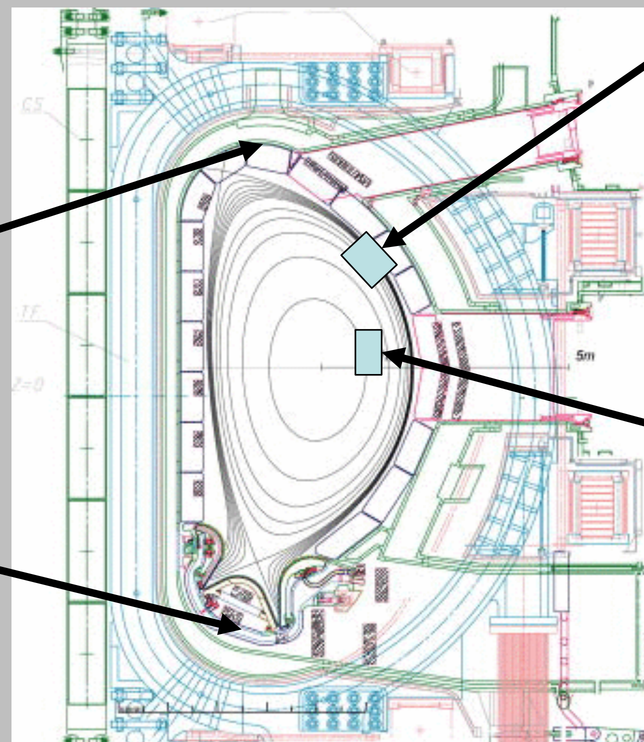




Disruption is a prompt termination of a plasma confinement in a tokamak and can be a showstopper for ITER. Mitigate to control thermal and current quench evolution.



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

Concluding Remarks

- General mathematical libraries and components 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
- Every library and component can also add a RISK to production and R&D application software.
  - Applications have 15 to 30+ year lifetimes
  - Scope creep – promotes inevitable tension in *flexibility vs performance* tradeoffs
  - Long term *stable sufficient funding and resources* are critical for fully supporting and enhancing capabilities.
- Components really help getting started quickly, but can sometimes hurt getting finished. Tend to be general solutions that greatly improve productivity and not specific solutions that could be much faster.
- Complex components can make it difficult for new users to orient themselves in large code

Trilinos Package Summary

	Objective	Package(s)
Discretizations	Meshing & Discretizations	Intrepid, Pamgen, Sundance, Mesquite, STKMesh, Panzer
	Time Integration	Rythmos, Tempus
Methods	Automatic Differentiation	Sacado
	Mortar Methods	Moertel
Services	Linear algebra objects	Epetra, Tpetra
	Interfaces	Xpetra, Thyra, Stratimikos, Piro, …
	Load Balancing	Zoltan, Isorropia, Zoltan2
	“Skins”	PyTrilinos, WebTrilinos, ForTrilinos, CTrilinos
	Utilities, I/O, thread API	Teuchos, EpetraExt, Kokkos, Phalanx, Trios, …
Solvers	Iterative linear solvers	AztecOO, Belos, Komplex
	Direct sparse linear solvers	Amesos, Amesos2, ShyLU
	Direct dense linear solvers	Epetra, Teuchos, Pliris
	Iterative eigenvalue solvers	Anasazi
	Incomplete factorizations	AztecOO, Ifpack, Ifpack2
	Multilevel preconditioners	ML, CLAPS, MueLu
	Block preconditioners	Meros, Teko
	Nonlinear solvers	NOX, LOCA
	Optimization	MOOCHO, Aristos, TriKota, GlobiPack, OptiPack, ROL
	Stochastic PDEs	Stokhos