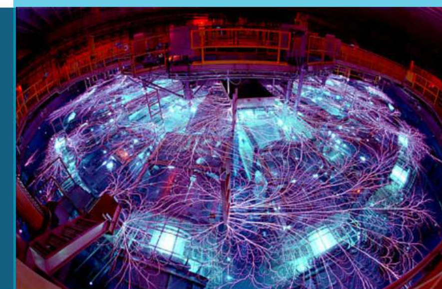
SAND2019-14894C

Sandia National Laboratories

Scalable Block Preconditioning of Implicit / IMEX FE Continuum Plasma Physics Models



John N. Shadid

Center for Computing Research

Sandia National Laboratories

and

Department of Mathematics and Statistics

University of New Mexico

CCR Center for Computing Research

U.S. DEPARTMENT OF ENERGY Office of Science

ASCR

U.S. DEPARTMENT OF ENERGY Office of Science Fusion Energy Sciences

Unclassified Unlimited Release
SAND2019-xxxx C
12/09/2019

U.S. DEPARTMENT OF ENERGY NNSA

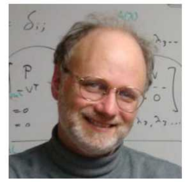
Collaborators

Long-time-scale Collaborators:

Ray Tuminaro

Roger Pawlowski

Paul Lin (LBL)



Howard Elman (U. MD)

Luis Chacon: (LANL)

Current Research Team:

Sidafa Conde

Michael Crockatt (PD)

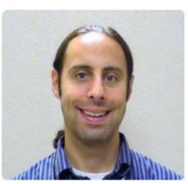
Sibu Mabuza
(PD, now Assistant
Prof. Clemson)

Ari Rappaport
(student)

Tom Smith

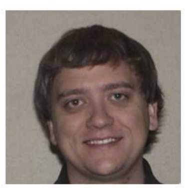
Ignacio Tomas (PD)

Past Research Team Members



Eric Cyr

Edward Phillips



Sean Miller

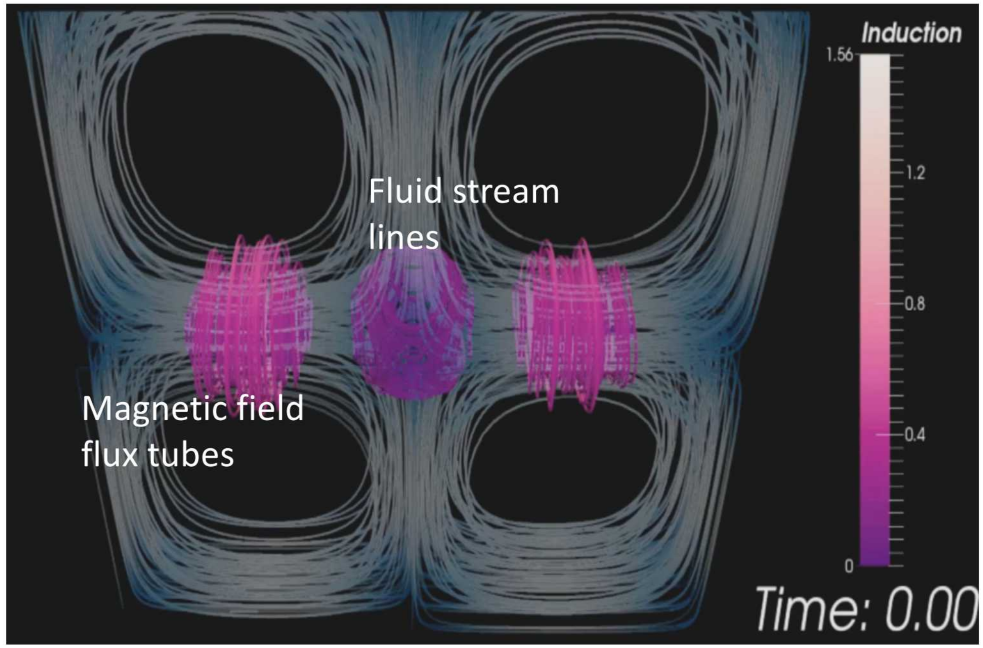
Outline

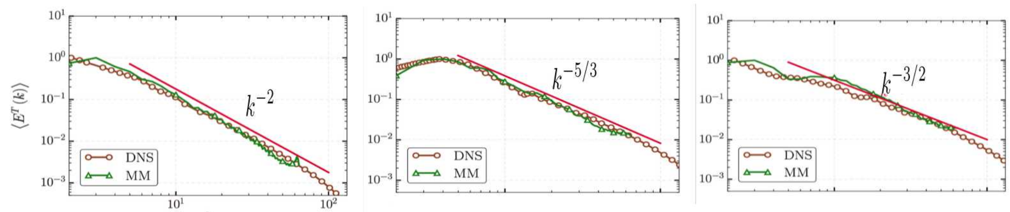
- General Scientific and Mathematical/Computational Motivation
- Comments on Multiple-time-scale Plasma Systems
  - Magnetic Confinement Fusion: Tokamak Device
  - Magnetic Inertial Fusion: Z-pinch (not discussed but a strong motivation)
- Brief Description on Continuum PDE Models (Kinetic, Navier-Stokes (NS), MHD, multifluid plasma)
- Discussion on Newton-Krylov Methods and Time Integration
  - Illustrations of Operator-split vs. Implicit 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)
- 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:**
  - **Magnetic reconnection, instabilities,**
  - **Solar flares, Coronal Mass Ejections.**
- **Planetary-physics:**
  - **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.
Non-universality of total 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.

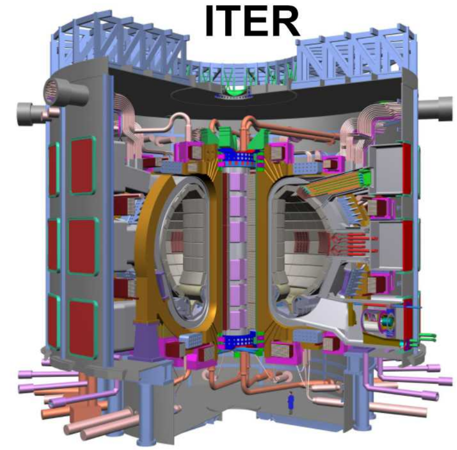
These mechanisms:

- **can be dominated by one, or a few processes, that drive a short dynamical time-scale consistent with these dominating modes,**

- **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.**

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

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



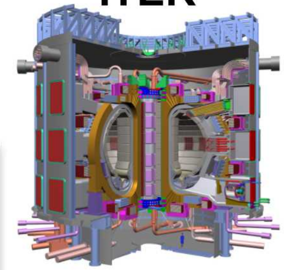
<u>**Goal for Fusion Device:**</u>

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

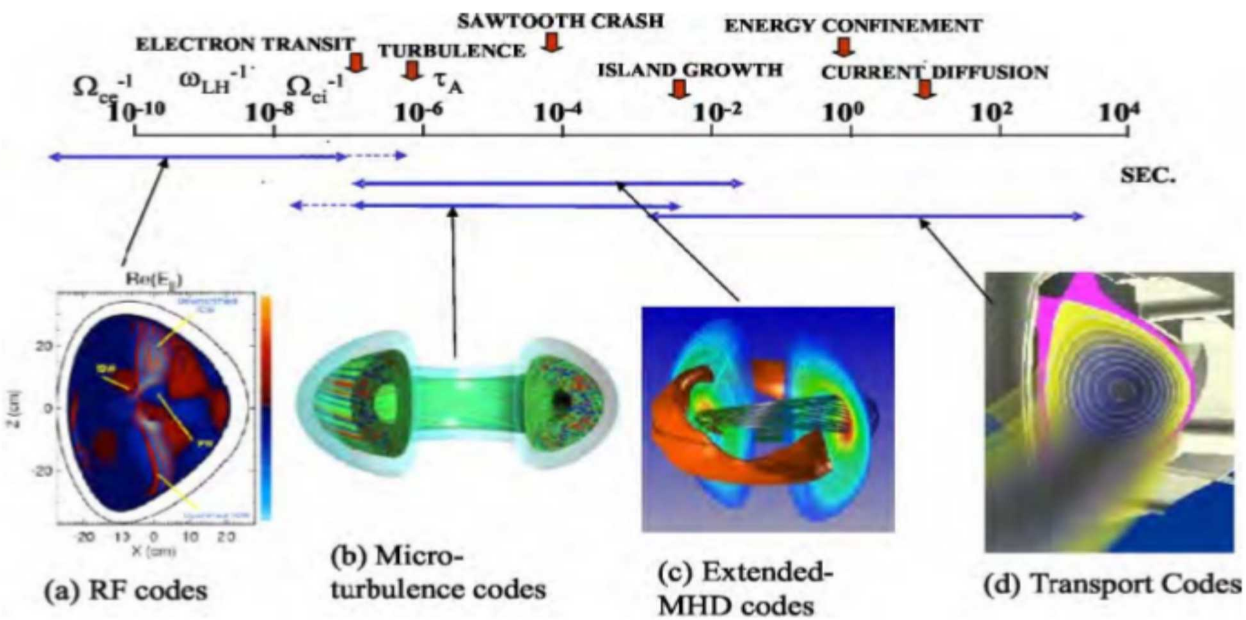
  - **Plasma disruptions can cause break of confinement, huge thermal energy loss, and discharge very large electrical currents (~20MA) to surface and damage the device.**
  - **ITER can sustain only a limited number of significant disruptions, O(1 – 5).**

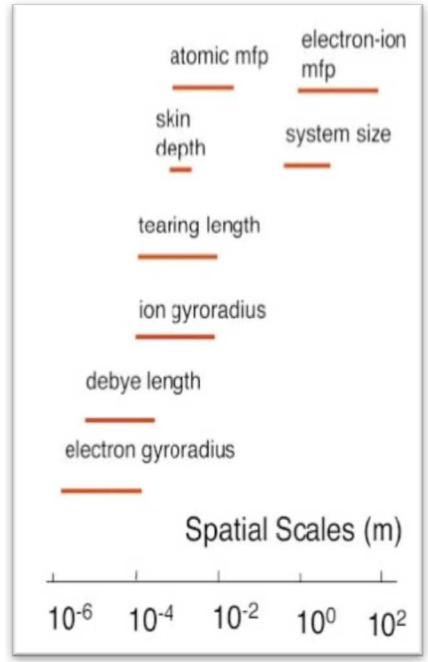
E.g. Multiple-time-scale Multiphysics System: Magnetic Confinement Fusion

ITER



MCF Devices are characterized by large-range of time and length-scales

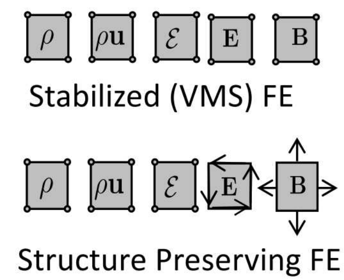




DOE Office of Science ASCR/OFES Reports: Fusion Simulation Project Workshop Report, 2007, Integrated System Modeling Workshop 2015

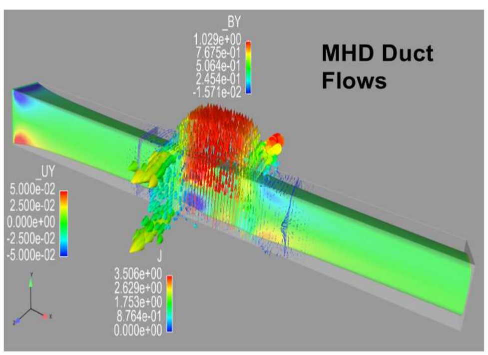
Our Mathematical Approach - develop:

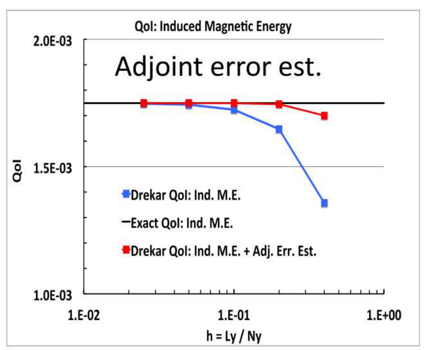
- **Stable, higher-order accurate implicit/IMEX formulations for multiple-time-scale systems**
- **Stable and accurate unstructured FE spatial discretizations. Options enforcing key mathematical properties (e.g. structure preserving forms: div B = 0; positivity ρ , P; DMP)**

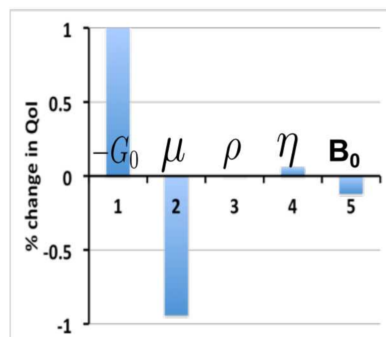


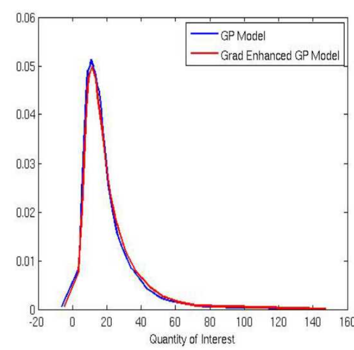
- **Robust, efficient fully-coupled nonlinear/linear iterative solution based on Newton-Krylov methods**
- **Scalable and efficient multiphysics preconditioners utilizing physics-based and approximate block factorization/Schur complement preconditioners with multi-level (AMG) sub-block solvers**

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









Notional Outline of Plasma Modelling Hierarchy

Equation of Motion for charged particle in EM field (neglects relativistic effects)

$$\frac{\mathrm{d}\mathbf{V}_i}{\mathrm{d}t} = q_s(\mathbf{E} + \mathbf{V}_i \times \mathbf{B})/m_s$$

Maxwell Eq. (E,B): Lorentz force

Discrete particle total density view:
Defining total particle density sum $N_s(x,v,t)$, with Lagrangian coordinates ($X_p(t)$, $V_p(t)$)

$$N_s(\mathbf{x},\mathbf{v},t) = \sum_i \delta(\mathbf{x} - \mathbf{X}_i(t))\delta(\mathbf{v} - \mathbf{V}_i(t))$$

Klimontovich Eq.

$$\frac{\partial N_s}{\partial t} + \mathbf{v}\cdot\frac{\partial N_s}{\partial \mathbf{x}} + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v}\times\mathbf{B})\frac{\partial N_s}{\partial \mathbf{v}} = \left.\frac{\partial N_s}{\partial t}\right|_c$$

Phase space distribution function: Statistical model - distribution function describes probability that a number of particles occupy a differential volume in phase space (x,v).

$$\frac{\partial f_s}{\partial t} + \mathbf{v}\cdot\frac{\partial f_s}{\partial \mathbf{x}} + \frac{q_s}{m_s}\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right)\cdot\frac{\partial f_s}{\partial \mathbf{v}} = \left.\frac{\partial f_s}{\partial t}\right|_c$$

Boltzmann, Valasov/Maxwell Eq.

$$\rho = m\int f(\mathbf{v})\mathrm{d}\mathbf{v},$$

$$\rho u_i = m\int v_i f(\mathbf{v})\mathrm{d}\mathbf{v},$$

$$\mathcal{P}_{ij} = m\int v_i v_j f(\mathbf{v})\mathrm{d}\mathbf{v},$$

PIC - Method of Characteristics: Lagrangian particle view + MCC/DSMC collisions
3D space + many particles

Discretization of Boltzmann Eq.: FE, FV, Spectral, .. + collision operator approximations
6D space (x,v)

Moment Approx. of Boltzmann: Assumed distribution function and closure approx.
3D space

Reductions to continuum fluid systems:

- **E.g. Maxwellian dist. and *5 moment multifluid EM plasma model* (electrons, ions, neutrals)**
- ***Extended MHD* (retaining aspects of electron dynamics)**
- ***Resistive MHD* approx. (long length scales, …..)**

Reduced unknowns, and time- / length-scales

(w/ S. Bond)

5 Moment Multifluid EM Plasma Model: Multiple Atomic Species, Full Maxwell EM with Collisions/Ionization/Recombination

$\mathcal{C}_s^{\mathrm{sc}}$: elastic scattering
$\mathcal{C}_s^{\mathrm{ion}}$: ionization reactions
$\mathcal{C}_s^{\mathrm{rec}}$: recombination reactions
$\mathcal{C}_s^{\mathrm{cx}}$: charge exchange
$\mathcal{C}_s^{\mathrm{rad}}$: radiative loss

	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]	$\partial_t (\rho_s \mathbf{u}_s) + \nabla \cdot (\rho_s \mathbf{u}_s \otimes \mathbf{u}_s + p_s \underline{\mathbf{I}} + \underline{\mathbf{\Pi}}_s) = q_s n_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) + \boldsymbol{\mathcal{C}}_s^{[1]} + \boldsymbol{\mathcal{S}}_s^{[1]}$
Total Energy[2]	$\partial_t \mathcal{E}_s + \nabla \cdot [(\mathcal{E}_s + p_s) \mathbf{u}_s + \mathbf{u}_s \cdot \underline{\mathbf{\Pi}}_s + \mathbf{h}_s] = q_s n_s \mathbf{u}_s \cdot \mathbf{E} + \mathcal{C}_s^{[2]} + \mathcal{S}_s^{[2]}$
Charge / Current	$q = \sum_s q_s n_s$ $\qquad$ $\mathbf{J} = \sum_s q_s n_s \mathbf{u}_s$
Maxwell's Eqn.	$\frac{1}{c^2} \partial_t \mathbf{E} - \nabla \times \mathbf{B} + \mu_0 \mathbf{J} = \mathbf{0}$ $\qquad$ $\nabla \cdot \mathbf{E} = \frac{q}{\epsilon_0}$ $\partial_t \mathbf{B} + \nabla \times \mathbf{E} = \mathbf{0}$ $\qquad$ $\nabla \cdot \mathbf{B} = 0$

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

Notional Discussion of Plasma Modelling Hierarchy (Contd.): Reduction to MHD

Assume Infinite speed of light (low frequency EM)

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

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

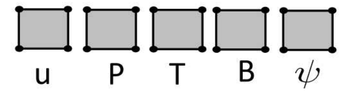
Center of mass description for Equation of Motion (essentially ions), neglect electron momentum inertia ($m_e/m_i = 0$) and develop a generalized Ohm's law description for E

$$\mathbf{E} = -\underbrace{\mathbf{u} \times \mathbf{B}}_{\text{Ideal}} + \underbrace{\eta \mathbf{J}}_{\text{Resistive}} + \underbrace{\frac{d_i}{n}(\mathbf{J} \times \mathbf{B} - \nabla P_e)}_{\text{Hall}}$$

Further neglecting Hall physics terms, produces a resistive MHD a resistive MHD model (written in magnetic induction equation form):

$$\mathbf{E} = -\underbrace{\mathbf{u} \times \mathbf{B}}_{\text{Ideal}} + \underbrace{\eta \mathbf{J}}_{\text{Resistive}} \longrightarrow \frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{v} \times \mathbf{B}) + \nabla \times \left(\frac{\eta}{\mu_0} \nabla \times \mathbf{B} \right) = \mathbf{0}$$

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



Resistive MHD Model in Conservative Form

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

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

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

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

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

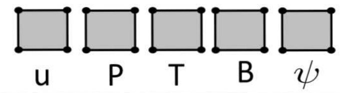
$$\Sigma_{tot} = \rho e + \frac{1}{2}\rho\|\mathbf{u}\|^2 + \|\mathbf{B}\|^2/2\mu_0$$

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

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

- Divergence free involution enforced as constraint with a Lagrange multiplier (Elliptic, parabolic, hyperbolic) [GLM: 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)

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



Navier-Stokes Compressible Flow Model (Conservative Form)

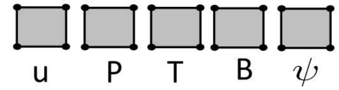
$$\mathbf{T} = -[P - \frac{2}{3}\mu(\nabla \cdot \mathbf{v})]\mathbf{I} + \mu[\nabla \mathbf{v} + \nabla \mathbf{v}^T]$$

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

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

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

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



Additional terms from EM:

- Magnetic Stress
- Poynting Flux and Magnetic Energy
- Magnetic Induction Evolution Eq. and GLM Solenoidal Constraint Eq.

<u>Resistive MHD Model in Conservative Form</u>

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

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

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

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

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

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

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

- 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]

Why Newton-Krylov Methods?

Newton-Krylov

Direct-to-steady-state

Fully-implicit transient /IMEX

<u>Convergence properties</u>

- 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

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

<u>Inexact Newton-Krylov</u>

Solve $\mathbf{J}\mathbf{p}_k = -\mathbf{F}(\mathbf{x}_k)$; until $\dfrac{\|\mathbf{J}\mathbf{p}_k + \mathbf{F}(\mathbf{x}_k)\|}{\|\mathbf{F}(\mathbf{x}_k)\|} \le \eta_k$

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

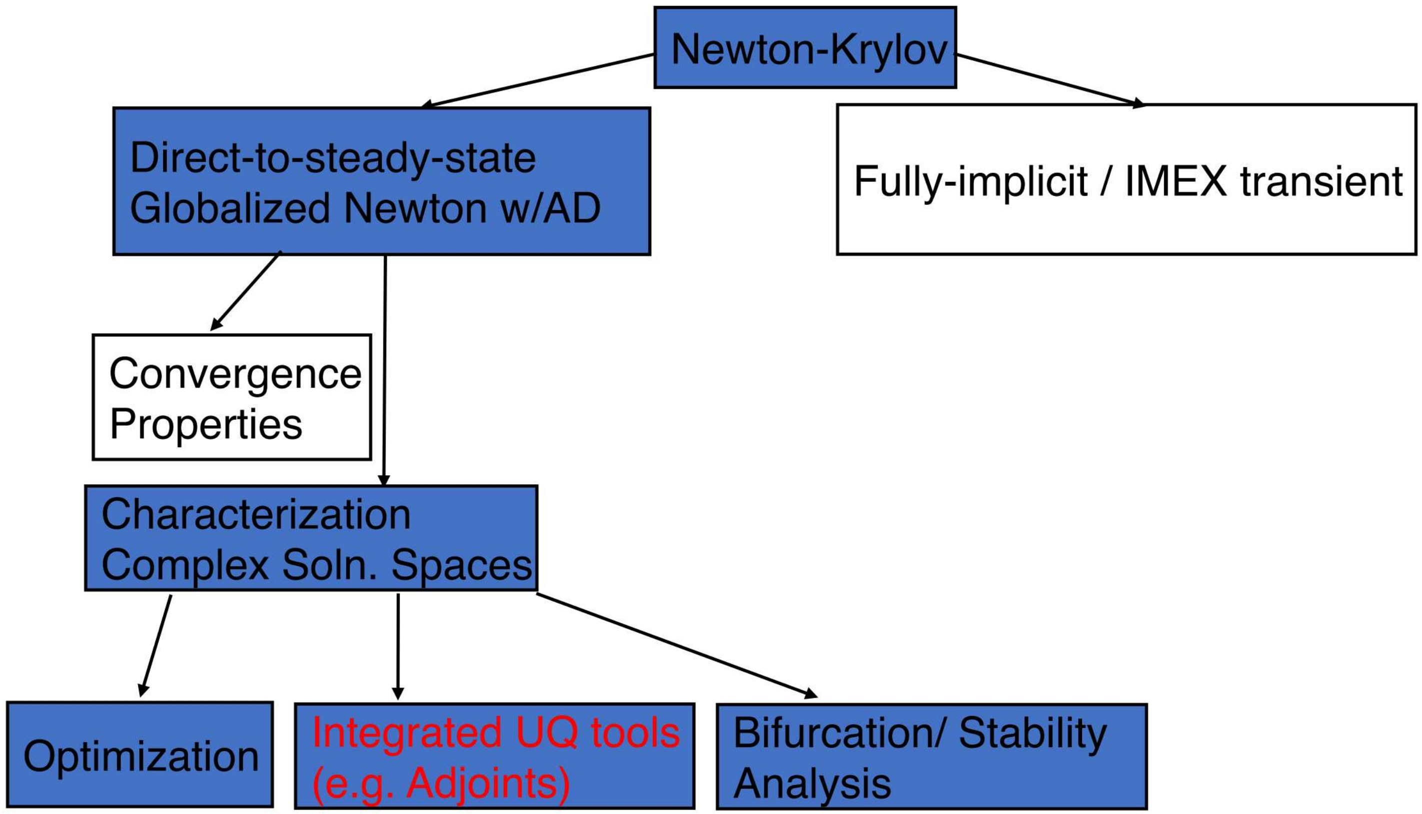
<u>Jacobian Free N-K Variant</u>

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

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

See e.g. Knoll & Keyes, JCP 2004

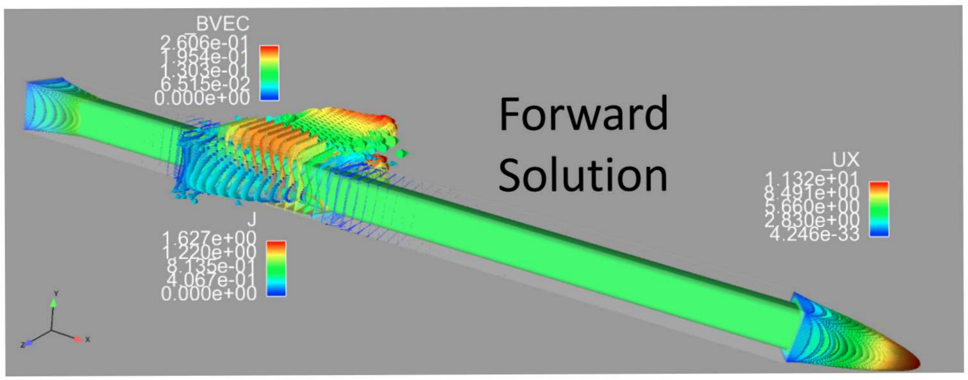
Why Newton-Krylov Methods?

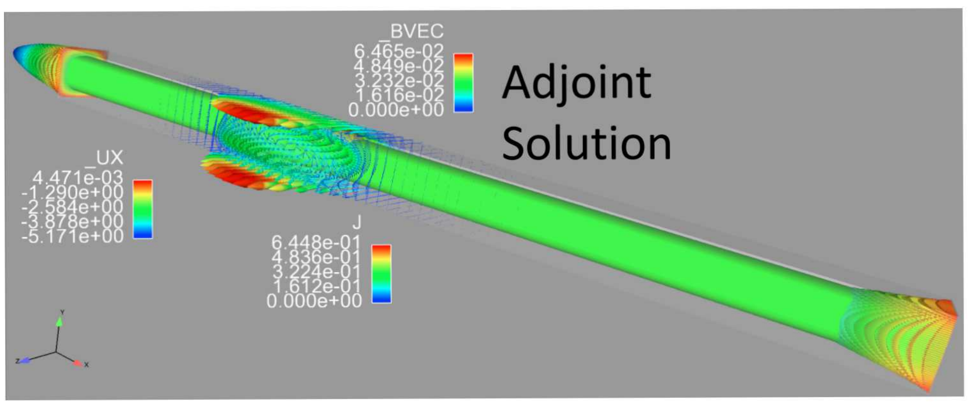


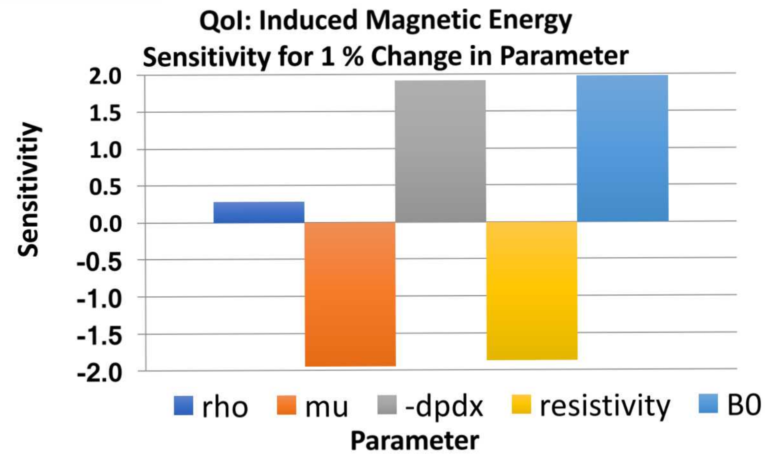
Multiple-time-scale systems: E.g. Adjoint Error-estimation and Sensitivity Study for 3D Steady State MHD Generator (Re ~ 2500, Re_m ~ 10, Ha = 5)

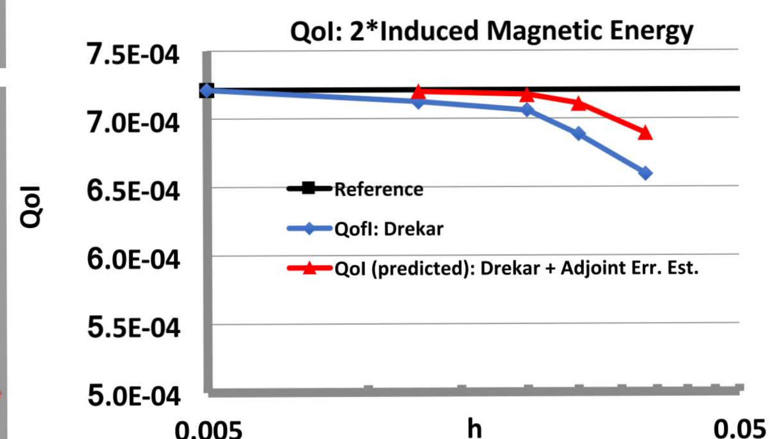
- QoI (1): Induced Magnetic Energy (M.E.)

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









Why Implicit / IMEX Newton-Krylov Methods?

Newton-Krylov

Direct-to-steady-state

Fully-implicit transient / IMEX

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

e.g.

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

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 run at the dynamical time-scale of interest in multiple-time-scale systems (See e.g. Knoll et. al., Brown & Woodward., Chacon and Knoll, S. and Ober, S. and Ropp)

Why Newton-Krylov Methods?

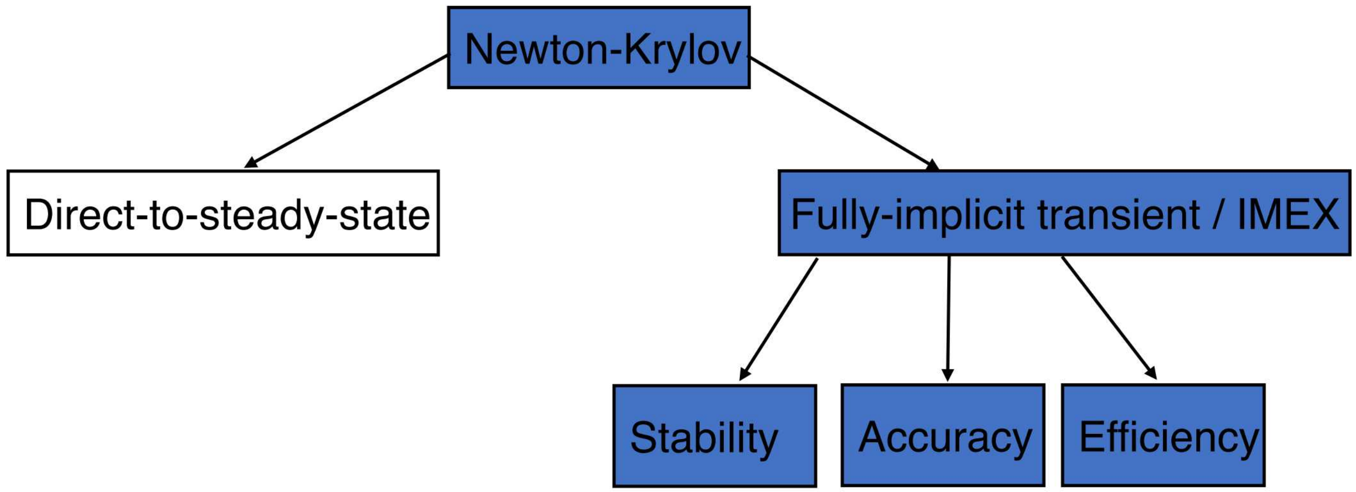


Illustration of Time-scales and an IMEX Partition for Multi-fluid Plasma System Model

Ionization/recombination

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

Cyclotron frequency

Collisional

Strong off diagonal coupling for plasma oscillation

Light wave off diagonal coupling

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

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.;

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

Eigen-values for 5M Euler
Eqn. for each species

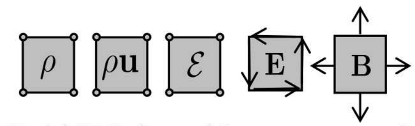
$$\lambda_\alpha = (u_\alpha, u_\alpha \pm \sqrt{\gamma T_\alpha / m_\alpha})$$

Time-scales from Maxwell
Eqn. & EM source terms

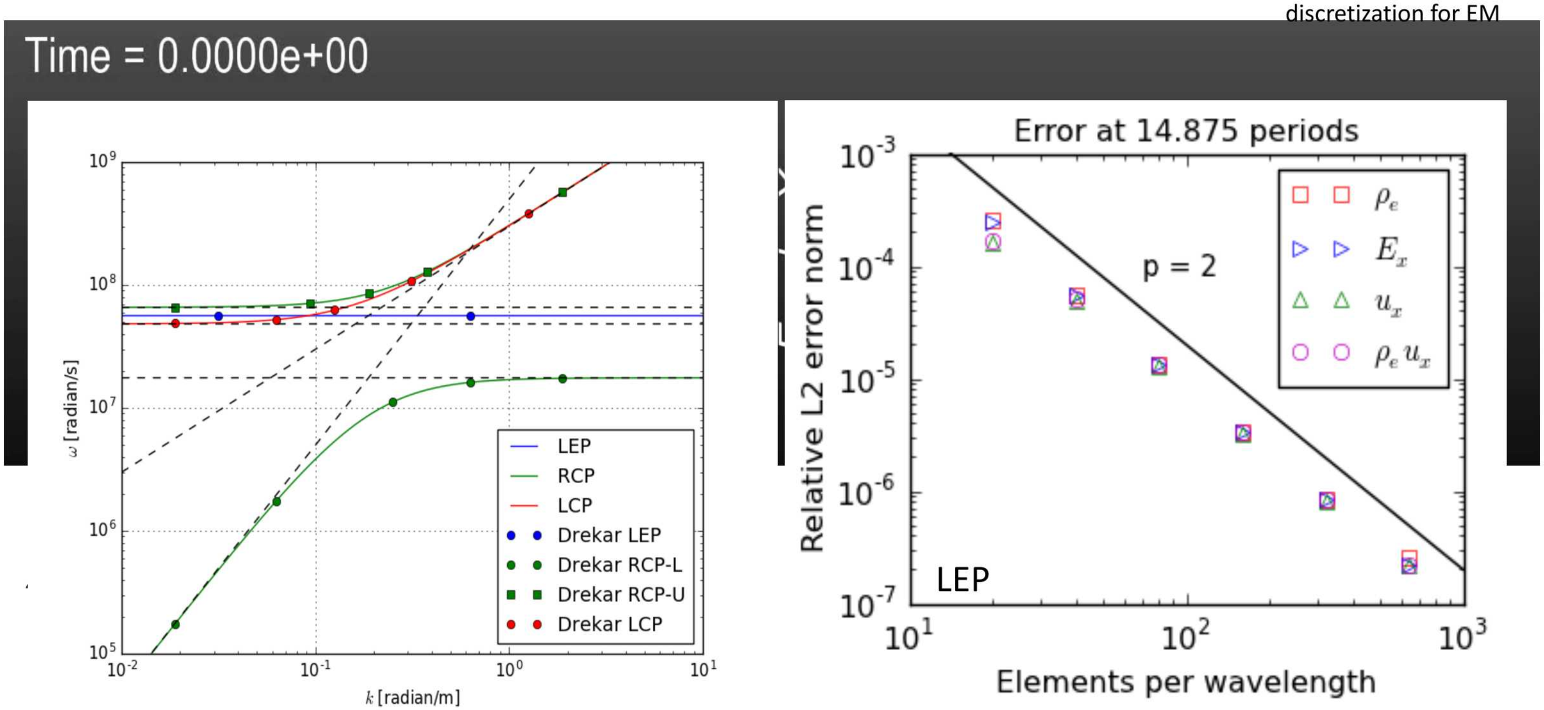
$$\tau_{EM} = \Delta x / c; \quad \tau_{\omega_{p\alpha}} = \frac{1}{\sqrt{\frac{n_\alpha q_\alpha^2}{\epsilon_0 m_\alpha}}}; \quad \tau_{\omega_{c\alpha}} = \frac{1}{\frac{q_\alpha B}{m_\alpha}}$$

EM Wave | Plasma Freq. | Cyclotron Freq.

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



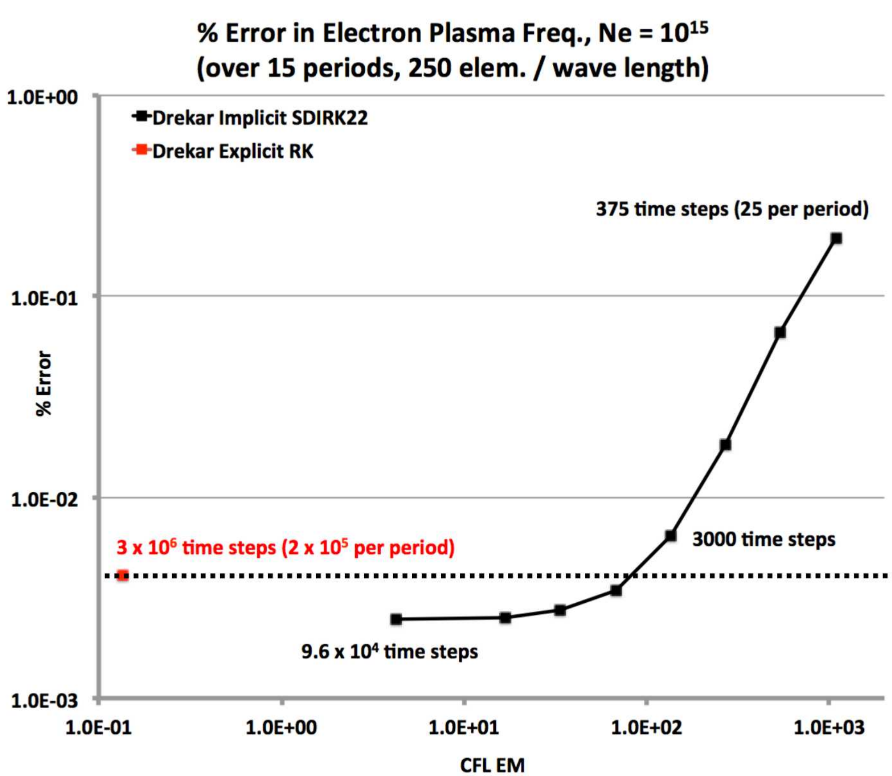
Nodal FE Hydro and Structure-preserving discretization for EM

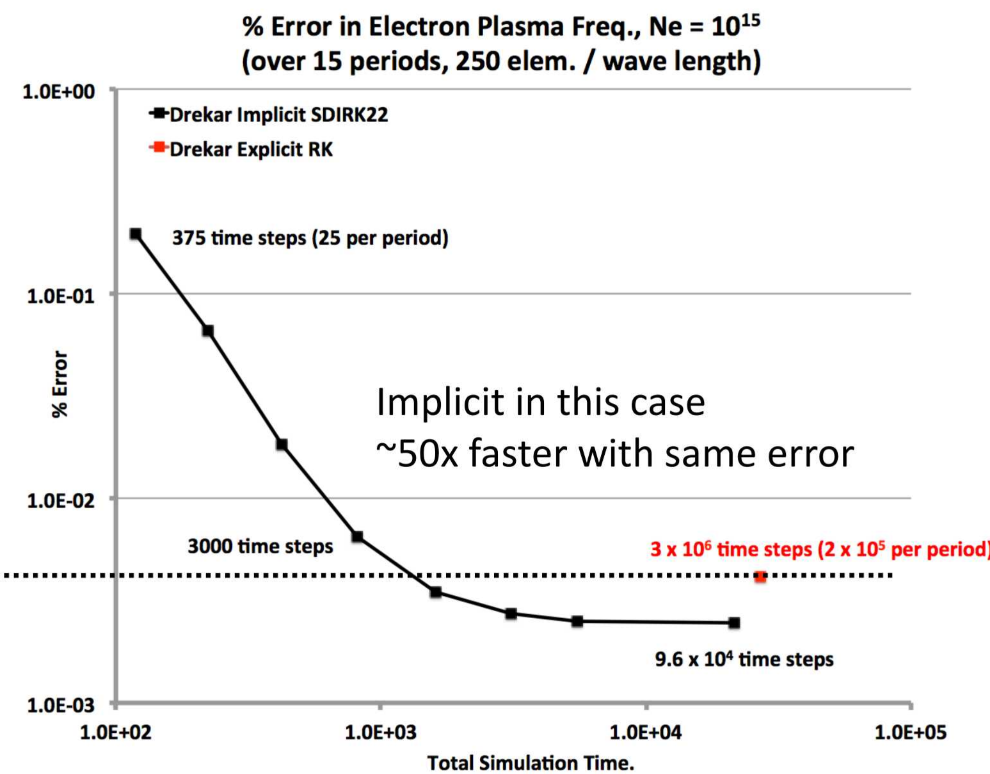


LEP: Longitudinal Electron Plasma Wave
RCP: Right Hand Circularly Polarized Wave
LCP: Left Hand Circularly Polarized Wave
(Cold plasma)

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

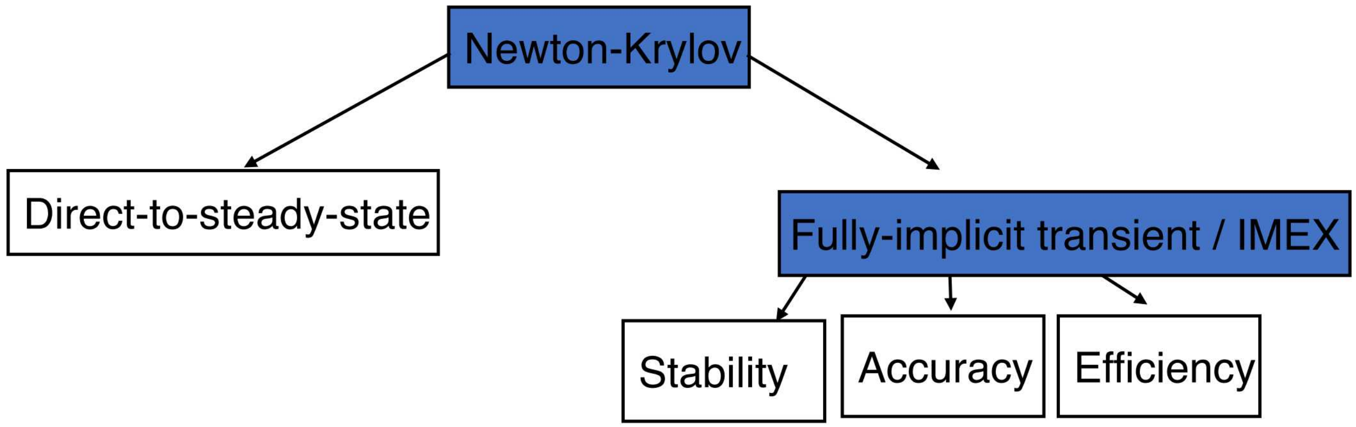
Demonstration of Accuracy for Implicit Solution Methods for Langmuir wave (i.e. Longitudinal Electron Plasma [LEP] Oscillation): Fast time-scale unresolved transverse EM (light) waves (Ne = 10^{15})





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

Why Newton-Krylov Methods?



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

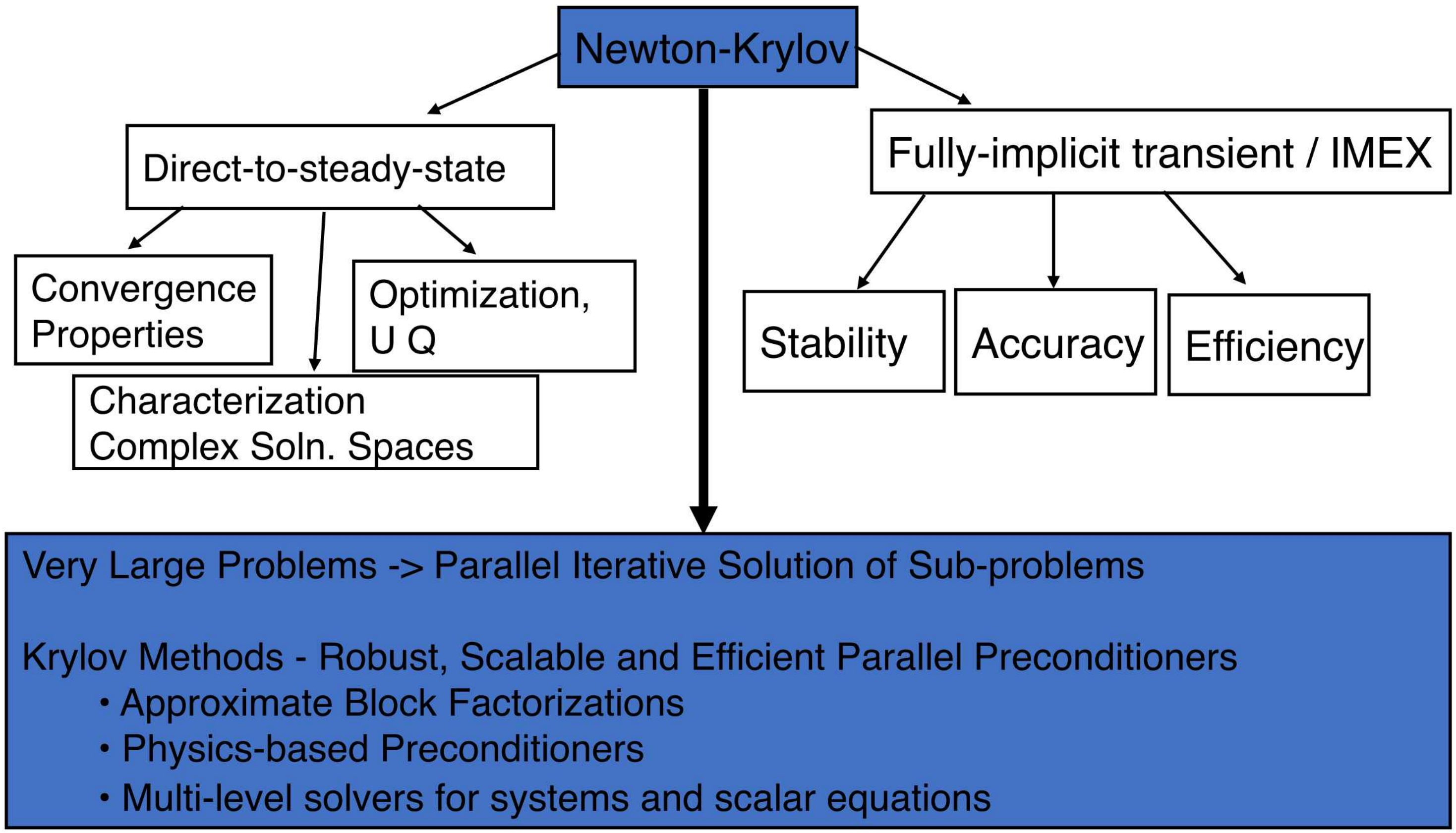
- Well characterized operator splitting methods
in specific application areas (e.g. Combustion – P. Colella, J. Bell, …)

- Spectral deferred correction (M. Minion et. al.)

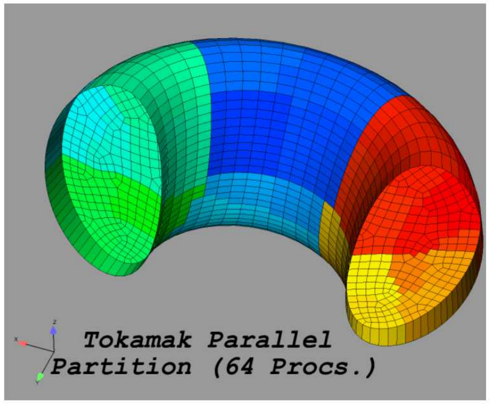
- Etc

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 Newton-Krylov Methods?



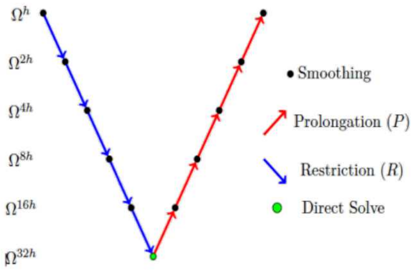
Scalable Preconditioning for Systems



1. Multilevel Methods for Systems: (ML & Muelu; Tuminaro, Hu et. al.))

Fully-coupled Algebraic Multilevel methods

- **Consistent set of DOF-ordered blocks at each node (e.g. 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, Shadid, Tuminaro)

- **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 coupled hyperbolic sys.)**
- **Enables specialized optimal AMG, e.g. H(grad), H(curl) for disparate discretizations.**
- **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 Relevant Continuum / PDE-based Models for

- Resistive MHD,
- Multifluid Plasmas,

and Associated Solution Methods

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

Resistive MHD Model in Residual Notation

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

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

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

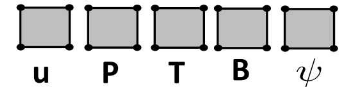
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

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

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

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

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



All nodal H(grad) elements using stabilized weak from

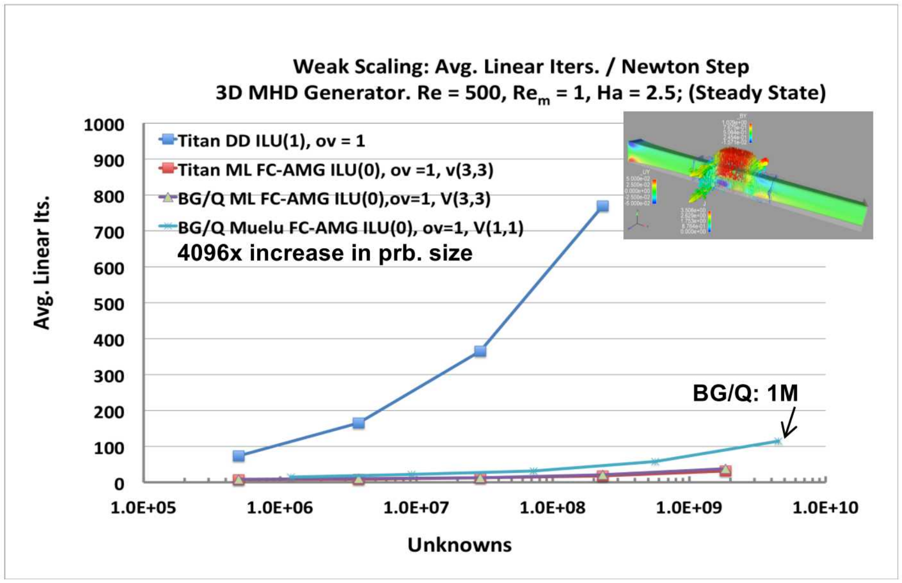
- Divergence free involution enforced as constraint with a Lagrange multiplier (Elliptic, parabolic, hyperbolic) [Dedner et. al. 2002; Elliptic: Codina et. al. 2006, 2011, JS et. al. 2010, 2016]
  - Only weakly divergence free in FE implementation (stabilization of B -ψ coupling)

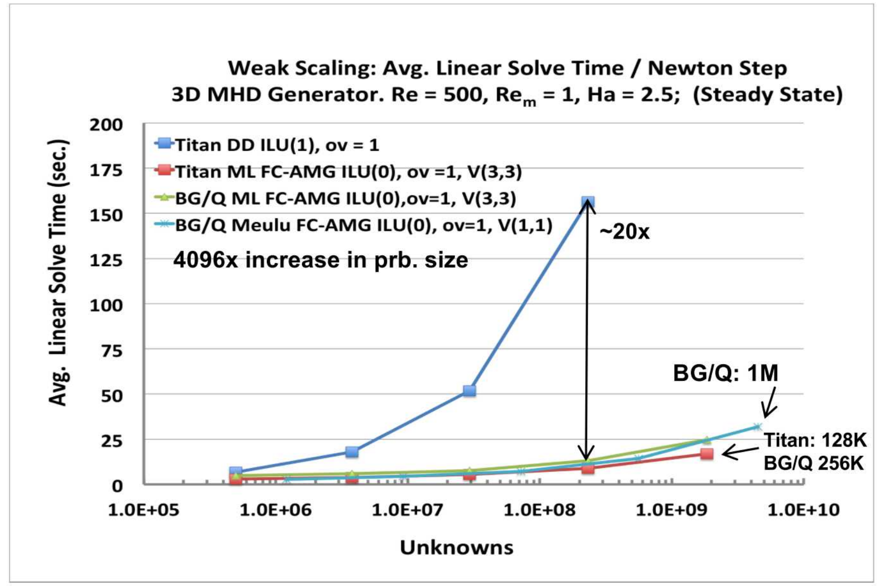
- Can show relationship with projection (e.g. Brackbill and Barnes 1980), and elliptic divergence cleaning (Dedner et. al, 2002) [JS et. al. 2016].

- 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)





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

MHD (steady) weak scaling studies to 256K Cray XK7, 1M BG/Q

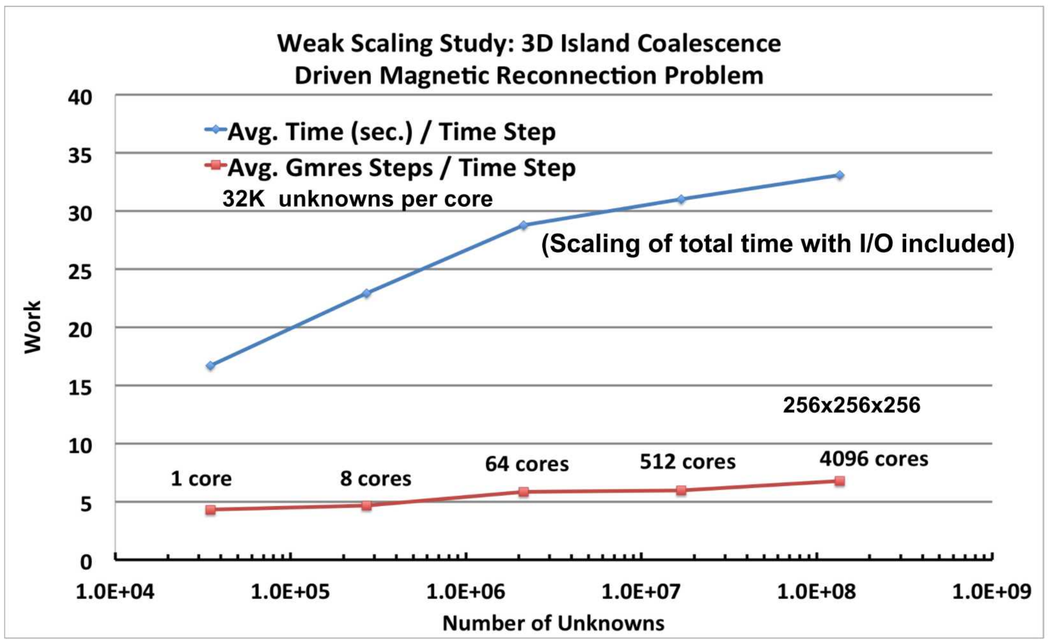
Large demonstration computations

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

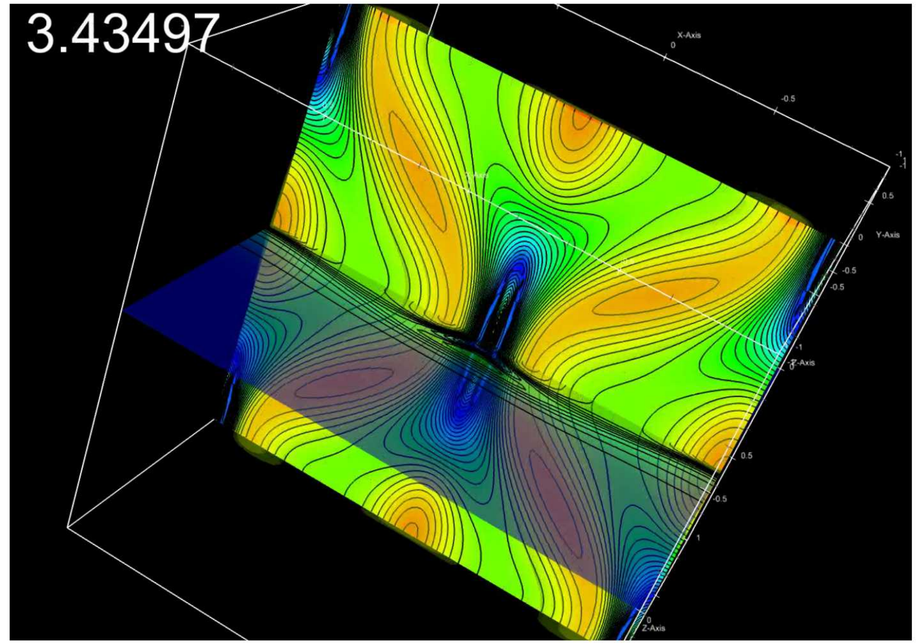
Poisson sub-block solvers: 4.1B DoF, 4.1B elem, on 1.6M cores BG/Q

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



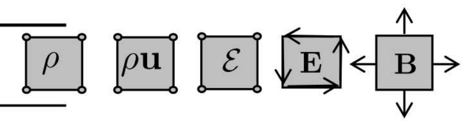
$S = 10^4$

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.

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



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

Density

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

Cyclotron frequency

Momentum

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

Collisional

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

Energy

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

Strong off diagonal coupling for plasma oscillation

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

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

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

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

Light wave off diagonal coupling

IMEX: Time Integration

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

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.;

Physics-based and Approximate Block Factorizations:

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

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

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!

[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) 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)]

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 Prec. for Stable Mixed Nodal and Edge FE Incompressible Resistive MHD," SISC 2016.
- 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

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.

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

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

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

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

$$\mathcal{P}^*_{SC} = \begin{pmatrix} \frac{1}{\Delta t}I + dD + aC & cC \\ 0 & S \end{pmatrix} \qquad \boxed{S = \frac{1}{\Delta t}I + dD + aC - c^2C\left(\frac{1}{\Delta t}I + dD + aC\right)^{-1}C}$$

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

*Only the upper diagonal of the block LU factorization is used as in Murphy, Golub, Wathen SISC 2000.
Exact computation/inversion of operators will be used for illustrative purposes in example of outer iteraction convergence.

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

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

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

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

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

Outer iterations in the dof based block factorization linear solver

CFL_c	10^{-2}	10^{-1}	10^{0}	10^{1}	10^{2}
GS	2	[illegible]	[illegible]	[illegible]	[illegible]
J	3	[illegible]	[illegible]	[illegible]	[illegible]
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	[illegible]	[illegible]	[illegible]	13	30
J	[illegible]	[illegible]	[illegible]	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

*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 XXXX)

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

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

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

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

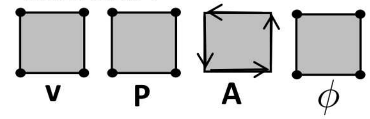
$$R_P = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

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

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

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

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**

$$\begin{tikzcd}
H^1 \arrow[r, "\nabla"] \arrow[d, "I"] & H(curl) \arrow[r, "\nabla\times"] \arrow[d, "I"] & H(div) \arrow[r, "\nabla\cdot"] \arrow[d, "I"] & L^2 \arrow[d, "I"] \\
H^{-1} & H(curl)^* \arrow[l, "-\nabla\cdot"] & H(div)^* \arrow[l, "\nabla\times"] & L^2 \arrow[l, "-\nabla"]
\end{tikzcd}$$

$$\begin{tikzcd}
nodes_1 \arrow[r, "\hat{G} = Q_E^{-1}G"] \arrow[d, "Q_\rho"] & edges \arrow[r, "\hat{K} = Q_B^{-1}K"] \arrow[d, "Q_E"] & faces \arrow[r, "\hat{D} = Q_\phi^{-1}D"] \arrow[d, "Q_B"] & nodes_0 \arrow[d, "Q_\phi"] \\
nodes_1^* & edges^* \arrow[l, "\hat{G}^t = G^t Q_E^{-1}"] & faces^* \arrow[l, "\hat{K}^t = K^t Q_B^{-1}"] & nodes_0^* \arrow[l, "\hat{D}^t = D^t Q_\phi^{-1}"]
\end{tikzcd}$$

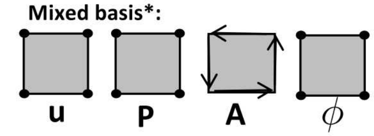
- **Mixed basis, Q1/Q1 VMS FE Navier-Stokes, A-edge, Q1 Lagrange Multiplier**

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

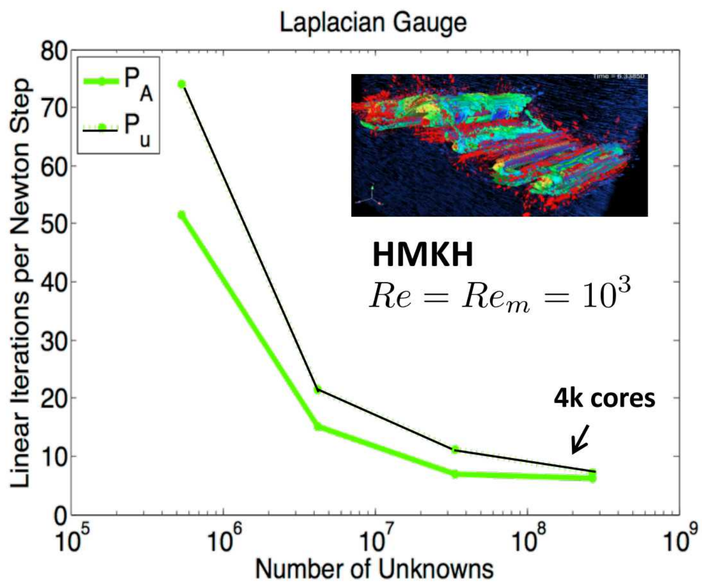


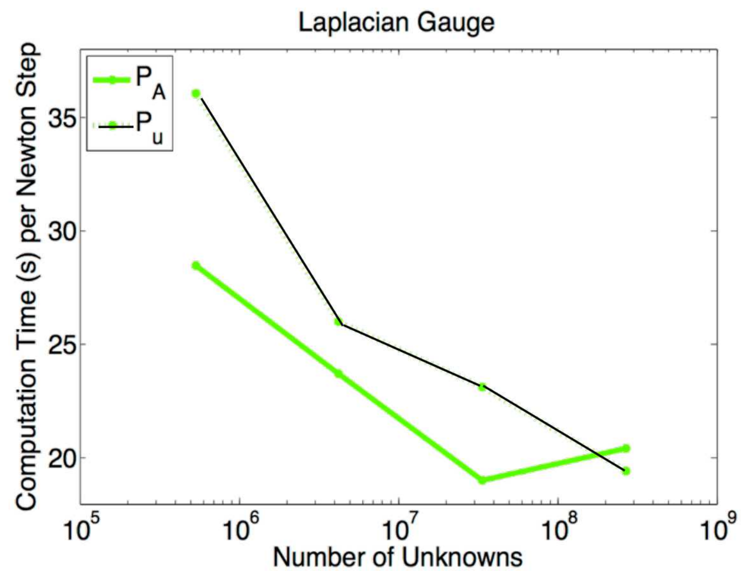
$$\mathcal{A}_{GSG} = \left(\begin{array}{ccc|c} F & B^t & Z & 0 \\ B & C & 0 & 0 \\ Y & 0 & G & D^t \\ \hline 0 & 0 & 0 & L \end{array}\right) \quad \mathcal{P}_{\mathbf{A}} = \begin{pmatrix} F & 0 & Z \\ 0 & I & 0 \\ Y & 0 & G \end{pmatrix} \begin{pmatrix} F^{-1} & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix}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

$$\hat{S}_{\mathbf{A}} = G - Y\hat{F}^{-1}Z$$ (SIMPLEC: see eg. Elman et al.)

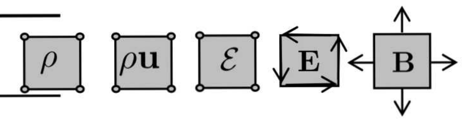
$$\hat{S}_P = C - B\hat{F}^{-1}B^t$$ (PCD: Kay, Loghin, Wathan)

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

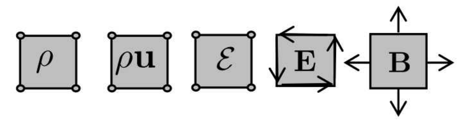
Other work on multifluid plasma formulations, solution algorithms:

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

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

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

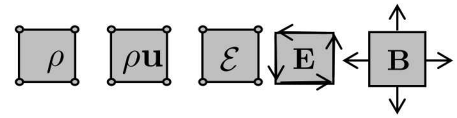
$$
\begin{bmatrix}
\mathbf{D}_F & \mathbf{Q}^F_E & \mathbf{Q}^F_B \\
\mathbf{Q}^E_F & \mathbf{Q}_E & \mathbf{K}^E_B \\
0 & \mathbf{K}^B_E & \mathbf{Q}_B
\end{bmatrix}
\begin{bmatrix} \mathbf{F} \\ \mathbf{E} \\ \mathbf{B} \end{bmatrix}
\Rightarrow
\begin{bmatrix}
\mathbf{Q}_B & \mathbf{K}^B_E & 0 \\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

Reordered 3x3

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(grad) AMG with grad-div stab.
or H(curl) AMG

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

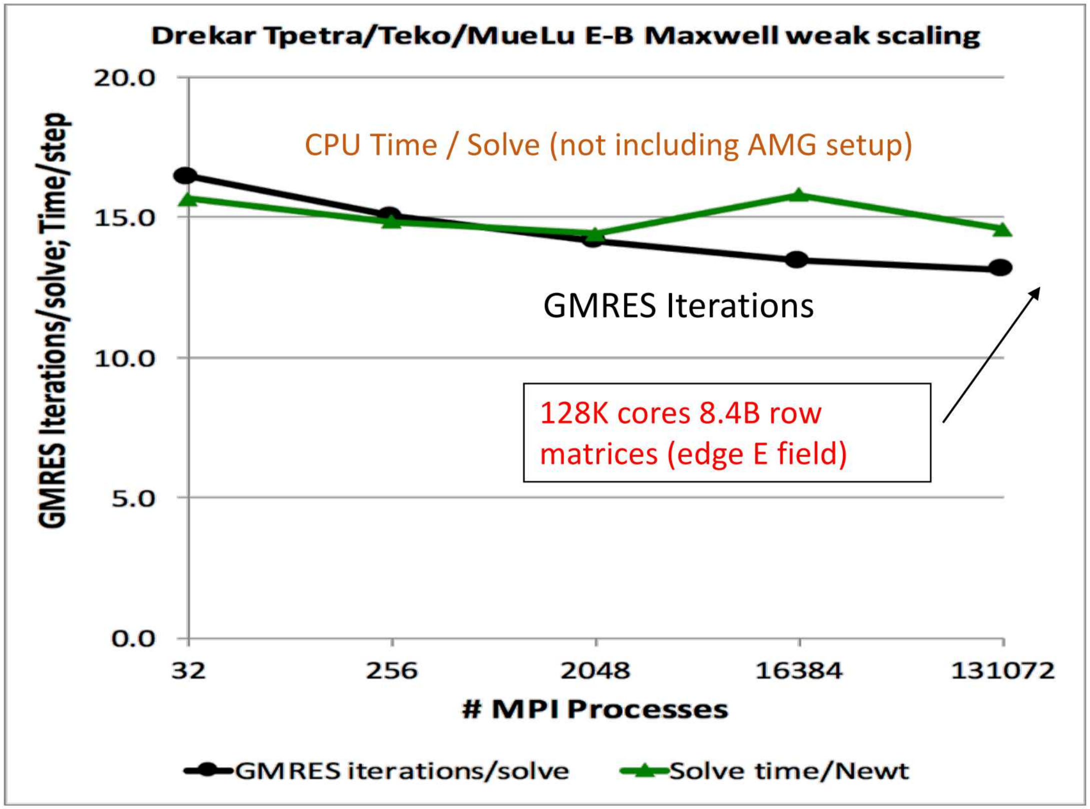
Face-based simple
mass matrix Inversion.
V-cycle Gauss-Seidel

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 to Ampere's law, i.e. adding zero $\nabla \cdot (\varepsilon \mathbf{E}) = \rho$
- 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 H(grad) 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 (Ref. Maxwell) and Hyper (AMS) can also 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 $CFL_c > 10^4$

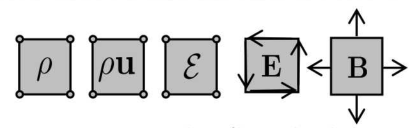
Drekar

GS smoother with H(grad) AMG

Max CFL_c ~ 200

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

$$\Delta x \approx 1 \mu m$$

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

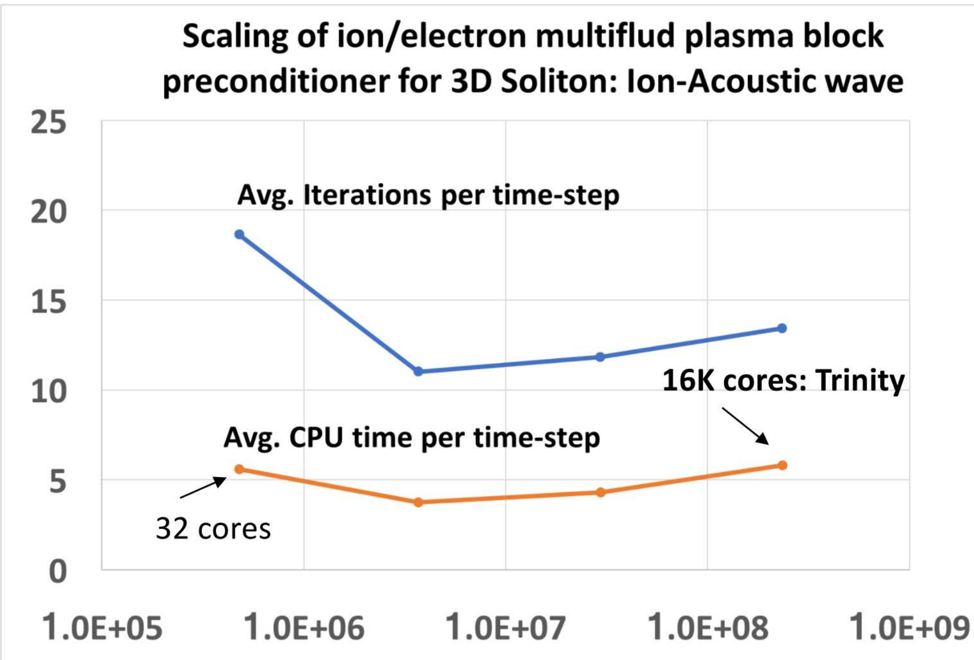
Initial weak scaling of ABF preconditioner

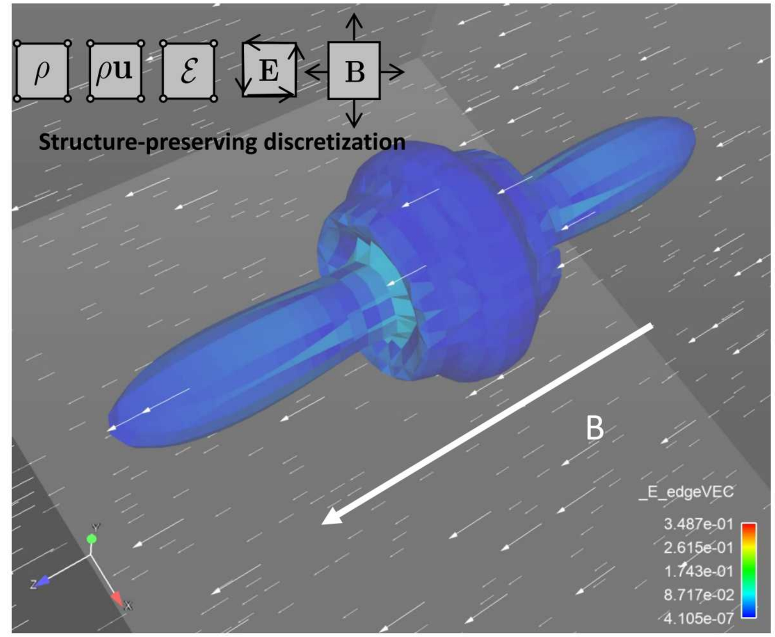
- Domain [0,0.01]x[0,0.0004]x[0,0.0004]; Periodic BCs in all directions
- N elements in x-direction;
- Fixed time step size for SDIRK (2,2): (not resolving TEM wave)

<u>Proof of Principle</u>

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

Demonstration of scalable physics-based preconditioners
3D Gaussian high density/pressure
for isentropic ion-acoustic wave propagation





Iso-surface of ion density colored by electric field magnitude

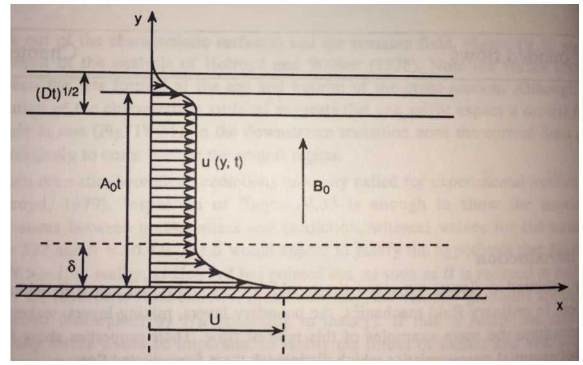
Isentropic flow $\frac{P}{P_0} = (\frac{\rho}{\rho_0})^{\gamma}$

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

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

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

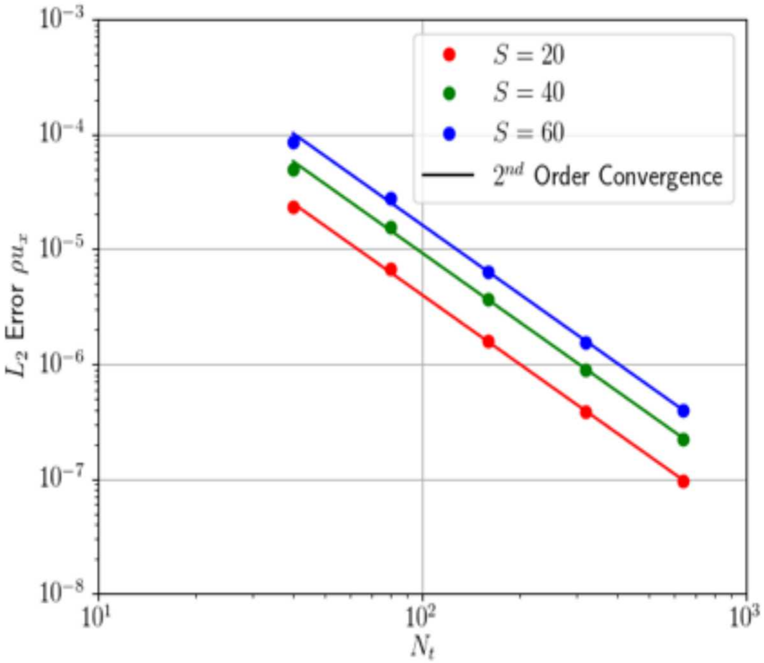
$$u_x = \frac{U}{4}\left(1 + \exp\left(\frac{v_A y}{\lambda}\right)\right)\mathrm{erfc}(\eta_+) + \frac{U}{4}\left(1 + \exp\left(-\frac{v_A y}{\lambda}\right)\right)\mathrm{erfc}(\eta_-)$$

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

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

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.

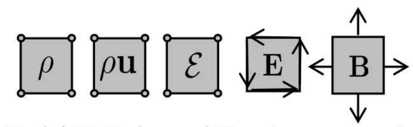


Accuracy in MHD limit (IMEX)

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

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



Nodal FE Hydro and Structure-preserving discretization for EM

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

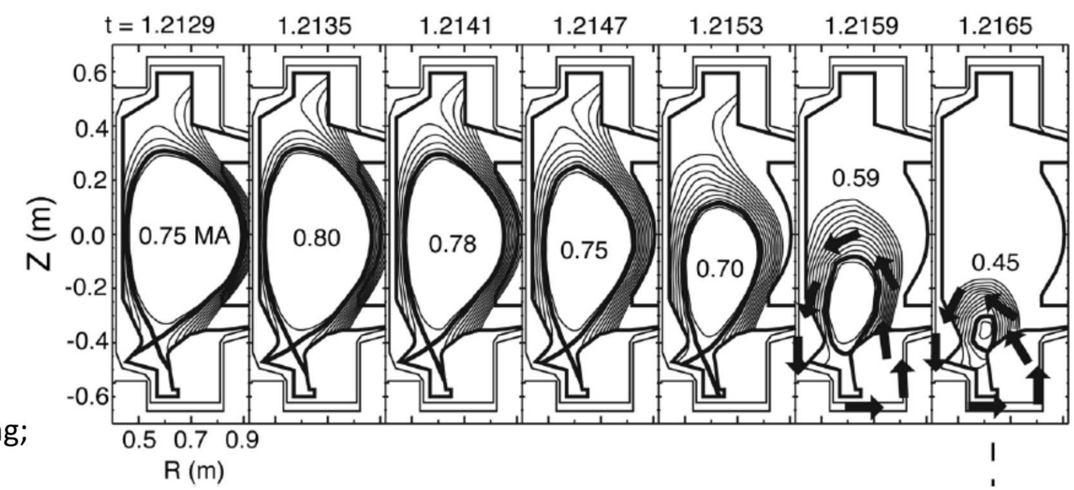
Tokamak Disruption Simulation (TDS) Center SciDAC-4 Partnership (OFES/ASCR)

<u>Computational Goal</u>
Develop and evaluate advanced hierarchy of plasma physics models and solution methods to understand disruption physics and explore mitigation strategies.

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

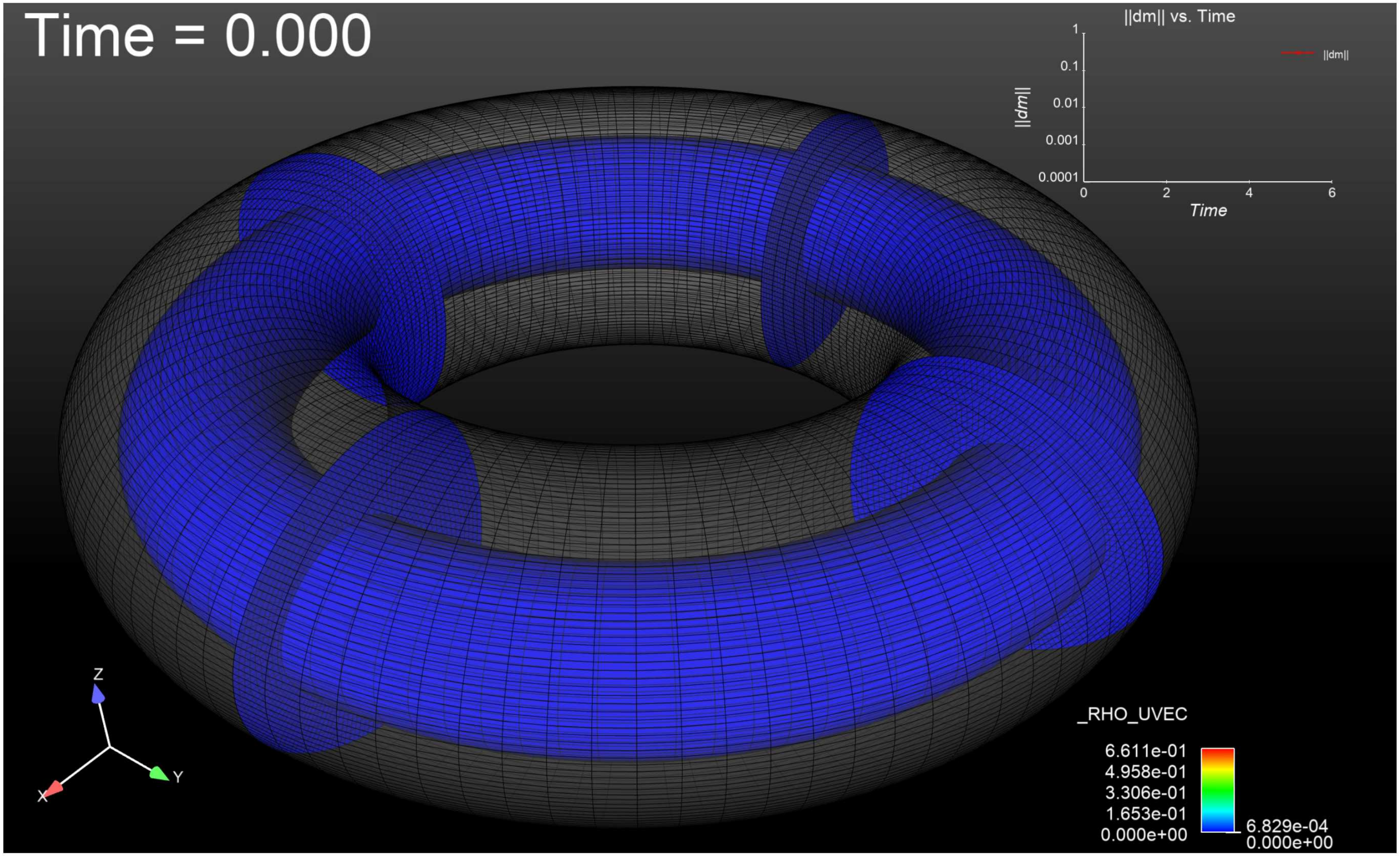
- **Plasma instabilities can cause break of confinement, huge energy loss, and discharge very large electrical currents (~20MA) into structure.**

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



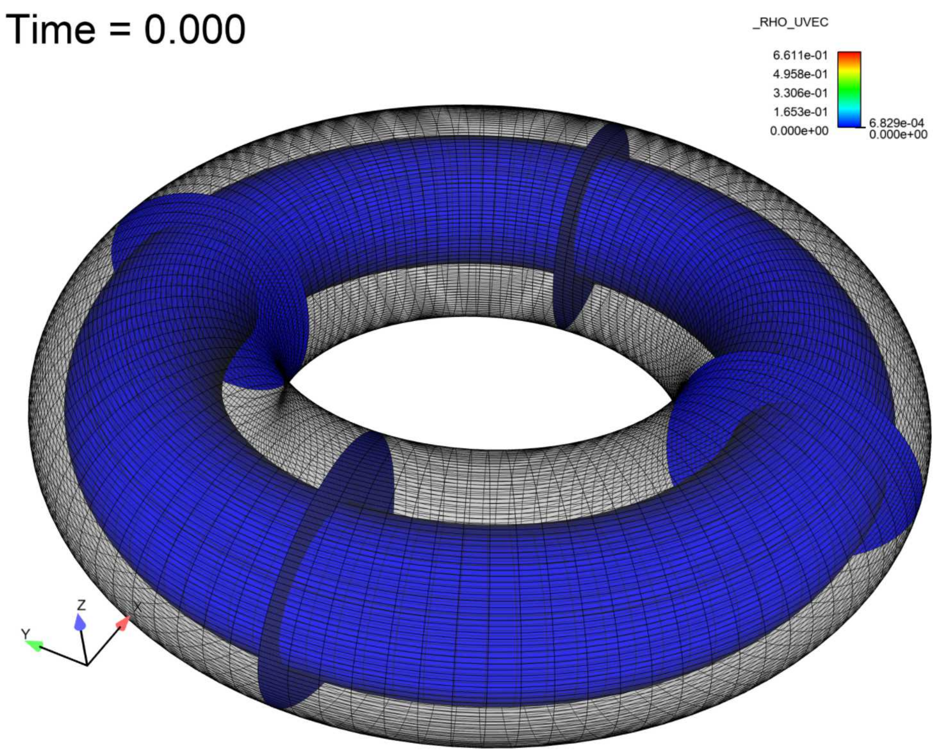
ITER Physics Expert Group on Disruptions, Nucl. Fusion 39, 2251 (1999).

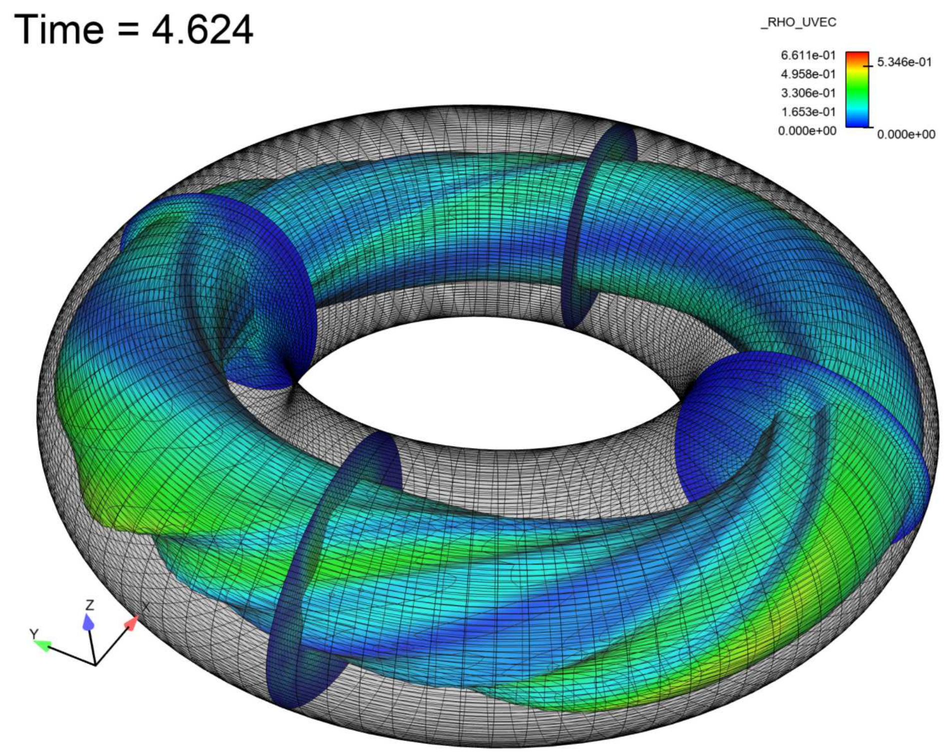
(Overall PI, OFES PI and LANL-PI, X. Tang;
J. Shadid ASCR-PI, SNL-PI):



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.





Neutral gas transport, ionization, and recombination with multifluid model

- The plasma internal energy can fall from 10 keV -> ev in the thermal quench in a few ms (plasma transport/radiation)

- Plasma current takes energy from the poloidal magnetic field and in 30 – 150 ms it can be channeled through runaway electrons.

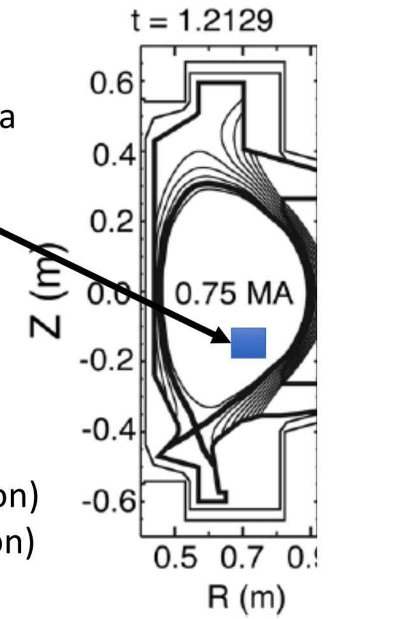
- For thermal quench mitigation one idea is to inject higher Z impurities to enhance radiation loss.

- To mitigate the current quench, an idea is to inject neutrals to enhance dissipation of runaways.

Goal: Understand impurity penetration and assimilation into plasma.

Preliminary 1D Gas Injection Problems

1D Sim. of Higher Z Neutral Gas (He, Ne, Ar) Cores Expanding 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). E.g.

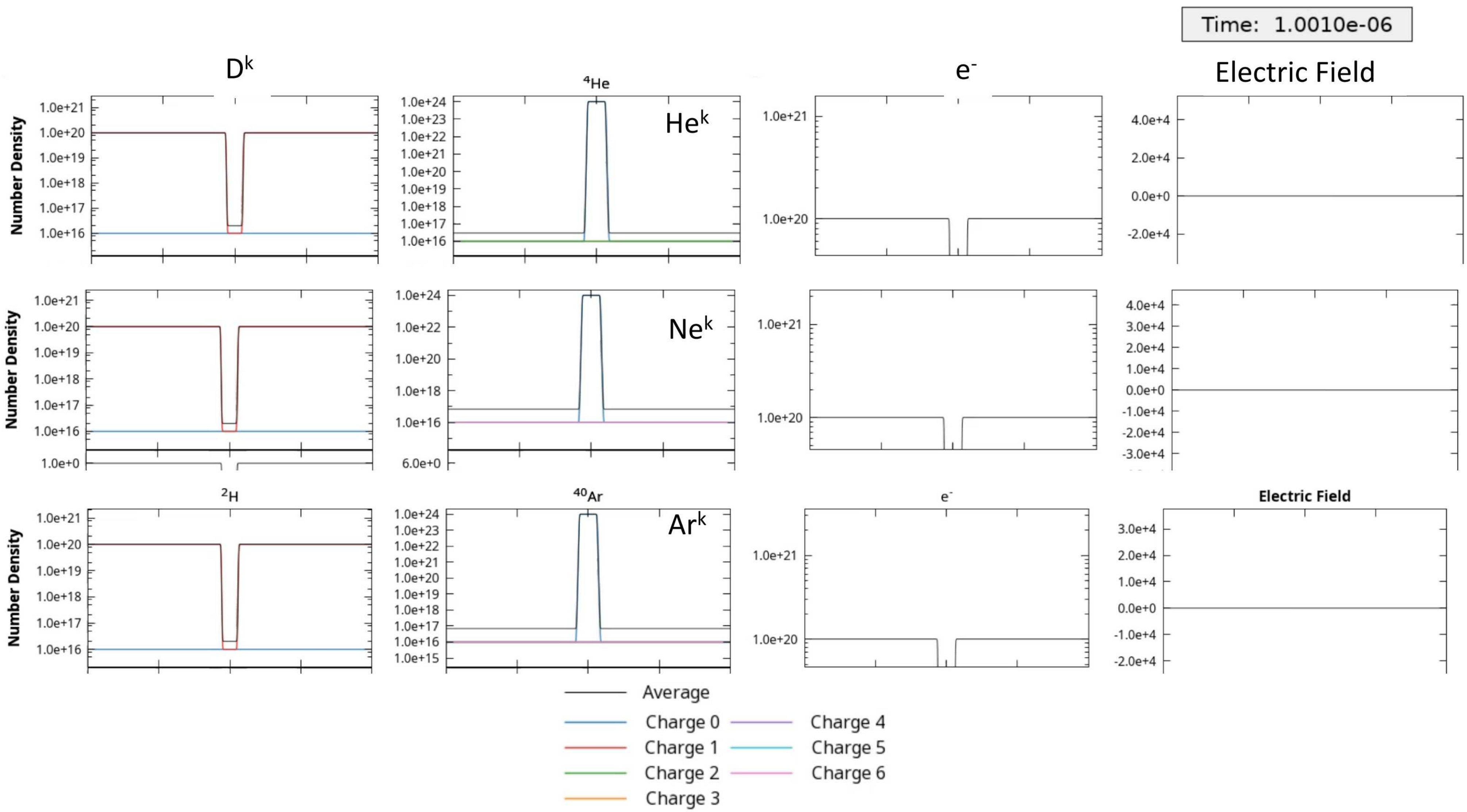
$$(D^0, D^+, e^-, Ar^0, Ar^{+1}, Ar^{+2}, Ar^{+3}, Ar^{+4}, Ar^{+5}, Ar^{+6})$$

and electromagnetics for (E,B).

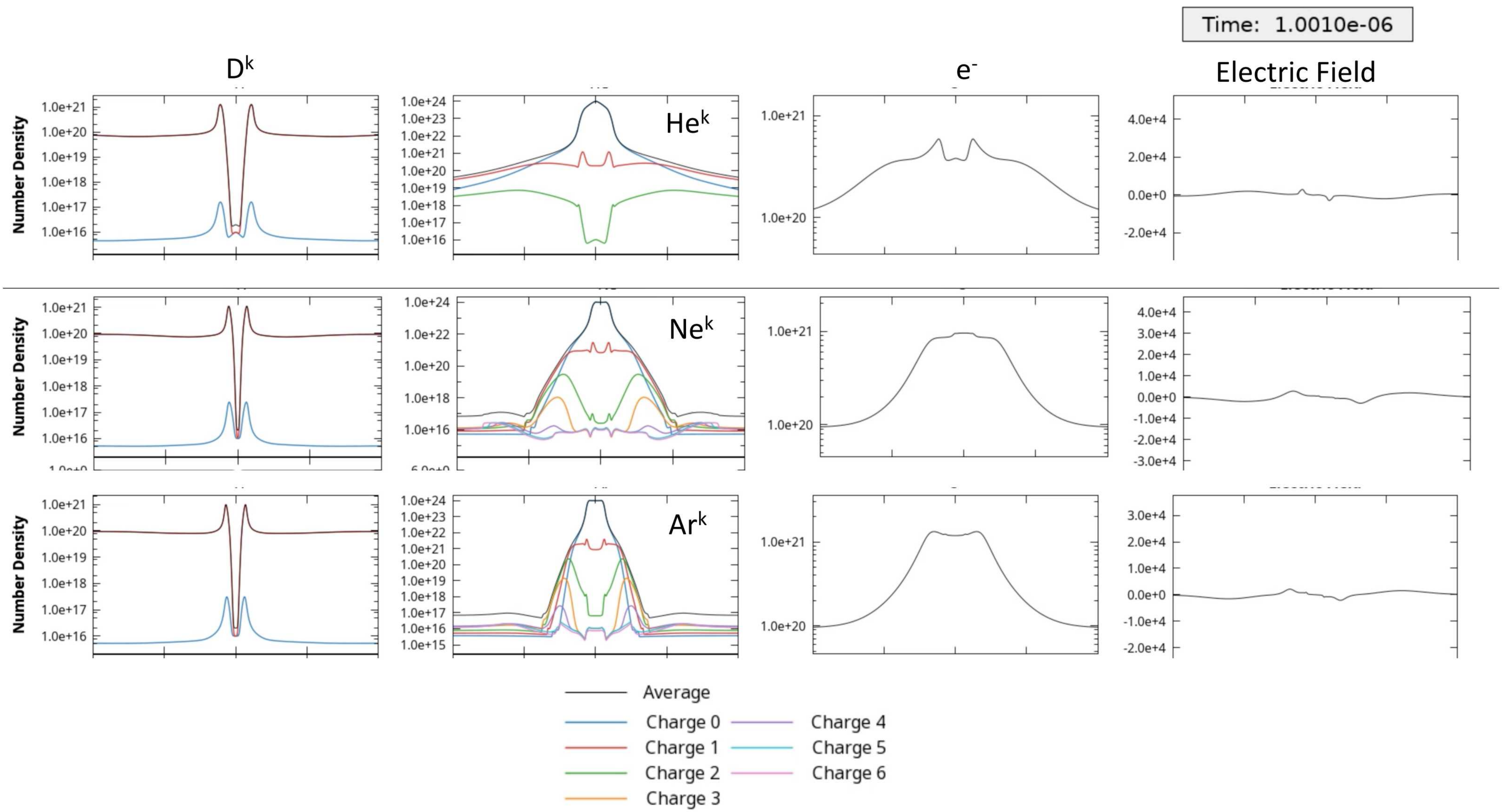
E.g. 5 moment plasma model x 10 species = 50 equations (solved in 3D but only a 1D solution)
Maxwell Equations E,B field = 6 equations (solved in 3D but only a 1D solution)
56 PDEs

Problem outline: Representative of the core plasma

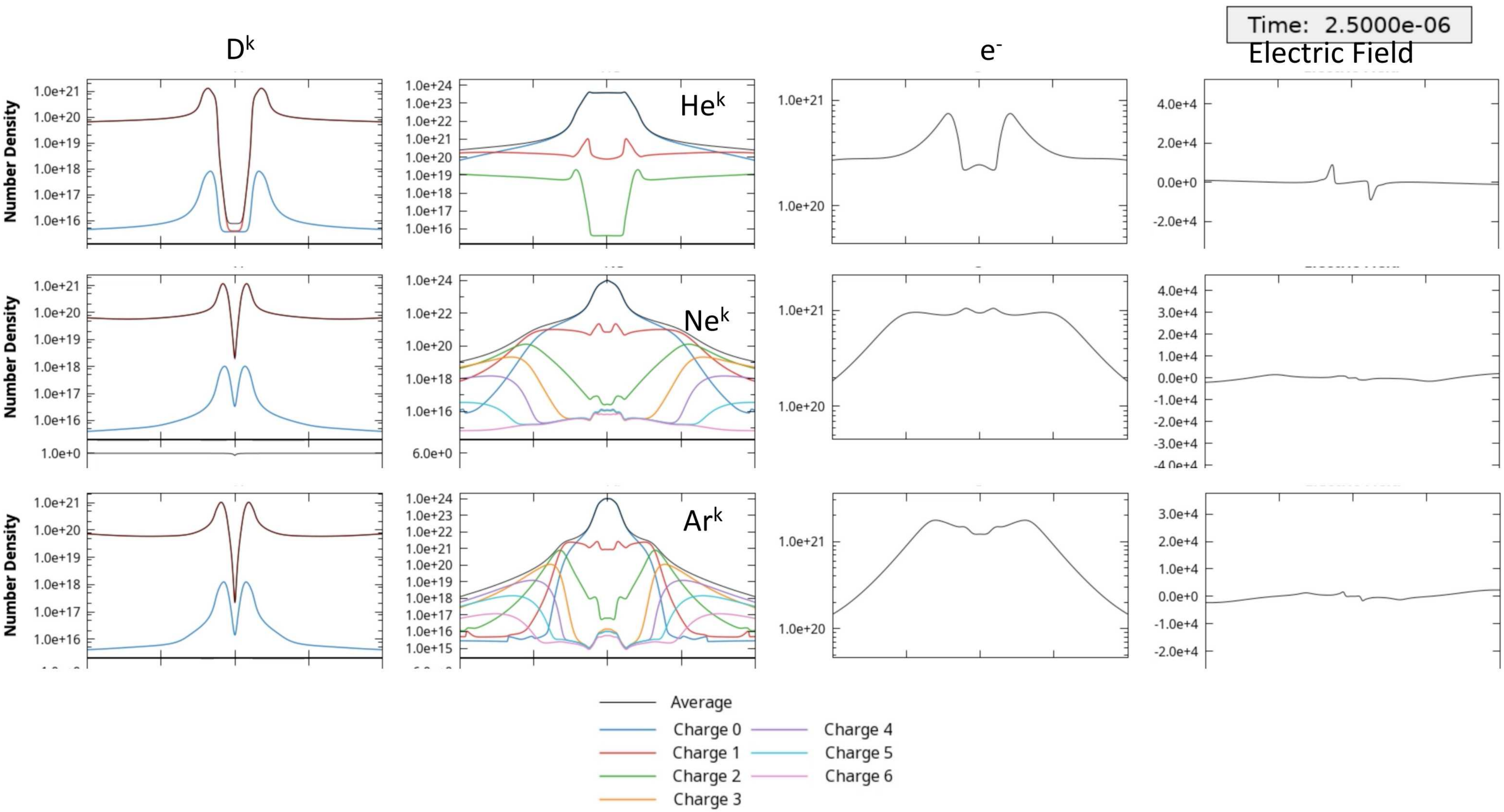
- Initial ~fully ionized Deuterium plasma at n = 10^{20}, T = 100ev (~1M degrees K)
- Neutral Argon (Ar^0) core introduced at n = 10^{24} , T = 10^{-1}ev (~1000 degrees K)
- Parallel B – field is ignorable (due to geometry in 1D so B does not modify transport)
- Domain in x is [0.3m,0.3m]; mesh is 4096 x 1 x 1 elements



Time: 1.0010e-06
D^k
^4He
He^k
e^-
Electric Field
Ne^k
^2H
^{40}Ar
Ar^k
Number Density
Average
Charge 0
Charge 1
Charge 2
Charge 3
Charge 4
Charge 5
Charge 6

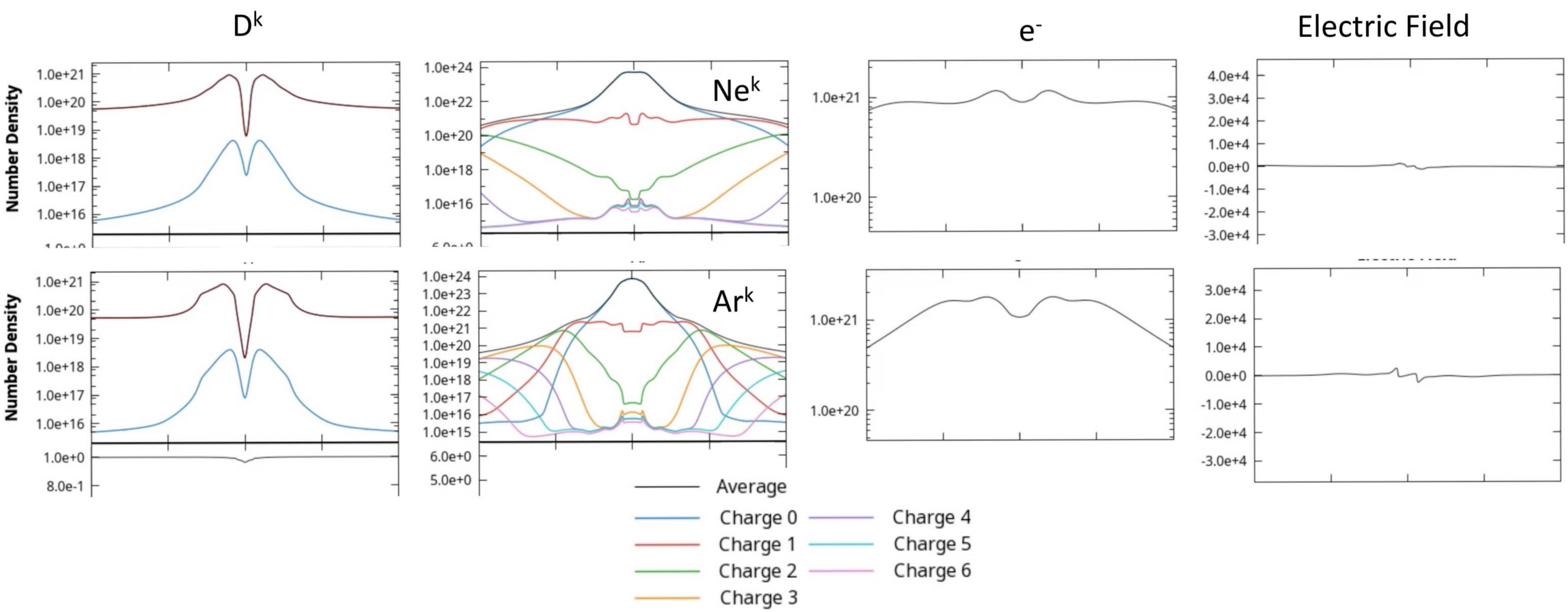


Time: 1.0010e-06
D^k
He^k
e^-
Electric Field
Ne^k
Ar^k
Number Density
Average
Charge 0
Charge 1
Charge 2
Charge 3
Charge 4
Charge 5
Charge 6



Time: 2.5000e-06
D^k
e^-
Electric Field
He^k
Ne^k
Ar^k
Number Density
Average
Charge 0
Charge 1
Charge 2
Charge 3
Charge 4
Charge 5
Charge 6

Time: 5.0000e-06



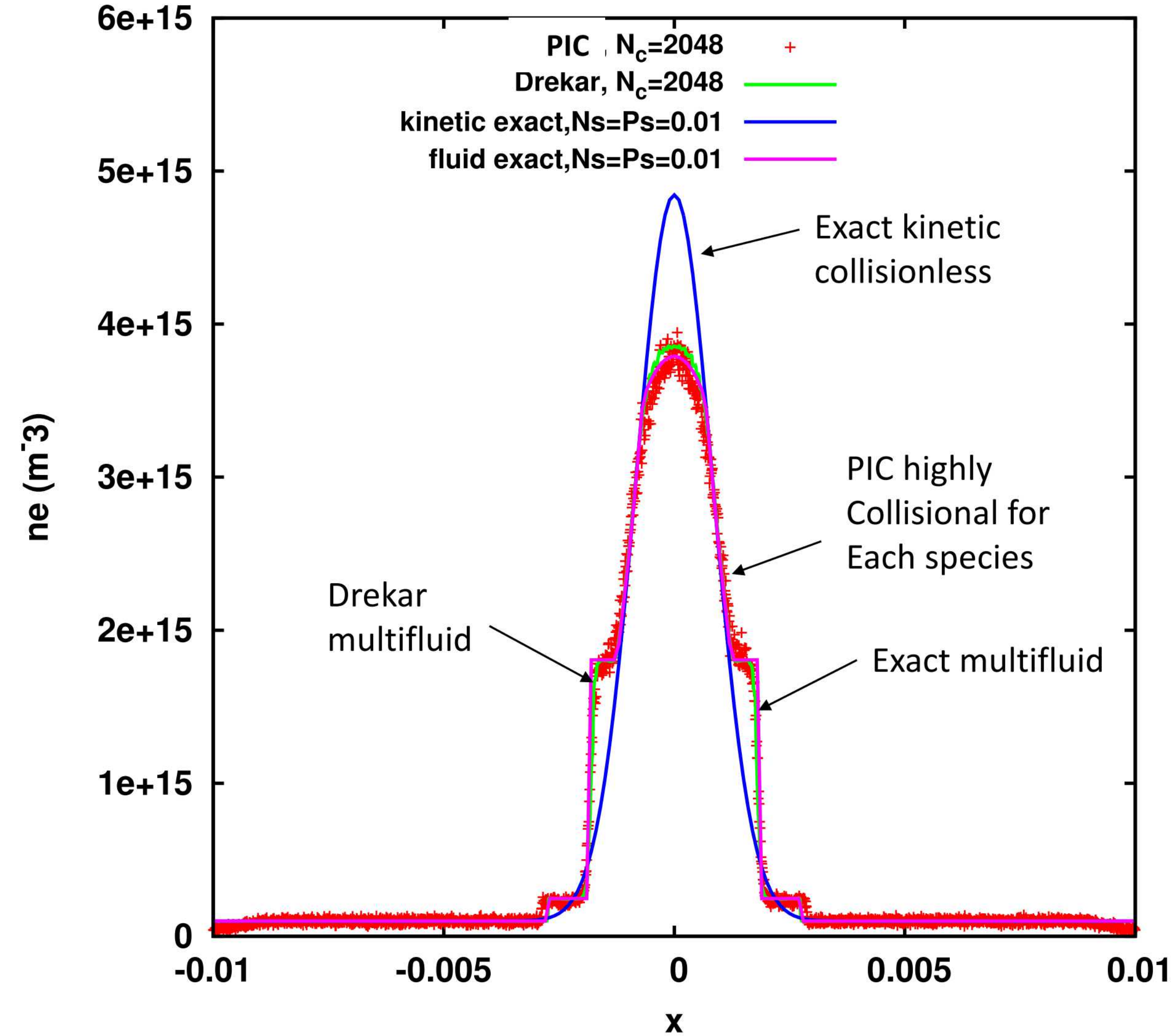
Comparison of multifluid to an exact solution for an electron / positron multfluid collisionless plasma for a quasi-neutral expanding core*.

PIC solution is for highly-collisional self interactions and collisionless between species. I.e.

$$\text{large } \nu_{ii}, \nu_{ee}$$

$$\nu_{ei} = \nu_{ei} = 0$$

*Allen C. Robinson (Sandia) exact kinetic/fluid solution



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. Can provide scalable solution of complex multiphysics plasma models.**

- **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**