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Enabling Multiphysics Plasma Simulations by the Development of Stable, Accurate and Scalable Computational Formulations and Solution Methods

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Motivation: Science/Technology and Mathematical / Computational

Science / Technology Motivation:

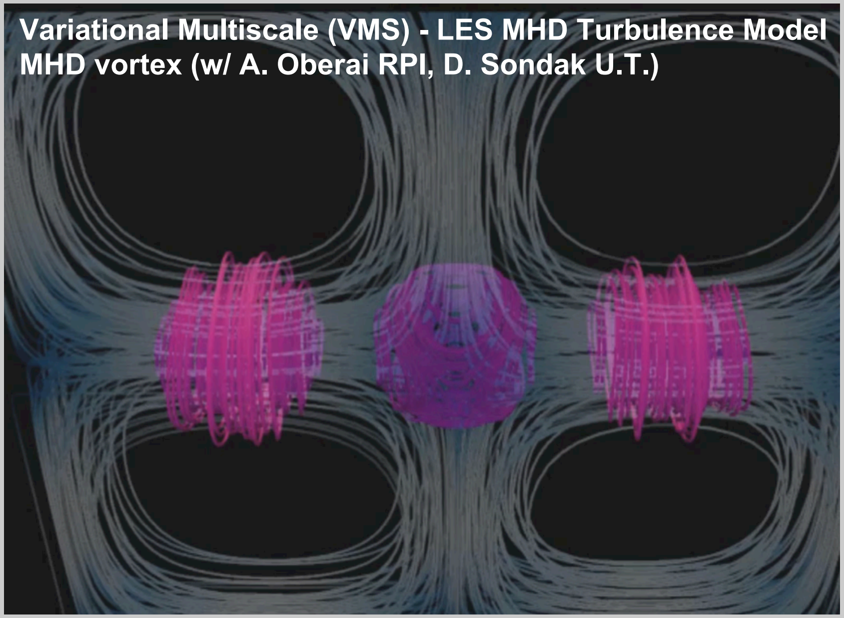
Resistive and extended MHD models are used to study important plasma physics systems

- **Astrophysics**: Magnetic reconnection, solar flares, sunspots, turbulent plasma flows, …
- **Planetary-physics**: Earth's magnetospheric sub-storms, Aurora, geo-dynamo, planetary-dynamos
- **Fusion**: Magnetic Confinement [MCF] (e.g. ITER), Inertial Conf. [ICF] (e.g. NIF, Z-pinch)
- **Technology/Engineering**: Liquid Metal Fusion **Blankets, MHD Generators, Plasma Reactors ..**

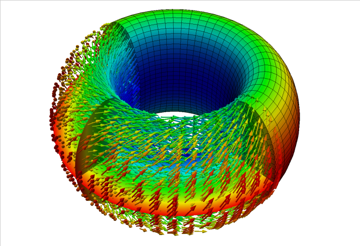
Mathematical / Computational Motivation:

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

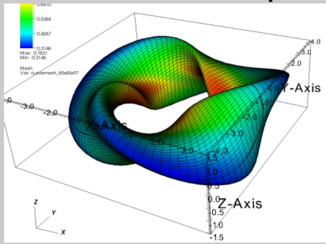
- Predictive Computational Simulations
- Scientific Discovery with Extreme-scale Simulations
- Physics / Mathematical Model Validation
- Beyond Forward Simulation: Inversion, Optimization, Design, Uncertainty Quantification
- Experimental Data Interpretation and Inference

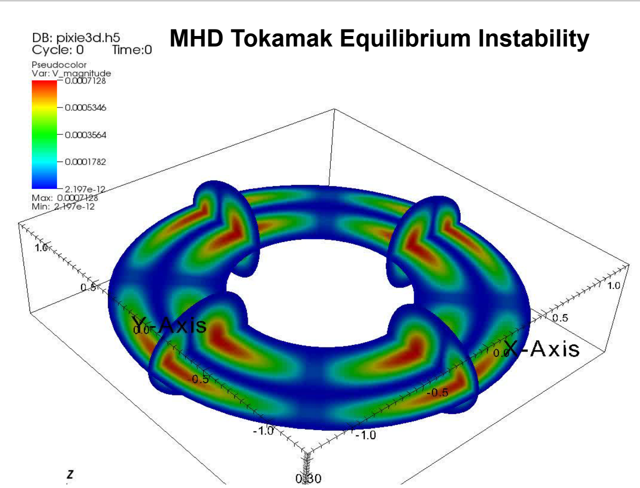

Variational Multiscale (VMS) - LES MHD Turbulence Model
MHD vortex (w/ A. Oberai RPI, D. Sondak U.T.)

MHD Tokamak Equilibrium



MHD Stellarator Equilibrium





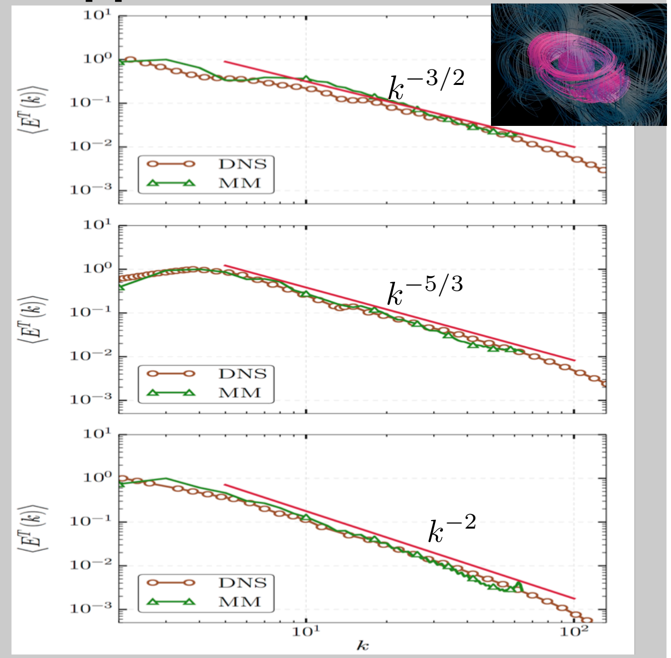
MHD Tokamak Equilibrium Instability

Relevance to DOE and the Mathematical Approach

Relevance to DOE (incomplete list):

- **Basic Plasma Physics**: Magnetic reconnection and island formation, Magnetic Kelvin-Helmholtz and Rayleigh-Taylor, MHD turbulence models
- **Fusion Reactors:** MCF stability and confinement, anisotropic transport, design, and optimization relevant to ITER-Tokamak, Reverse Field Pinch
- **Astrophysics with hybrid fluid – kinetic modeling: Two-fluid MHD solver for moment** closure to allow charge separation for kinetic simulations
- **Fusion Pulsed Power Concepts**: symmetry, stability, Hall physics and two-fluid effects (Z-pinch)
- **High Energy Density Physics**: Experiment design, optimization, and UQ (e.g. Z-pinch implosions and launching magnetic flyer plates)

Scalable implicit fully-coupled MHD solution methods can provide the required robustness and efficiency for accurate integration of complex multiple-time-scale multiphysics MHD simulations

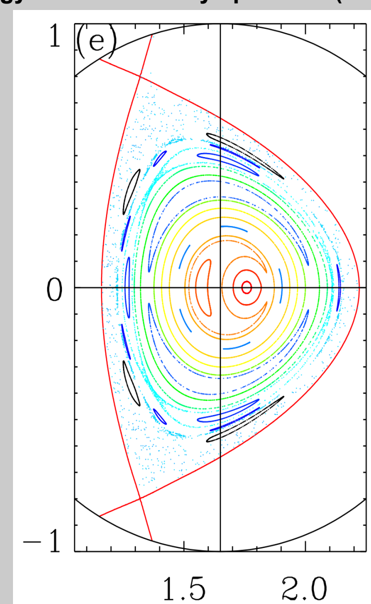


MHD Taylor-Green Vortex Decay: Non-universality of total energy turbulent decay spectrum (MHD VMS – LES)

Mathematical Approach:

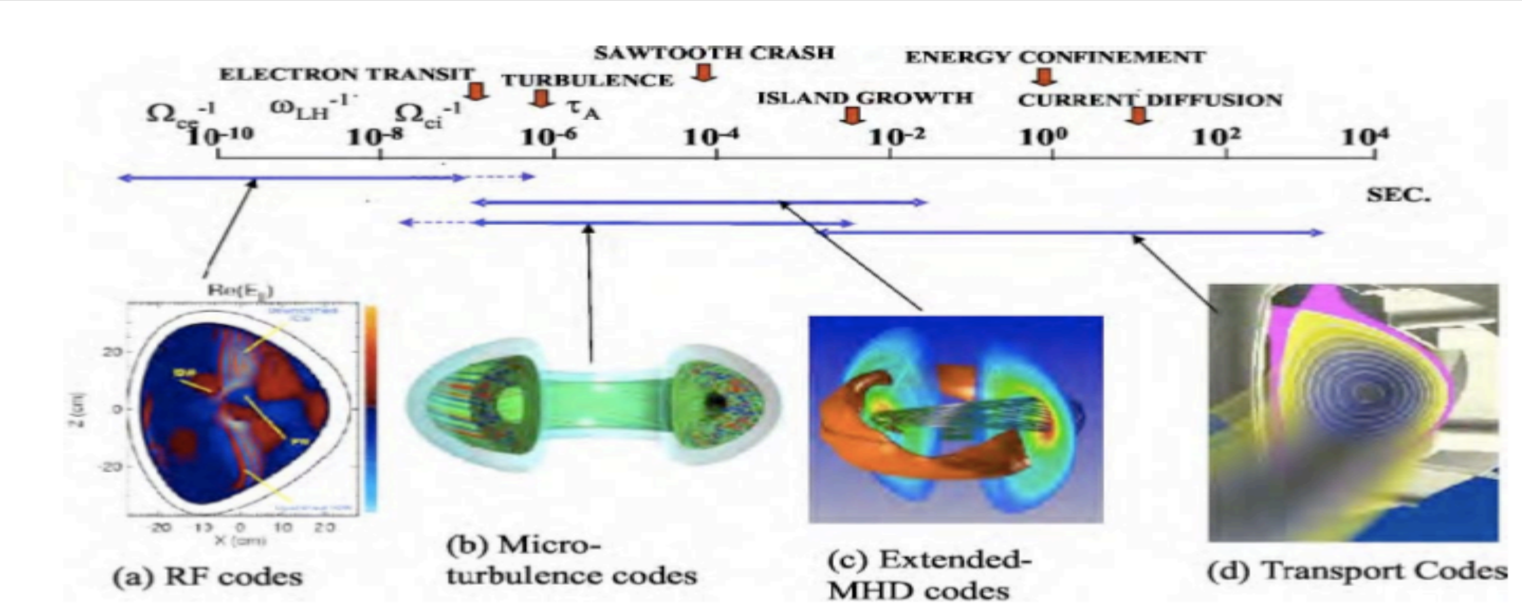
- Hierarchy of advanced plasma physics models (continuum [resistive and extended MHD, multifluid electromagnetic plasma], kinetic, and Hybrid)
- Stable asymptotic preserving and higher-order accurate implicit formulations
- Stable and accurate spatial discretizations for complex geom., Options enforcing key mathematical properties (e.g. positivity, div B = 0)
- Robust and efficient fully-coupled nonlinear/linear iterative solution methods based on Newton-Krylov (NK) methods
- Scalable and efficient preconditioners utilizing multi-level (AMG) methods (Fully-coupled AMG, physics-based, approx. block factorization)

=> Also enables beyond forward simulation and integrated UQ

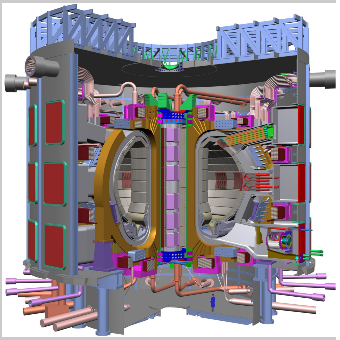


XMHD D-shaped Tokamak ????

Magnetic Confinement Fusion: Understanding and controlling instabilities in plasma confinement is critical. Very Large range of time-scales; Some implicit aspect required.



(a) Time scales in fusion plasmas (FSP report)



ITER

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(10) significant instabilities.

Strong external magnetics field used to:

- **Confine the hot plasma and keep it from striking wall,**
- **Attempt is to achieve temperature of about 100M deg K (6x Sun temp.),**
- **Energy confinement times O(1 – 10) seconds is desired.**

(See e.g. DOE Office of Science ASCR/OFES Reports:
Fusion Simulation Project Workshop Report, 2007; Integrated System Modeling Workshop 2015)

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Why Newton-Krylov Methods?

Newton-Krylov

Fully-coupled nonlinear solves

Fully-implicit transient

<u>Robustness, Convergence and Flexibility</u>

- **Strongly coupled multi-physics often requires a strongly coupled nonlinear solver**
- **Quadratic convergence near solutions**
- **Enables: bifurcation, stability, optimization, error estimation, sensitivity, UQ**

(see e.g. Shadid, Pawlowski, et. al. - CMAME, JFM, JCP; Shadid, Cyr, Wildey – SISC, submitted to CMAME)

<u>Stability, Accuracy and Efficiency</u>

- **Stable (stiff systems)**
- **Pseudo-transient possible**
- **High-order and variable-order methods**
- **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; Shadid. and Ober & Shadid and Ropp - JCP)

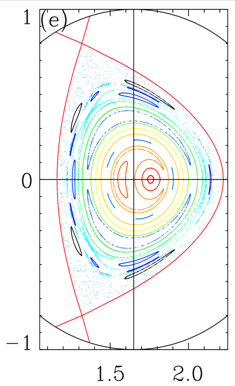
Very Large Problems -> Parallel Iterative Solution of Sub-problems

Robust Krylov Methods -> **Requires Scalable and Efficient Multilevel Preconditioners**

- **Fully-coupled AMG** [specialized uniform discretizations, e.g. VMS all H(grad)]
- **Physics-based (PB) and Approximate Block Factorization (ABF)** [General discretizations]

[Multigrid and AMG Multi-level methods for sub-systems and scalar equations]

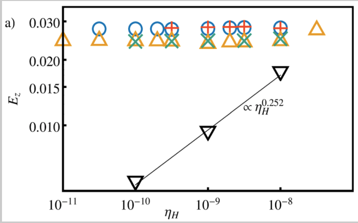
Brief Incomplete list of Accomplishments in this Funding Cycle and how this Aligns with the FY18-20 ASCR Guidance.



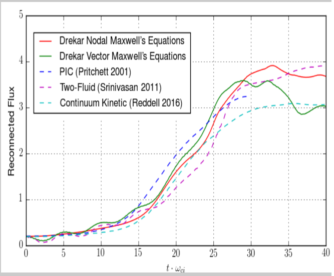
Relevance of research to DOE missions or DOE scientific grand challenges

- **Magnetic Confined Fusion (MCF) – Reactor simulations.** Computed equilibrium & instabilities in Tokamak geometries (FV, FE), and in Reverse Field Pinch (RFP, FV). Code used for realistic discharge studies for RFX (RFP,FV) experiment in Padova, Italy. First VMS FE computations for Solovev instability comparable to our FV methods.

- **Inertial Confinement Fusion (ICF) – Pulsed Power Magnetic Inertial Fusion (MIF).** Beginning to carry out base-line MHD implosion efforts. Developing appropriate multifluid electromagnetic plasma problem description, geometries, anisotropic transport capabilities.



- **Fundamental plasma physics – magnetic reconnection phenomena.** New results for fluid (extended MHD), hybrid (fluid electrons, kinetic ions), and fully kinetic models. Concluded that a hybrid description provides a sufficiently accurate description of magnetic reconn. in arbitrary magnetic fields. New multifluid electromagnetic plasma results for GEM challenge.



- **Our work addresses critical gaps called out in ASCR, DOE-SC, DOE-FES, and National Academies of Science reports** by developing robust and efficient solution methods for general multiphysics multiple-time-scale systems. These include stability, higher-order accuracy, efficient and accurate long-time-scale integration, efficient implicit methods, algorithmic and parallel scalability, and utilization of high-concurrency node architectures. **Specifically addressing advanced plasma physics models/formulations.**XMHD, multifluid electromagnetic plasmas, and hybrid continuum/ kinetic.

Red text – Topic related to research highlights presented

Brief Incomplete list of Accomplishments in this Funding Cycle and how this Aligns with the FY18-20 ASCR Guidance.

Mathematical and algorithmic challenges arising in computational simulations at scale

- New ABF preconditioners for structure-preserving resistive MHD formulations have been developed. Scaling only achievable by new ABF preconditioners.

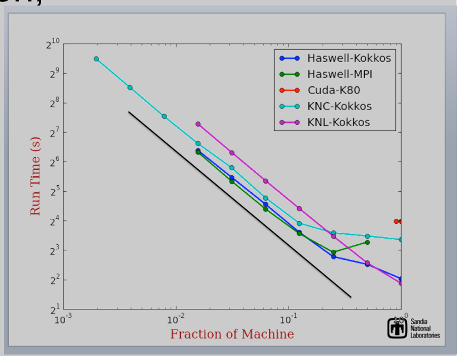
- New ABF Preconditioners for full-Maxwell Equations and initial ABF for Multifluid Electromagnetic Plasmas Equations have been developed. Scaling only achievable by new ABF preconditioners.

- Scalable Kinetic Solvers with Two-fluid-based Physics-based Preconditioning.

- Evaluation and improvement of scaling for 3D FE resistive MHD with Newton-Krylov & FC-AMG preconditioning for > 0.5M cores. In the process of carrying out large core-count scaling studies on an IBM BG/Q platform, we identified and helped correct a significant scaling bottleneck (≥ 128K cores) for the new 64-bit Tpetra/Muelu AMG packages in Trilinos. We also made very substantial progress in decreasing the AMG setup time (≥ 10x for large core counts).

- A New scalable XMHD physics-based preconditioner based on ion equation of motion and novel development of critical Schur complement operators to be approximated in the PB preconditioner.

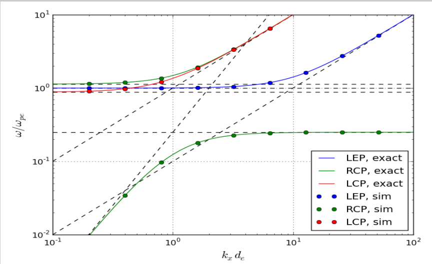
- **High-performance multiphysics FE integration and assembly on high concurrency nodes.** Began studies of our Directed Acyclic Graph (DAG) approach for physics evaluation, element integration, residual computations, and the generation of Jacobian matrix by automatic differentiation (AD) on Intel MIC and GPUs.



Red text – Topic related to research highlights presented

Brief Incomplete list of Accomplishments in this Funding Cycle and how this Already Aligns with the FY15-17 ASCR Guidance to PIs.

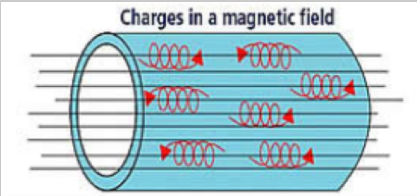
Advances and innovations in mathematical models, methods and/or numerical algorithms



- Initial development and demonstration of an implicit structure-preserving FE formulation for the multifluid full-Maxwell electromagnetic plasma system. Initial demo of scalability for ion/electron plasma oscillation with uncoupled TEM waves.

- Development of a scalable implicit 3D VMS FE resistive MHD solver for incompressible, low flow-Mach-number asymptotic approximation, anelastic, and low flow-Mach-number compressible. Based on a B-field / Lagrange multiplier formulation that allows fully-implicit and direct-to-steady-state solutions. Large-scale parallel performance studies.

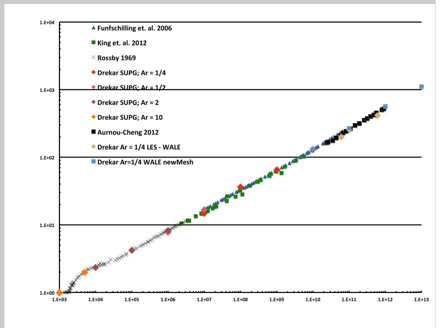
- **Novel Mathematical Formulations for Extremely Anisotropic Transport.** Achieves high-accuracy and enforces positivity.



- Completion of the development of the first truly **algorithmically scalable fully-implicit XMHD solver** (to our knowledge), on structured finite-volume grids.

- **Comprehensive stability and accuracy results for Spectral Deferred Correction (SDC) applied to anisotropic transport and the continued Development of asymptotic preserving operator-split Lagrangian approach.**

- **A new FE Variational Multi-Scale (VMS) MHD turbulence model with thermal convection effects has been developed.** A fully residual-based dynamically adaptive formulation. Demonstrated computations of non-universality MHD Turbulence comparisons with DNS. Comparisons for thermal convection with WALE-LES and experiments are very encouraging.



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Brief Incomplete list of Accomplishments in this Funding Cycle and how this Already Aligns with the FY15-17 ASCR Guidance to PIs.

- **The transition path for past and future research**

Spurring New and Continuing Research Directions (informal collaborations – i.e. not funded).

- MHD Modeling of RFP reactors (w/RFX experiment in Padova Italy)
- VMS MHD - LES Turbulence models (w/ Prof. Oberai – RPI, D. Sondak – UT)
- VMS MHD modeling / experimental validation for Geo-dynamo (w/ J. Aurnou - UCLA)
- ABF preconditioning for mixed FE and edge-elements (w/Elman – UMD)
- Locally coupled smoothers (Vanka-type) (w/Adler, MacLachian, Benson - Tufts)
- High-resolution methods/multiphysics MHD – Algebraic Flux Correction (w/Kuzmin - Univ. Dortmund)

Algorithms in Libraries and Software

- New high-concurrency node capability for **Trilinos/Phalanx** (DAG mulitiphysics dependencies) & **Trilinos/ Panzer** (FE multiphysics assembly) using **Trilinos/Kokkos** performance portability abstraction layer.
- Supporting targeted dev./opt. of fully-coupled AMG for multiphysics stabilized FE [**Trilinos/ML & Muelu**]
- New 64 bit capability for block-oriented preconditioning package (e.g. phyiscs-based, ABF) [**Trilinos/Teko**]
- New capability for utilization of developed ABF preconditioners in **Trilinos/Teko** as smoothers for AMG in **Trilinos/Muelu**

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

Methods/algorithms adopted by other DOE offices

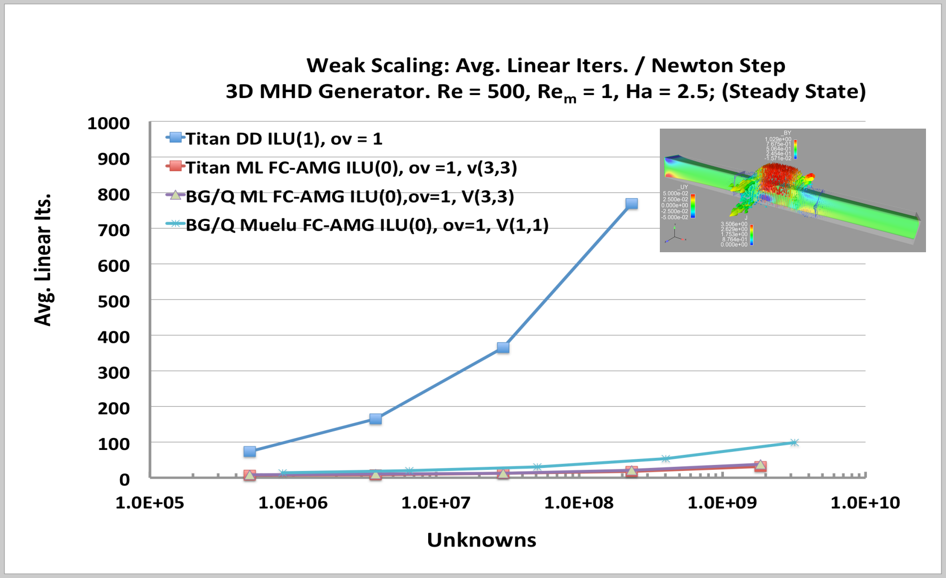
- DOE-NNSA: Charon2 next gen. semiconductor modeling developed on our app./solution method software.
- DOE-NNSA (ATDM) developing next gen. multifluid/PIC plasma using Phalanx, Panzer, Teko software.
- DOE-NNSA: SNL LDRD on magnetic implosions using multifluid electromagnetic plasma model; the research is using our implicit formulations, scalable ABF preconditioners for more realistic EOS, geometries, and high energy density physics (HEDP) pulsed power experiments (just begun).
- DOE-OFES (Basic Plasma Physics program): LANL to model magnetic reconnection experiments in the US. Using extended MHD and hybrid continuum/kinetic algorithms and solvers.

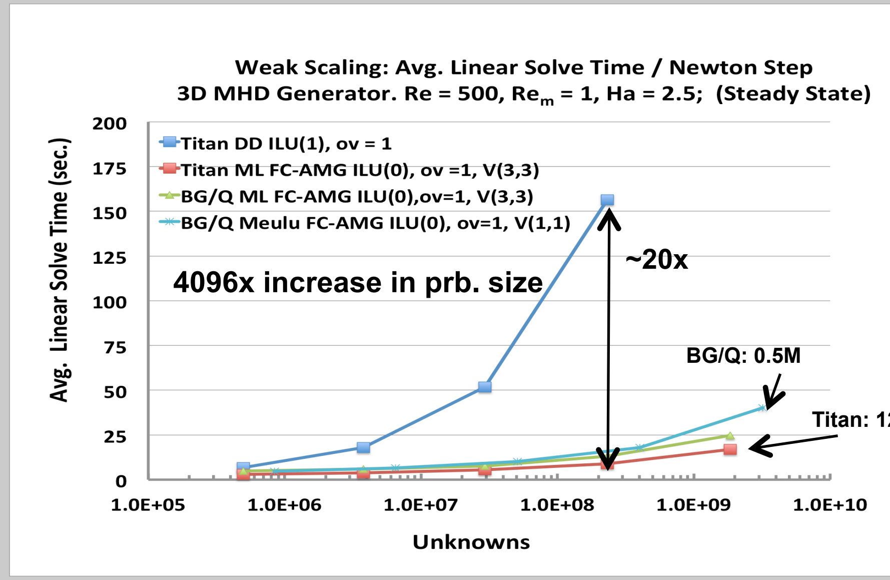
Red text – Topic related to research highlights presented

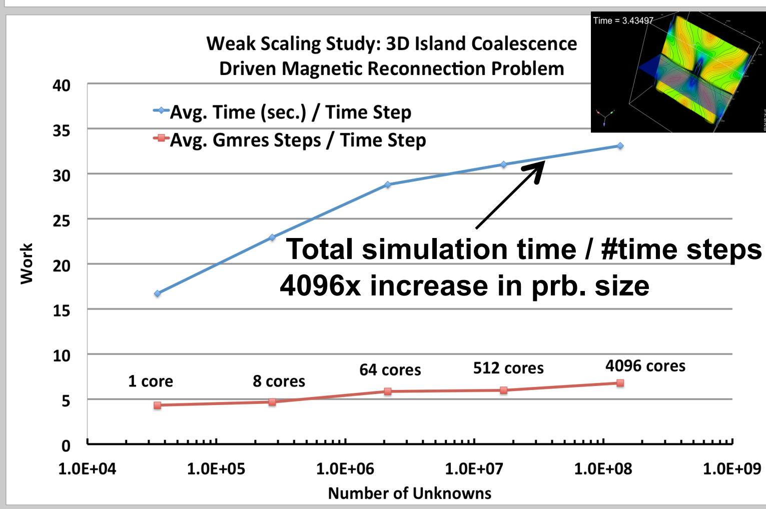
Large-scale Scaling Studies for Cray XK7 AND BG/Q; VMS 3D FE MHD

VMS, Q1 interpolation,

v P B r







Largest fully-coupled unstructured FE MHD solves demo. to date:

- MHD (steady) weak scaling studies to 128K Cray XK7, 0.5M cores 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: 3.2B DoF, 3.2B elem, on 1.6M cores

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

(DOE/ORNL Titan Cray XK7: Joule Metric test runs)

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

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

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

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

Result:

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

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

3) MAIN RESULT: Partitioning of coupled physics into sub-systems enables *SCALABLE* AMG (e.g. Our **Trilinos/Teko block-precondioning** using optimal AMG e.g. H(grad), H(curl) from **ML**)

Background on Our Work in Scalable Block Preconditioning Alg. and App. to MHD/XMHD/Plasmas

Physics-Based and Approximate Block Factorization Methods/Algorithms/Software

- Chacon ???? (more general type of references)
- Chacon ???? (more general type of reference)
- Knoll and Chacon et. al. "JFNK methods for accurate time integration of stiff-wave systems", SISC 2005
- Elman, Howle, Shadid, Shuttleworth, Tuminaro, " Block prec. based on approximate commutators", SISC, 2006
- Elman, Howle, Shadid, Shuttleworth, Tuminaro," A Taxonomy of Mulit-level Block Prec. for the Incomp. Navier-Stokes", JCP, 2008
- Cyr, Shadid, Tuminaro, "**Teko** an **abstract block preconditioning capability** .....", SISC, 2016 (**Trilinos Package**)

Physics-Based Preconditioning Algorithms for MHD, XMHD, Implicit PIC Methods

- ???
- ???
- 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-complement Methods for MHD/ Multifluid Plasmas

- 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 prec. capability with concrete app. to Navier-Stokes and resistive MHD, SISC, 2016
- Shadid,et. al., "Towards Scalable and Eff. Soln of Full Maxwell EM - Multifluid Plasmas", NECDC 2016 (Extended Abstract)
- Phillips, Shadid et. al., Fast Linear Solvers for Multifluid Continuum Plasma Simulations, NECDC 2016 (Extended Abstract)
- Phillips and Shadid, Approximate Block Factorization Preconditioners for 3D Magnetic Vector Potential MHD, in preparation

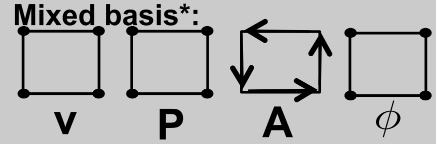
Block Preconditioners for Multiple-time-scale Maxwell Electromagnetics

- Phillips, Shadid, Cyr, "Scalable Precond. for Structure Preserving Discretizations of Maxwell Equations in First Order Form", in prep.

Magnetic Vector-Potential Formulation: Structure Preserving

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

Mixed basis*:



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

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

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

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

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

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

- Divergence free involution for B enforced to machine precision by structure-preserving edge-elements*.

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

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

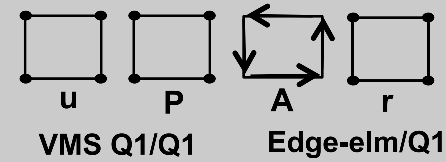
- Residual defect-correction factorization procedure used to strongly couple operators producing the Alfven wave and reduce N-S / vector potential to two 2x2 blocks for the ABF:

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

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

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

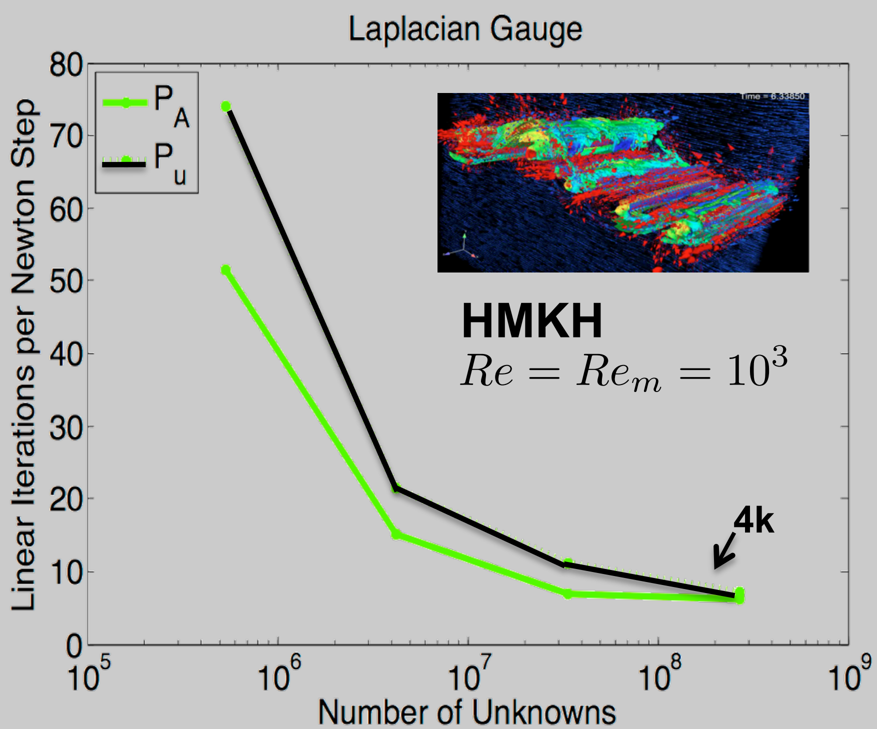
Weak Scaling 3D Unstructured FE Implicit MHD Approximate Block Factorization AMG-based Preconditioners (structure-preserving discretization)

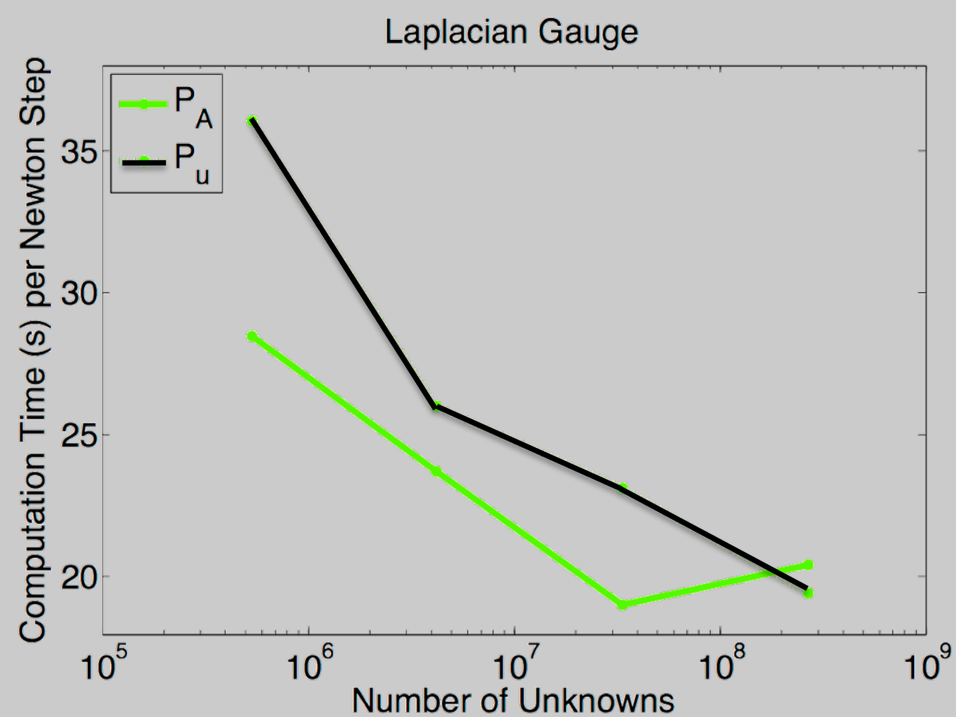


$$\mathcal{A}_{GSG} = \left(\begin{array}{ccc|c} F & B^t & Z & 0 \\ B & C & 0 & 0 \\ Y & 0 & G & D^t \\ \hline 0 & 0 & 0 & L \end{array}\right) \qquad \mathcal{P}_{\mathbf{A}} = \begin{pmatrix} F & 0 & Z \\ 0 & I & 0 \\ Y & 0 & G \end{pmatrix} \begin{pmatrix} F^{-1} & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I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

$\hat{S}_P = C - B\hat{F}^{-1}B^t$ PCD, H(grad) AMG

$\hat{S}_{\mathbf{A}} = G - Y\hat{F}^{-1}Z$ SIMPLE, H(curl) AMG

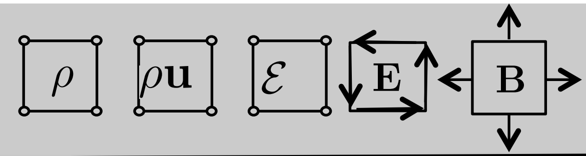




Structure of right preconditioned matrix using $\mathcal{P}_A$; Further analysis required.

$$\mathcal{A}_{GSG}\mathcal{P}_A^{-1} = \begin{pmatrix} I & 0 & 0 & -ZS_{\mathbf{A}}^{-1}D^tL^{-1} \\ 0 & I & 0 & 0 \\ YF^{-1}(I + B^tS_{\mathbf{p}}^{-1}BF^{-1}) & -YF^{-1}B^tS_{\mathbf{p}}^{-1} & (S_{\mathbf{A}} - YF^{-1}B^tS_{\mathbf{p}}^{-1}BF^{-1}Z)S_{\mathbf{A}}^{-1} & (I - GS_{\mathbf{A}}^{-1})D^tL^{-1} \\ 0 & 0 & 0 & I \end{pmatrix}$$

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

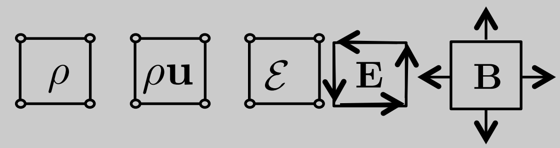
Other work on formulations, solution algorithms: See e.g. U. Shumlak et. al.; T. Barth; J. Rossmanith et. al.

(with R. Kramer, A. Robinson – SNL)

Scalable Physics-based Preconditioners for Physics-compatible Discretizations

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

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

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

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 Approach Enables Optimal AMG Sub-block Solvers

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

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

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

Electric field system
Edge-based curl-curl type
ML: H(curl) AMG
(lumped mass)

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

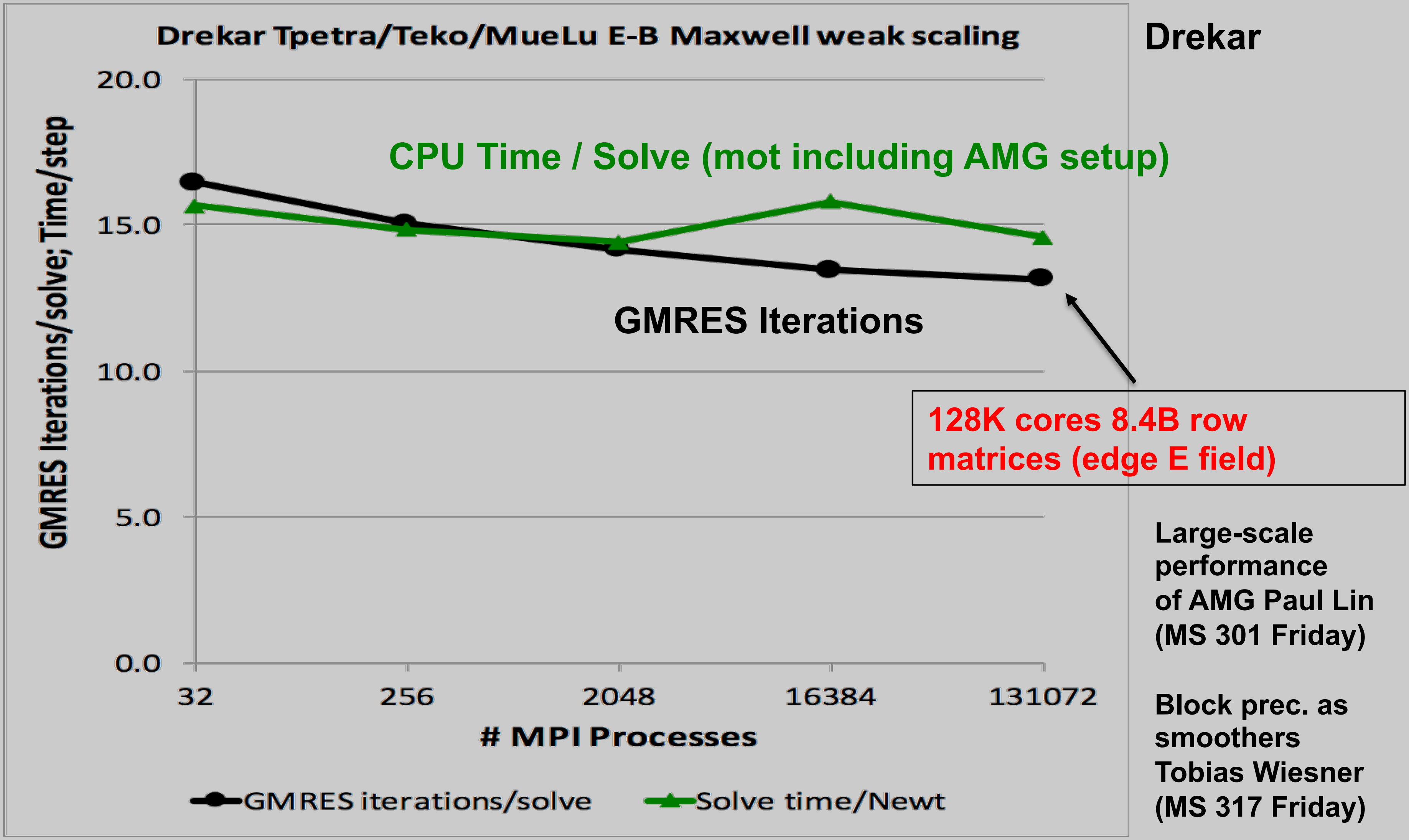
Face-based simple
mass matrix Inversion.

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

Weak Scaling for 3D EMP with Block Maxwell Eq. Preconditioners on Trinity



Drekar

Large-scale performance of AMG Paul Lin (MS 301 Friday)

Block prec. as smoothers Tobias Wiesner (MS 317 Friday)

GS smoother with H(grad) AMG

Max CFL_c ~ 200

Sandia National Laboratories

Transient artificial current source (EMP) in Mid-to-high Atmosphere EM Field Propagation and Cold Electron Plasma Response ($8\mu s$)

Atmosphere with realistic electron density, and Earth's magnetic field.

$$\tau_{EM} = \Delta x / c = 8 \times 10^{-8}$$

$$\tau_{\omega_{pe}} = \frac{1}{\sqrt{\frac{n_e q_e^2}{\epsilon_0 m_e}}} = 5 \times 10^{-7}$$

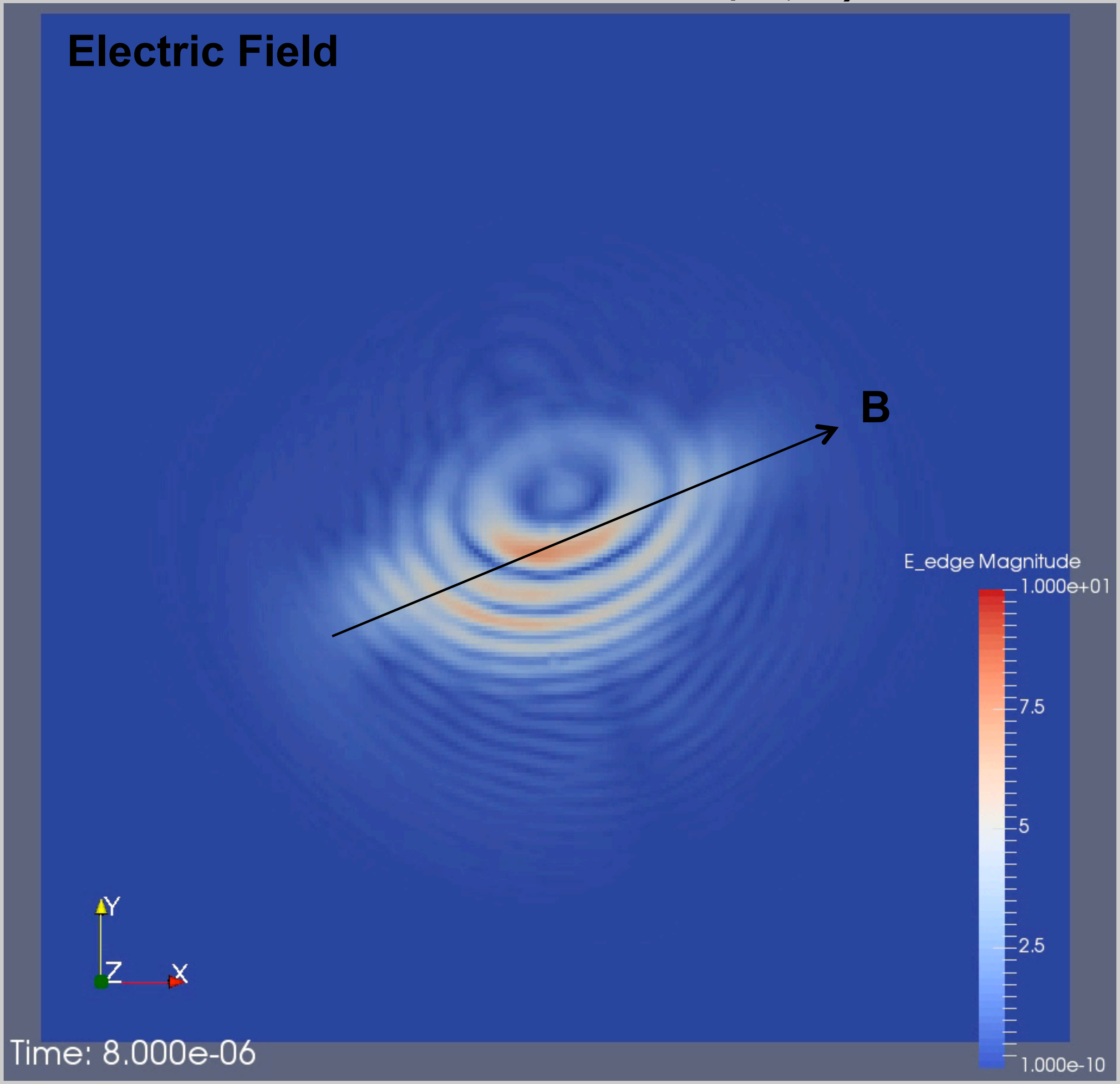
$$\tau_{\omega_{ce}} = \frac{1}{\frac{q_e B}{m_e}} = 1 \times 10^{-6}$$

$$\tau_{source} = 100 \times 10^{-9}$$

For physics included has correct qualitative behavior:

- **Anisotropic structure**
- **Strongly dispersive**
- **Phase and group velocities appear reasonable**

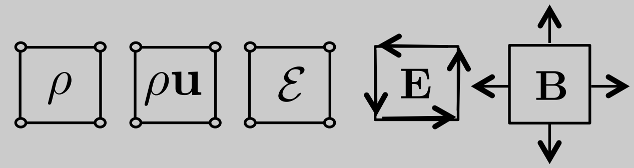
EMPIRE/Drekar full-Maxwell, electron plasma simulation, with SNL ATDM Team



UUR From: SAND2016-5223 PE

Electron / Ion Plasma Oscillation Results (Full Maxwell – two-fluid)

- **Longitudinal Ion/Electron plasma wave and an initialized under resolved transverse EM wave**
- **Formulation: Structure-preserving discretization***



- **Problem: Ion density perturbation to a cold electron / ion plasma**

$$n_i(x) = N; n_e(x) = N\left(1 + \delta sin(200\pi x)\right); \quad N = 10^{18}$$

$$E_x(\mathbf{x}, 0) = \frac{\delta q_i N}{200\pi\epsilon_0} cos(200\pi x)$$

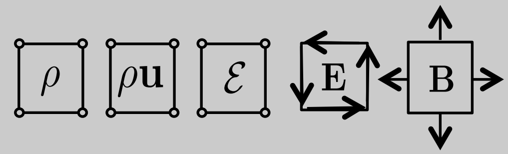
$$E_y(\mathbf{x}, 0) = -\frac{\delta q_e N}{200\pi\epsilon_0} sin(200\pi x)$$

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

(with R. Kramer, A. Robinson, G. Radtke, J. Niederhause, M. Bettencourt, K. Cartwright)

Initial Weak Scaling for Electron / Ion Plasma Oscillation and TEM Wave Results

$$\tau_{EM} \approx 3.3 \times 10^{-13} \quad \text{on coarsest mesh}$$
$$\tau_{\omega_{pe}} \approx 1.1 \times 10^{-10}$$
$$\tau_{\omega_{pi}} \approx 4.8 \times 10^{-9}$$
$\Delta t = 0.1 * \tau_{\omega_{pe}}$ (not resolving TEM wave)



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

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

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

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):

Proof of Principle

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

<u>**Summary of ABF / Physics-based preconditioners developed**</u>

2D and 3D resistive MHD models for a wide range of flows and EoS

- **True incompressible, Low-Mach & anelastic approx.**
  - **Vorticity-streamfunction**
  - **Primitive variable**

- **Low Mach number compressible**
  - **Conservative variables**
  - **Primitive variables**

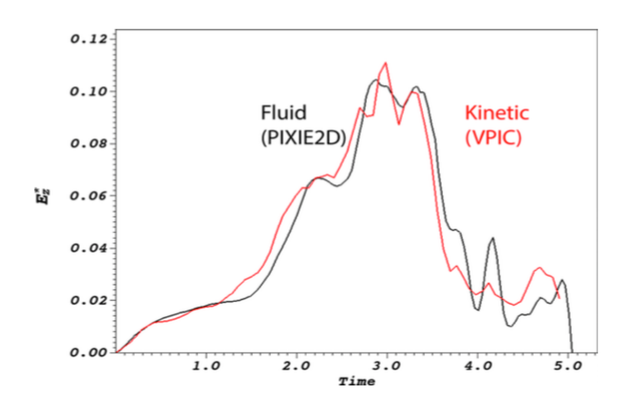


FIG. 10. Normalised reconnection rate E_z^* against time for Harris-sheet run

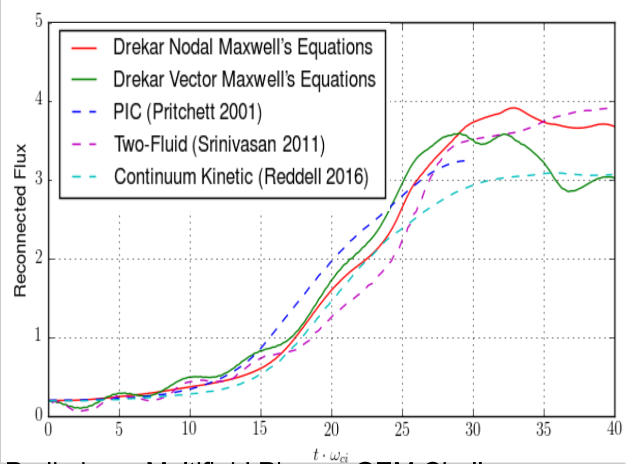
XMHD Magnetic reconnection …

2D and 3D Hall physics / extended MHD

- **Incompressible: vorticity-streamfunction**
- **Low Mach number compressible: Conservative**

3D multifluid / full-Maxwell plasma

- **Compressible (Conservative variables)**



Preliminary Multifluid Plasma GEM Challenge

Kinetic

- **Implicit PIC (Moment accelerated form)**

Wide Range of Discretizations:

- **FV, mapped FV, AMR FV, edge & face FV,**
- **VMS/Stabilized FE, mixed FE, structure-preserving FE (node/edge/face)**