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

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Abstract

We are developing advanced ***stable, accurate, and scalable, formulations for a hierarchy of important plasma physics models used for DOE science and national security missions. These models include resistive [1,2] and extended MHD [3], multifluid electro-magnetic (EM) plasmas [5,6], and initial hybrid fluid/kinetic systems [7,8].*** For efficient and accurate long-time integration, implicit treatment of a sub-set of the multiple-time-scale physics, and appropriate structure-preserving spatial discretizations are required. The key numerical solution methods we are developing are stable and higher-order accurate implicit, and implicit/explicit (IMEX) formulations [1,6], and scalable and robust Newton-Krylov (NK) nonlinear iterative solvers [1,2,5,9,10]. For efficient solution of the implicit operators, we employ novel scalable physics-based block preconditioners with optimal AMG sub-block solvers.

Motivation (e.g. multifluid plasmas)

Multifluid EM plasma models are being developed for simulation of moderately-dense to dense / collisional systems in support of DOE magnetic and inertial confinement fusion (MCF, ICF) and magneto-inertial fusion (MIF) systems. The models can be used as continuum solvers, and as moment–based accelerators for multiscale continuum/kinetic models.

$$\frac{\partial \rho_a}{\partial t} + \nabla\cdot(\rho_a \mathbf{u}_a) = \mathcal{R}_{\rho_a}$$

$$\frac{\partial(\rho_a \mathbf{u}_a)}{\partial t} + \nabla\cdot(\rho_a \mathbf{u}_a \otimes \mathbf{u}_a + p_a I + \Pi_a) - q_a n_a(\mathbf{E} + \mathbf{u}_a \times \mathbf{B}) = \mathcal{R}_{\rho_a u_a}$$

$$\frac{\partial \mathscr{E}_a}{\partial t} + \nabla\cdot((\mathscr{E}_a + p_a)\mathbf{u}_a + \Pi_a\cdot\mathbf{u}_a + \mathbf{h}_a) - q_a n_a \mathbf{u}_a\cdot\mathbf{E} + Q_a^{src} = \mathcal{R}_{\mathscr{E}_a}$$

$$\epsilon_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla\times\frac{1}{\mu_0}\mathbf{B} + \mathbf{J} = 0; \quad \frac{\partial \mathbf{B}}{\partial t} + \nabla\times\mathbf{E} = 0; \quad \mathbf{J} = \sum_k q_k n_k \mathbf{u}_k$$

Scalable Solution Approach

Key Gaps: Efficient and scalable implicit formulations and solution methods that account for unresolved time-scales in wave physics (hydrodynamics and EM), plasma / cyclotron frequencies, ionization / recombination and collisional effects.

Our approach develops stable, higher-order IMEX formulations with partitions for slow (explicit) and fast (implicit) operators [6]. As well we design scalable multiphysics solvers **based on physics-based preconditioners tailored for structure-preserving finite elements (FE)**. For example for multifluid EM plasmas hydrodynamic variables (**F** –nodal) are partitioned, from the electric (**E** –edge), and magnetic (**B** –face) fields, and approximate block factorizations and Schur complements are designed.

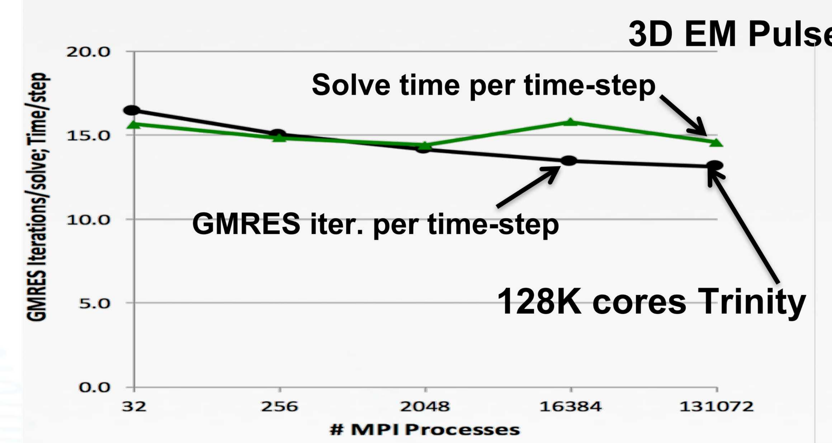
$$\begin{bmatrix} \mathbf{Q}_B & \mathbf{K}_E^B & 0 \\ \mathbf{K}_B^E & \mathbf{Q}_E & \mathbf{Q}_F^E \\ \mathbf{Q}_B^F & \mathbf{Q}_E^F & \mathbf{D}_F \end{bmatrix} \begin{bmatrix} \mathbf{B} \\ \mathbf{E} \\ \mathbf{F} \end{bmatrix}; \quad \begin{bmatrix} \mathbf{Q}_B & \mathbf{K}_E^B & 0 \\ 0 & \hat{\mathcal{D}}_E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

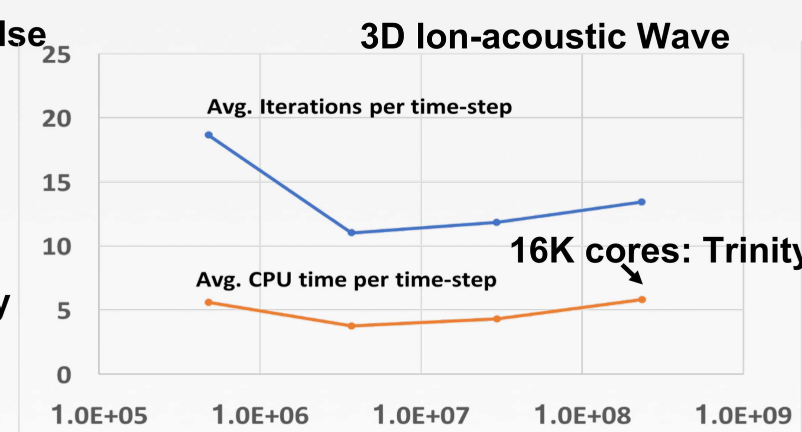
$$\underbrace{\mathbf{S}_F = \mathbf{D}_F - \mathcal{K}_E^F \mathcal{D}_E^{-1} Q_F^E}_{\text{CFD – H(grad) AMG}} \; ; \quad \underbrace{\mathcal{D}^E = \mathbf{Q}_E - \mathbf{K}_B^E \bar{\mathbf{Q}}_B^{-1} \mathbf{K}_E^B}_{\text{E field – H(curl) AMG}}$$

The **E** field Schur complement is close to singular for large EM CFL_c. We use grad-div stabilization for weak forms dominated by the curl-curl operator. For the multifluid model these techniques allow overstepping of EM waves, plasma & cyclotron frequency, and collisional time-scales, by > 10^4 [6,10].

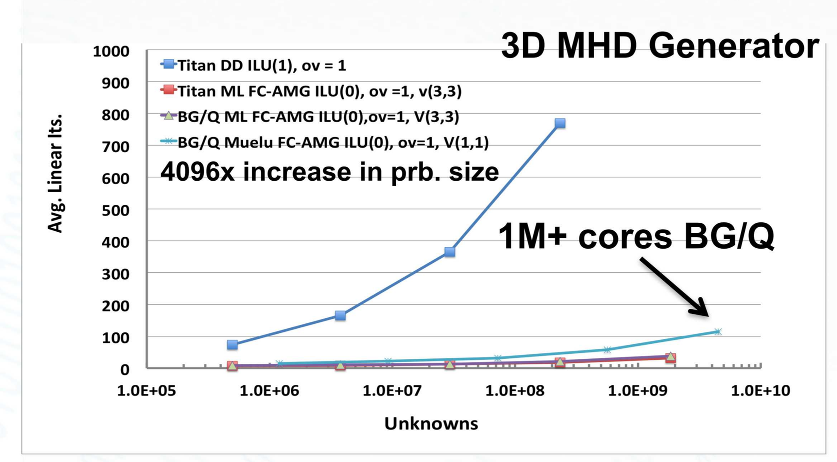
Highlighted Algorithmic Results:

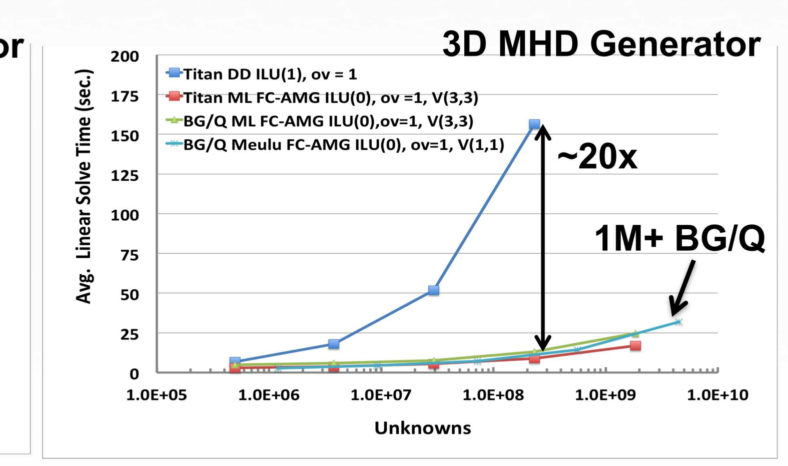
(1) Scaling of approximate block Schur complement for structure-preserving FE using H(curl) preconditioners for 3D EM Pulse (Maxwell eqns.), and a 3D ion-acoustic wave (multifluid ion/electron EM plasma system) with combined H(curl) and H(grad) sub-block AMG solve [4,10].





(2) Scaling of H(grad) coupled system AMG for variational multiscale (VMS) nodal FE resistive MHD up to **1M+ cores**. This solver is also used in the hydrodynamic sub-block $\mathbf{S}_F$ above [1,9].





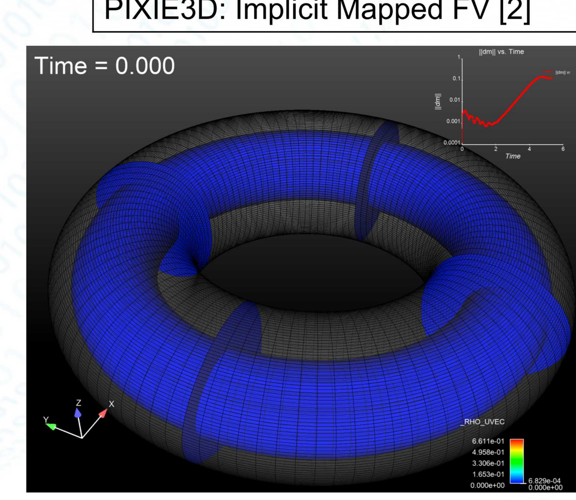
(3) Demonstrated utilization and optimal algorithmic strong scaling of H(grad) AMG to **entire full-scale 1.6M cores of Sequia BG/Q** for Poisson sub-block solves that are used in block preconditioners [9].

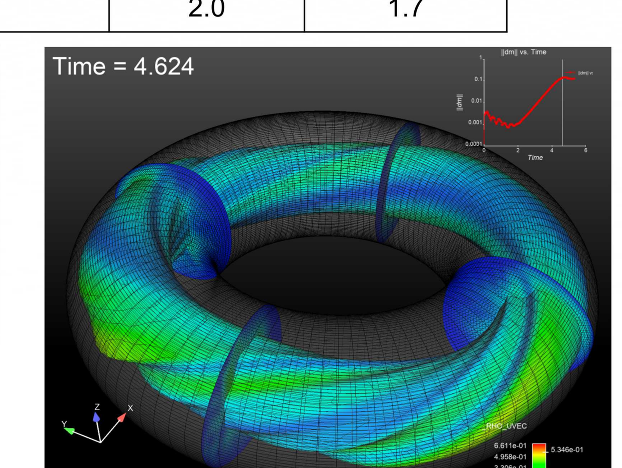
Preliminary Scientific App. Results:

Demonstrations of implicit VMS resistive MHD formulations have been carried out for MCF and MIF relevant idealized problems.

(1) Initial comparison of linear growth rates and transformation of constant pressure surface for unstable Soloveev tokamak relevant equilibrium.

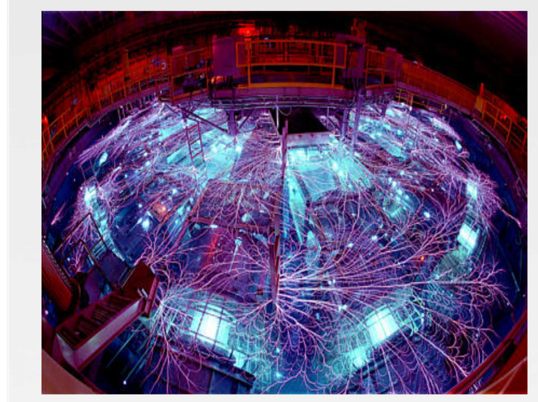
	$\gamma = 1$	$\gamma = 5/3$
Drekar: Implicit Unstructured FE [1]	1.94	1.69
PIXIE3D: Implicit Mapped FV [2]	2.0	1.7

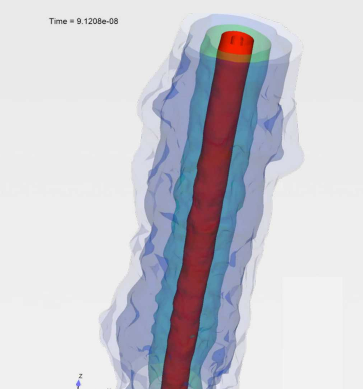




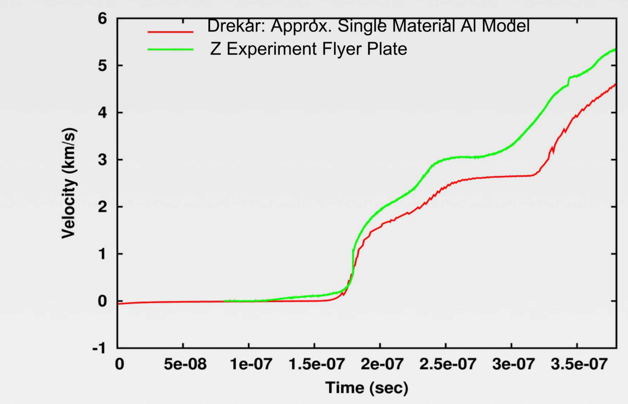
Left: Soloveev ($\kappa = 1$) equilibrium configuration constant pressure surface. Right: Constant pressure surface after nonlinear saturation of kink and interchange instability.

(2) Idealized simulations of magnetic implosions of gas puffs and solid Aluminum in Z-pinch configurations. Z-pinch device experiments (left) are relevant for shock and material interactions, high energy density physics (HEDP), MIF, and ICF.





3D Gas Puff z-pinch Drekar MHD



1D VISAR Al Flyer Plate Exp. and 1st Drekar Approx. Single Material Model - Blind Test

Potential Impact

Our development of implicit / IMEX plasma physics formulations and block preconditioning approaches has demonstrated scalable solution for challenging multiple-time-scale plasma systems. Our novel Schur complement approximations (1) preserve critical off-diagonal hyperbolic and strong source term coupling, and (2) decompose the coupled system into sub-blocks to which optimal H(grad) and H(curl) AMG can be applied.

1 year: Incorporation of approaches into R&D and production MHD and multifluid continuum plasma solvers for DOE/SNL applications in MIF (e.g. z-pinch) and NNSA high-energy density physics (HEDP).

5 year: Demonstration and application for large-scale fusion applications for DOE Office of Science and OFES MCF (e.g. Tokamaks) through SciDAC-4 partnership (Tokamak Disruption Sim. (TDS) Center).

10 year: Advanced hierarchy of IMEX formulations and solution methods, combined with extreme-scale HPC, will enable plasma simulations using hybrid multiscale continuum / kinetic plasma models for the most challenging DOE SC and NNSA science apps.

Synergy

Areas in which we can help

R&D involving advanced continuum plasma models both as continuum solvers and accelerators for multiscale continuum/kinetic models. New ASCR/OFES SciDAC and OFES plasma efforts, as well as NNSA plasma physics R&D would strongly benefit from collaboration on these topics.

Areas in which we need help

Continued development of efficient and scalable H(grad) / H(curl) AMG algorithms / software at extreme scale and R&D for these methods on next generation architectures.

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