Whitepaper for **DOE Workshop on Integrated Sim. for Magnetic Fusion Energy Sci.** Topic D: Multiphysics and Multiscale Coupling. Prepared by J. Shadid, Cyr, Lin, Pawlowski, Phillips, Tuminaro, Wildey (SNL), L. Chacon (LANL). (No Presentation) [SAND2015-2929 W].

Motivation: Magnetic fusion plasma energy systems are characterized by a complex interaction of strongly-coupled, highly-nonlinear, multiple-time-scale physical mechanisms. These can include very fast time-scales (electron plasma oscillations), fast wave phenomena (e.g. magnetosonic, Alfven, and Whistler waves), transport (mass, momentum, energy, charged species), dissipative processes, atomic physics, radiation transport, and interacting electromagnetic fields [18]. Computational models range from continuum MHD fluid formulations (e.g. resistive, Hall physics, and multifluid), kinetic descriptions approximated by direct discretization and particle-in-cell type methods, and hybrid fluid/kinetic techniques. These characteristics make the robust, accurate, efficient and scalable computational solution of these systems, over relevant dynamical time-scales of interest, extremely challenging. This whitepaper addresses a few of the most important open issues related to time-integration and the scalable computational solution methods for multiphysics PDE systems that are critical aspects of mathematical models for magnetic fusion plasma simulation.

Time Integration Issues: Current standard-practice production time integration for multiphysics MHD systems relies on operator-splitting expressed as a sequential evaluation of physics operators in a time-loop. Operator-splitting results in a loose-coupling, which can lead to inaccurate and unstable results when physical mechanisms are strongly coupled, highly-nonlinear and have overlapping time-scales. These characteristics often require very small time-step sizes that can make longer-time-scale integration costly and inaccurate. Additionally, the complex loosely coupled mathematical structure makes higher-order temporal integration and direct integration of efficient sensitivity analysis, error estimation, and advanced UQ techniques difficult and therefore often sampling-only black-box techniques (that require many expensive function evaluations/multiphysics solves) can be employed. The use of fully-implicit methods with advanced coupled non-linear solvers and scalable linear solvers have shown significant promise in this context. These methods can provide stable, variable- and higher- order techniques with local and global error control. They can also be stable and accurate when run at the dynamical time-scale of interest in multiple-time-scale systems. Recently progress has been made in developing fully-implicit formulations that robustly and accurately integrate these systems and follow the dynamical time-scales of interest (see e.g. [5, 15, 9, 16] and references therein). However significant critical developments are still required. These include:

1. Development, demonstration, and extensive evaluation of higher-order fully-implicit approaches for robust, accurate fusion relevant simulations of multifluid MHD approximations characterizing stability, accuracy, and the convergence to Hall physics and resistive MHD limits.
2. Development, demonstration, and evaluation of well-structured high-level mathematical models for extended MHD employing recent IMplicit-EXplicit (IMEX) time-integration methods. These methods have well-defined consistent nonlinear residual forms that enable the development of higher-order methods, strongly-coupled nonlinear solvers (e.g. Newton-Krylov), and adjoint-based beyond forward simulation computational analysis.
3. Develop, analyze, and evaluate IMEX time-integration coupled with physics-compatible discretizations and high-resolution methods for hyperbolic MHD. Including results for nonlinear stability (e.g. positivity and monotonicity results) for systems in the limit of small dissipative contributions and strong source-term coupling to Maxwell's equations.
4. Development, mathematical analysis, and evaluation of hybrid fluid/kinetic methods that use fluid equations and varying levels of implicitness to extend the accessible simulation time- and length-scales, and thereby the efficiency of the underlying kinetic approximations.

5. Theoretical analysis, and numerical evaluation of adjoint methods for IMEX methods to enable error estimation, sensitivity analysis, and fast integrated UQ techniques for general multi-stage (e.g. RK type) and multistep (e.g. BDF) methods. (e.g. a recent result [6])

Scalable Computational Multiphysics Solution Methods: Iterative solution algorithms for the implicit and IMEX time integration approaches described above must provide robust, efficient, and scalable solution to the complex coupled large-scale nonlinear/linear systems generated from a diverse set of plasma physics approximations. The most successful methods to date have been based on strongly-coupled preconditioned Newton-Krylov (NK) type methods that employ physics-based preconditioning techniques (see e.g. [12, 5, 15, 16]). These methods address numerical stiffness arising from fast normal modes and overlapping time-scales in multiphysics PDEs by effectively building a preconditioner from approximate block factorizations (ABF) and/or physics-based approaches, that approximate the critical off-diagonal hyperbolic-coupling that is encoded in block-diagonal Schur complement operators. By design these Schur complement approximations can be effectively solved by multilevel methods (AMG), and can result in optimal convergence rates of the coupled Newton-Krylov solver. Additionally these approaches allow AMG type methods to be applied to multiphysics problems for which disparate mixed spatial discretizations are employed (e.g. DG for fluid unknowns and edge/face elements for the electric field/magnetic induction) and no monolithic scalable AMG methods exist. While progress has been made, significant algorithmic advances and some software development is required. This includes:

1. Demonstration and evaluation of large-scale MHD fluid (resistive and Hall physics) simulations employing fully-implicit and IMEX time integration and existing physics-based and ABF preconditioners on leadership-class machines for realistic fusion relevant simulations, both transient and equilibrium calculations. Extensively evaluate stability, accuracy and scalability in comparison to current generation production MHD solver algorithms.
2. Develop variants/extensions of existing physics-based / ABF MHD preconditioners for use as local multigrid smoothers (as opposed to preconditioners) within monolithic AMG Methods.
3. Develop monolithic AMG methods suitable for mixed discretizations and in particular physics-compatible discretizations. Here, coarsening techniques and grid transfer operators are needed for each component such that coarse level operators preserve key properties (e.g., stability).
4. Development and evaluation of efficient physics-based / ABF preconditioners and approximate Schur complements for more complex coupled multiphysics effects including anisotropic transport/diffusion and two-temperature (ion/electron) formulations.
5. Development and evaluation of new physics-based / ABF preconditioners for two-fluid and multifluid MHD approximations coupled to full Maxwell equation electromagnetics models with physics-compatible discretization approaches.
6. Develop preconditioners for implicit part of hybrid fluid/kinetic models in the highly magnetized regime.

Impact: This research will address a number of critical open issues (e.g., stability and higher-order accuracy for multiphysics simulations, efficient and accurate long-time-scale integration for multiple-time-scale systems, development of efficient implicit methods, along with algorithmic and parallel scalability). These challenging issues represent unresolved gaps that have been specifically identified as critical components of future predictive computational capabilities for important scientific and technological applications in a number of recent DOE-SC reports. These include DOE-OFES reports [7, 14, 13], as well as several scientific grand-challenge [17, 4, 8, 19, 3], multiphysics systems [10, 11], and exascale reports [2, 1] from DOE-ASCR.

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