Whitepaper for **DOE ASCR Workshop on Turbulent Flow Simulation at the Exascale: Opportunities and Challenges** Prepared by D. Sondak (UW-Madison), J.N.Shadid (SNL), L.M.Smith (UW-Madison), F.Waleffe (UW-Madison), T.M.Smith (SNL), A.A.Oberai (RPI).

Motivation: Computational physics can be thought of as the scientific discipline that uses the computer as a microscope. In this way, exascale simulations will allow us to peer deeper into turbulence than ever before. In so doing, we can hope to dissect the inner workings of this phenomenon as well as to work with turbulence when designing and exploring systems for use in practical applications. In this whitepaper, we discuss directions for fundamental turbulence research in hydrodynamics, thermal convection and magnetohydrodynamics (MHD), new approaches to turbulence modeling in MHD and new developments and challenges in solution methods for MHD and plasma physics.

Towards a Fundamental Understanding of Turbulence: Exascale simulations bring forth the possibility of exploring the building blocks of turbulence beyond statistical theories [5]. High resolution simulations of a turbulent flow field may provide a glimpse at the quantization of turbulence; the underlying universal coherent structures that govern turbulence dynamics. Exploration of these structures to date has been limited due to computational resources. Some progress in finding these coherent structures has been made at low Reynolds numbers in shear flows [10], Rayleigh-Bénard convection [11, 8] and in MHD [12]. Ongoing work seeks to detect the signature of these structures in fully turbulent flows and to assess their impact on governing the dynamics of turbulence. Assessment of coherent structures in governing real-world dynamics such as those found in astrophysical (e.g. solar and galactic processes) and geophysical (e.g. atmospheric and oceanic dynamics) systems will require significant computational power. Although enticing, exploiting these structures for the development of numerical algorithms and turbulence models is prohibitively expensive with current computational resources [3]. Exascale simulations may potentially offer an opportunity to design numerical approaches to turbulence that incorporate these quanta of turbulence.

Development and Implementation of Turbulence Models: Direct numerical simulation (DNS) of geophysical and astrophysical systems will likely remain out of reach even with exascale simulations. On the other hand, mathematically consistent, scalable and robust large eddy simulations (LES) should now be within striking distance. Since its inception, LES has been an expensive compromise between DNS and Reynolds-averaged Navier-Stokes simulations. LES often falls back on classical eddy viscosity closure models which may destroy the true dynamics of turbulence. Recent LES models for incompressible MHD have found success on simple test problems [4, 7, 6, 9] by being flexible enough to incorporate distinct physical mechanisms from MHD such as transfer of energy from small to large scales. These capabilities are particularly important, for example, in LES for magnetoconvection and geodynamo simulations. The computational solution of the governing balance equations for mass, momentum, heat transfer and magnetic induction for such MHD systems can be extremely challenging. These difficulties arise from both the strong nonlinear, nonsymmetric coupling of fluid and electromagnetic phenomena, as well as the significant range of time- and length-scales that the interactions of these physical mechanisms produce in MHD flows.

Scalable Computational Multiphysics Solution Methods: Iterative solution algorithms for implicit and implicit-explicit (IMEX) time integration approaches must provide robust, efficient, and scalable solutions 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 type methods that employ physics-based preconditioning techniques (e.g [1, 7, 2, 6]). 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 coupling that is encoded in block-diagonal Schur complement

operators. By design these Schur complement approximations can be effectively solved by multilevel methods, and can result in optimal convergence rates of the coupled Newton-Krylov solver. While progress has been made, advances in both LES and MHD solvers are required. These include:

1. Development and testing of new LES models on challenging problems such as the geodynamo and astrophysical systems.
2. Incorporation of essential physics into LES models such as the coherent structures governing turbulence dynamics as well as important mechanisms including transfer of energy between scales.
3. Demonstration of large-scale MHD fluid simulations employing fully-implicit and IMEX time integration and existing physics-based and ABF preconditioners on leadership-class machines.

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