Accelerating Fusion Through Integrated Whole Device Modeling

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Executive Summary

The current challenge for fusion research is to increase the rate of progress toward development of an economically viable fusion energy source. Major recent advancements in theoretical understanding, validating physics models, computing infrastructure, and diagnosis of experiments provide important new opportunities for accelerating progress toward this objective. What is needed now is to comprehensively and self-consistently advance and integrate the many complex, nonlinear and multi-scale plasma descriptions into a suite of integrated whole device modeling (WDM) capabilities for magnetically confined plasmas. Because of the complexity of this goal and the wide range of time and length scales that need to be modeled, a diversity of approaches is required. This white paper explains: 1) what is involved in developing integrated WDM, 2) how WDM could make critical contributions to accelerating fusion research, 3) how the developing Department of Energy (DOE) exascale computing project (ECP) will be a major contributor to the development of many key aspects of WDM, and 4) advocates that development and utilization of integrated whole device modeling should become a major strategic element of the U.S. fusion program over the next two decades.

What is Whole Device Modeling?

Whole Device Modeling (WDM) is generally described as assembling physics models that provide an integrated simulation of the plasma.[1] All components that describe a magnetic confinement device, from macroscopic equilibrium to micro-turbulence and control systems, are included in WDM, which should describe the evolution of a plasma discharge from start-up to termination. The individual component models need to be validated with experimental databases. Such a modeling capability is required for assessments of device performance in order to minimize risks and qualify operating scenarios for next-step burning plasma experiments, as well as time-dependent or single-time-slice interpretive analysis of experimental discharges.

We envision such a capability to be applicable to tokamaks, stellarators, and other promising concepts for magnetic confinement. Fusion energy development is a worldwide coordinated research effort. Economical and safe operation of burning plasma devices requires integrated predictive modeling with a confidence level established by validation. In all future burning plasma facilities, the optimization of fusion performance

[1] This definition is taken from the *Report of the Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences, June 2-4, 2015, Gaithersburg, MD, USA*. Note that this Report (referred to hereafter as the Bonoli-Curfman Report) was written before the establishment of the ECP in 2016, now the largest program in the Office of Science. Subsequent to the establishment of the ECP, a new *Report on the Fusion Energy Sciences Exascale Requirements Review, January 27-29, Gaithersburg, MD, USA* (referred to hereafter as the Chang-Greenwald Report, DOI 10.2172/1375639) was completed.

and control scenarios will require predictive WDM with a quantified, validated uncertainty, as it is not feasible to determine operational limits by running trial discharges. Simulations covering the whole device, while they are not a substitute for experiments, are much more cost-effective than building multiple billion-dollar facilities to test new ideas or concepts, similar to how aircraft manufacturers used simulations to reduce the number of physical wings they needed to build in designing superior aircraft.[2]

The following three research elements are critical for realization of a successful WDM capability. These elements bring in expertise from basic fusion theory, applied mathematics, and computer science:

- It is necessary to continue efforts to better understand and distill the physics of gap areas in fusion theory. A list of critical gaps in theory (and associated gaps in simulation capability) has previously been identified by the community in the Bonoli-Curfman Report. Addressing the theoretical challenges associated with these gaps must take place in parallel to building a next-generation WDM capability.
- There must be increased development of and support for modular WDM frameworks. The magnetic fusion program today widely relies on large, complex legacy tools and emerging usage of newer efforts. A sustainable path forward will require support both for the most mission-critical legacy tools and for development and expansion of the newer efforts that can more effectively utilize leadership-class computing resources and execute next-generation work.
- There must be an increased connection to experiment through validation. Each of the challenges and opportunities identified in this paper will require either extensive validation against existing experiments or new development efforts. This will require the development and extensive use of tools that fulfill validation hierarchies and compute associated metrics. Such an approach will require expertise in large-scale data management and analysis for both leadership-class code output and the experimental observations they will be tested against.

Background

For over two decades now, the U. S. Department of Energy (DOE) Fusion Energy Sciences (FES) theory and simulation program, in collaboration with the Advanced Scientific Computing Research (ASCR) program has developed a powerful foundation for advanced simulation capabilities in fusion and plasma science. This has been accomplished through the work of several centers in the Scientific Discovery through Advanced Computing (SciDAC) program, and since 2016, through the establishment of a fusion simulation center in the DOE Exascale Computing Program (ECP). The recently completed "*Interim Report of the Committee on a Strategic Plan for US Burning Plasma Research*"[3] recognizes the important contributions realized by this collective effort:

> "In recent years, understanding of key areas….has advanced to the point where detailed predictions can be made in advance of experiments….These same predictive tools have been employed to develop high-performance scenarios for

[2] "Case Study: Boeing Catches a lift with High Performance Computing," *Report by Council on Competitiveness, 2009*

[3] National Academies of Sciences, Engineering and Medicine, Washington DC: The National Academies Press, https://doi.org/10.17226/24971 , pp. 22-23.

ITER and other planned devices. The capability exists to use theoretical understanding to optimize devices and achieve higher performance… While the U.S. theory program is focused primarily on tokamak research, key innovations have also been developed in other areas, such as the idea of quasi-symmetry in stellarators.

Exascale computing platforms present great opportunities for computational physics. The increased computing power should allow researchers to investigate new and previously inaccessible problems in burning plasma science. Equally important, exascale computing should greatly improve the community's ability to understand and predict experiments with validated sophisticated numerical models."

In the recently concluded Community Workshop on U.S. Magnetic Fusion Research Directions (USMFR) (December 11-15, 2017, Austin, TX), the critical role of theory and simulation in all strategic areas was emphasized by the Table below. A few Discussion Groups at the Austin Workshop expressed concurrence with this perspective. For example, Discussion Group 2 submitted the following summary on theory and simulation:

"It was agreed that the concept of Whole Device Modeling, including theory, verification and validation, has the potential to accelerate development of fusion energy science. Simulation is sufficiently mature that modeling can distinguish between competing concepts. Great strides have been made since the design of ITER leading to improved confidence.

We recognize that simulation is not a replacement for an experiment. Retaining strong partnership between FES and ASCR is needed to benefit from integrated simulation on high performance computers with mutually beneficial results. Exascale is a potential game changer for integrated simulation."

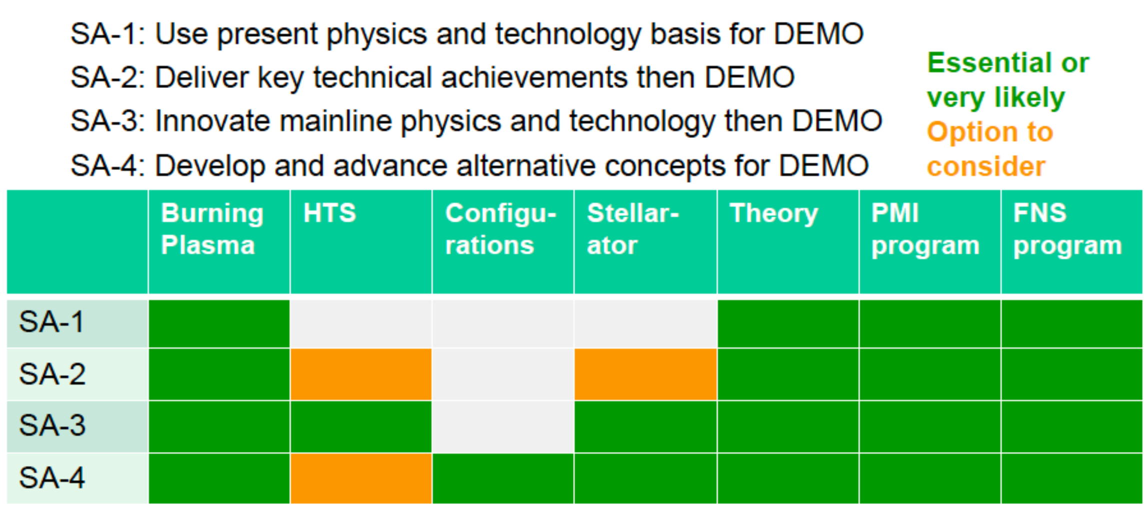

Table: This Table provides the potential mapping of Strategic Elements, listed in the top row, to the four Strategic Approaches (SA 1-4), listed in the first column. Theory and Simulation (represented by Theory in column 6) was considered essential or very likely in both community Workshops at Madison and Austin (see presentations by A. Hubbard and M. Wade at the USMFR website https://sites.google.com/site/usmfrstrategicdirections/home).

What is our 20-year objective?

Our 20-year objective is the development of a validated predictive modeling capability for device design, time-dependent simulation and real time control applications for magnetic confinement devices (including tokamaks, stellarators, and other promising concepts of magnetic confinement) integrating the effects of collision-induced and turbulent transport, large-scale MHD instabilities, energetic particles, plasma-material interactions, heating, and current drive.

Strategies for realizing 20-year objective

The integrated WDM requires a *fidelity hierarchy* of computational models. It is helpful to think of these models as a pyramid structure. The top of this structure is occupied by models, which are at the most detailed level of description (using the language of statistical mechanics), and will require leadership-class computing resources.[4] When physical scales and computational cost justify it, these highest-fidelity simulations may be used to calibrate reduced models that form the successive layers of the hierarchy. Fast, reduced models are used for large dataset validation of the physics basis. The validation process itself requires highly diagnosed experiments relevant to the burning plasma regime that obtain data at multiple levels of space and time, from small to large. The computing infrastructure needed depends on the level of the hierarchy, and can vary from resources that require exascale computing (or beyond) at the top levels of the hierarchy to capacity computing for midsized parallel processing models so that parameter scans and uncertainty quantification can be performed for many subsystem models simulating various aspects of the burning plasma environment. It is important to develop a large (statistically significant) database of simulations at multiple levels of the fidelity hierarchy so that the outcomes of present and planned machines can be predicted and the uncertainty in these predictions quantified. Machine learning can assist both in training reduced models based on the results database and extracting useful features from the larger-scale simulations.

Closing the theory gaps identified in the Bonoli-Curfman report requires a strong and sustained effort in analytical theory. Numerous aspects of burning plasma science are not well understood. These include, but are not limited to, the L-H transition, the coupling of core to pedestal to scrape-off-layer regions, plasma-material interactions for both solid and liquid interfaces, disruptions and their avoidance and mitigation, the nature of three-dimensional equilibrium, and coil configurations that produce magnetic fields with hidden symmetries optimized with respect to stability and transport. In some of these cases, even the appropriate theoretical frameworks are subjects of research and debate. While experiments, both physical and numerical, can provide valuable information, mathematical modeling is needed in many cases to elucidate underlying mechanisms and obtain solutions that cut through mazes of data. In many cases, mathematical models can help provide scaling laws that can be tested by existing databases and extrapolated to regimes that are not yet accessible by actual experiments or numerical computations. In the last couple of decades, plasma theory has reached a level

[4] This requirement is discussed in the Chang-Greenwald Report, DOI 10.2172/1375639.

of maturity whereby we can use advanced computation and analytical theory rather than phenomenological scaling laws to design next-step machines.

Integration Challenges and Opportunities

There are opportunities for theory and simulation to have an impact on all of the elements of an MFE Strategic Roadmap. The process of building a comprehensive WDM capability involves integration of multi-physics couplings in stages. The currently active areas of integration include but are not limited to:

1. Coupling core, edge, and plasma material interactions
2. Power threshold for the H-mode transition
3. Multi-scale gyrokinetic turbulence
4. Heating, fueling and current drive processes
5. Fast particle instabilities and transport
6. Boundary plasma and divertor optimization
7. Stellarator fast ion and thermal confinement optimization
8. Coupling of transport and MHD instabilities
9. Tokamak disruptions and runaway electrons
10. Pellet fueling and disruption mitigation
11. Edge Localized Mode control with external coils
12. Active control of MHD instabilities
13. Material resilience to neutron damage
14. Tritium breeding blankets
15. Impact of high-T_c superconducting magnets on confinement configurations

Not all of these elements need to be included in a particular WDM application but all of them, and more, need to be advanced to a level of verified, predictive accuracy.

Impact of Exascale Computing

The ECP, which is a partnership between the DOE Office of Science (SC) and the National Nuclear Safety Administration (NNSA), relies at the present time entirely on investments by ASCR and the NNSA. The first exascale computing facility is expected in the US in 2021, to be followed by a second in 2023. As we have evolved from the terascale to the petascale, the increasing power of computer hardware, coupled with important advances in software technologies (developed in collaboration with applied mathematicians and computer scientists), has enhanced significantly our ability to include more physics and technology in more complex geometries, moved us further along the path of higher fidelity to experiments and performance of next-step facilities. In particular, fault-tolerant and communication-avoidant schemes are recognized as critical aspects of next-generation high-fidelity codes in the areas of core, edge and multiscale turbulence in tokamaks and stellarators, disruption physics, and plasma-material interactions. Machine-learning strategies are also recognized as innovative tools to leverage the formidable datasets generated by leadership architectures. A validated WDM capability provides the confidence to explore the extreme parameter regimes of fusion reactors, informing decisions and lowering the future risks of building gigawatt-scale fusion power plants, and thus accelerating the fusion program.

Relevance of this White Paper to the Charge to the NAS Committee

The NAS Committee has been tasked to consider the following elements:

- *Ensure that US maintains a leadership role in the Program*

Thanks to the efforts of the US fusion community over the last few decades, and the strong support of FES and ASCR, the US does play a leading role in the world in the area of integrated simulations. The ASCR programs are a model for valuable partnerships with applied mathematicians and computer scientists, access to an evolving and growing base of software technologies and state-of-the-art hardware that is tuned to application development. Such synergisms give the US fusion community a strong edge.

This leadership is further reinforced now through the commitments of the DOE SC to the ECP. The ECP aims to maximize the benefits of high-performance-computing for US competitiveness and scientific discovery, one of the important considerations of the charge to the NAS Panel. We envision significant advances enabled by exascale computing, specifically in the areas core-edge coupled turbulence and transport, disruption physics, plasma-material interactions, and data management analysis and assimilation.

- *The Committee will consider the budget implications of its guidance but will not make recommendations about the budget for burning plasma research itself.*

This paper presents the rationale for developing a WDM capability, and advocates for an effort with the expectation of persistence: a long-term programmatic commitment, and support for community efforts. We consider the partnership between FES and ASCR vital for the objectives of WDM. The ECP, which is at present the largest program in the SC and is administered by ASCR, is a critical source of new resources for the US fusion community.

- *The Committee may take into account how unanticipated events or innovations may necessitate mid-course re-directions.*

This paper addresses a program that is salient to every "Strategic Approach" presently under consideration by the US Magnetic Fusion Community towards DEMO. As such it will contribute to any path the US magnetic fusion program may take towards DEMO. Aligning the program with the highest priorities of SC is a sound strategy in developing a robust program. The simulation program, and its close connections with experiments, may itself be the source of unforeseen innovations in fusion and plasma science. The primary risks in developing an integrated WDM capability as a major strategic element of the US fusion program are those posed by a softening of the support for theory and simulation research in fusion and plasma science at Universities, national laboratories, and industry, and a lack of nurturing of the human talent needed to support integrated WDM development. We refer the reader to a separate paper that articulates the broad importance of theory, computation and predictive modeling in the US Magnetic Fusion Energy Strategic Plan, based on the community input at the Madison and Austin Workshops.[5]

[5] F. Ebrahimi et al., *Importance of theory, computation and predictive modeling in the US Magnetic Fusion Energy Strategic Plan*, submitted to the NAS Committee (2018)

This white paper is endorsed by the following scientists in addition to its authors:

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