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Integrated simulations for fusion research in the 2030's time frame (white paper outline)

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Outline for a white paper to be prepared by the US Fusion Energy Theory Coordinating Committee, for input to the National Academy of Sciences

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This draft outline includes place-holders for more detailed material in italicized text which has been included to make clear what the LLNL group has in mind for the higher-level items.

This outline does not discuss the particulars of the end goal to be recommended in our white paper. We see several possibilities for what we might include:

- recommendation of a unified national project, such as the FSP.

- recommendation of the development a collection of flexible tools that would work with one or more frameworks.

- a paragraph listing some possible strategies, including the two above.

- neither recommendations nor discussion of options (with any specificity apart from exascale capability) along this axis.

We see the white paper as an effort to persuade the NAS to articulate a recommendation in their report that DOE/FES/ASCR establish a Whole Device Modeling program.

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Integrated simulations for fusion research in the 2030's time frame

I. Purpose and goals

1. Statement of purpose: *This white paper presents the rationale for developing a community-wide capability for whole-device modeling, and advocates for an effort with the expectation of persistence: a long-term programmatic commitment, and support for community efforts.*

2. Statement of 2030 goal (two suggestions):

(a) *Robust integrated simulation tools to aid real-time experimental discharges and reactor designs by employing a hierarchy in fidelity of* physics models.

(b) *To produce by the early 2030s a capability for validated, predictive simulation via integration of a suite of physics models from moderate through high fidelity, to understand and plan full plasma discharges, aid in data interpretation, carry out discovery science, and optimize future machine designs. We can achieve this goal via a focused effort to extend current scientific capabilities and rigorously integrate simulations of disparate physics into a comprehensive set of workflows.*

II. Definitions and relationship to earlier work

3. Definition of WDM:

Tools for simulation of a magnetic-fusion device over an entire discharge from startup to ramp-down, and from core through and into walls.

Environments enabling researchers to make deep connections to experiment and theory.

4. Relationship of this WP with the Bonoli/Curfman IS 2015 Workshop Report [1]. *The workshop was charged with identifying the technical state of the art, gaps, opportunities, etc., but not with advising a program plan. Most of the points touched on in this WP can be found elaborated therein.*

III. Importance of an integrated WDM capability

5. Importance of a unified research effort coupling experiments, data analysis, modeling for ongoing experiment guidance, detailed first principles simulations, and analytic theory. *Individual tools are at an increasingly high level of sophistication, but treat only isolated or a few selected aspects of the system; it remains to develop accurate reduced models from these and future tools (see 9. below). The community's current WDM codes integrate many physics components and together have an array of complementary strengths. These include demonstrations of (but not routine use of) coupling techniques for integrating high-fidelity models, e.g., core-edge coupling. As yet there is no WDM code that makes available all the codes' capabilities; and these codes, which have served experimental and design efforts for many decades, are in need of modernization.*

6. Value of integrated, whole-device modeling

Large parameter space, varied magnetic geometries can't all be tested in hardware. Simulation is more cost effective than building machines with sufficient confinement to test new ideas, e.g., exploration and scoping of high-field concepts (Whyte), advanced divertors, ...

Simulations already enable more efficient use of limited machine time; this can be brought to a higher level.

7 . Tasks requiring WDM capability

Design of new machines

Reactor-scale machines*, with their enormous cost, enormous stored energy (vulnerability to damage) and constrained number of shots, will need WDM not only for routine campaign planning: high-fidelity simulations will be required before finalizing shots, to ensure as well as possible that each shot will evolve as planned, and in particular that dangerous operating limits will not be approached.*

Discovery science. *This can happen in a WDM; with multiple consistently interacting high-fidelity models, things can pop up for the first time in WDM simulation. Reactor-scale machines cannot risk exploring novel new ideas, e.g., for burning-plasma experiments, without high-fidelity WDM-scale integrated simulation in advance.*

IV. Characteristics of an effective WDM capability

8. Desirable properties of a WDM: *Due to the large range of timescales in a reactor-scale MFE device, straightforward integration in time of a high-fidelity simulation on transport timescales is infeasible at present and will remain so even with the advent of exascale computing. Fortunately, there are significant scale separations which can be exploited to dramatically speed up computations using multiscale methods. These methods similarly speed up simulation with reduced models, which must be fast enough for wide-ranging exploration of operating points and scenarios, machine design, optimization, experimental analysis, etc. This leads us to adopt the "1.5D" approach (1D transport across 2D magnetic surfaces) employed by today's WDM codes. A partial high-level list of features follows*

Flexibility; support for a heterogeneous, modular approach; preserve and expand upon existing major workflows and frameworks

Hierarchy of physics models

Connection to experimental databases (two-way)

Utilizing the latest computer science developments and computing platforms.

Exploitation of new programming methods, e.g., Machine learning to give WDMs the ability to learn without being explicitly programmed.

Particular major areas to incorporate, not well addressed in present WDM codes: *PMI, slow 3D MHD (3D equilibria, providing capability for stellarator WDM and a WDM capability for simulating magnetic-island growth in tokamaks …)*

Tools for avoidance of large random transient events, such as disruptions and ELMs

V. Role of this effort within the overall program

9. How WDM fits within the overall theory program

This effort is one component, albeit a significant one, of a well-balanced theory program. *Analytic and numerical work should be supported independently of the WDM project. Examples include …*

Validation of component models and of full WDM fidelity

Analytic theory in relation to WDM *(Sovinec WP)*

Development of models for WDM and other applications *(Staebler's and J. Candy's remarks during 10/11 telecon)*

Smaller-scale-integration research *(Bonoli)*: *Development of high-fidelity components requiring some level of integration, for fundamental understanding, for the development of high-fidelity components for eventual coupling to a WDM, and for the basis from which to construct reduced models.*

There are things that WDM (as currently conceived) can't do: *Examples for transport-timescale simulation include: disruptions; 3D global non-linear ideal-MHD instability; stochastic magnetic fields with field lines not remaining in the vicinity of approximate surfaces; chronic avalanches; etc. Reasonable models can be developed for some fast but brief 3D events, such as sawteeth.*

10. US leadership; WDM and the international theory program; value with or w/o ITER *(Amitava)*

Re exascale computing: Note many references to exascale in [1]

Enhance the impact of the fusion research program beyond the fusion community. The integrated simulations program will engage and feed back into the broad scientific community, in fields such as advanced scientific computing, fluid mechanics, astrophysics, material science, and engineering.

VI. Path forward

11. How to get there from here, building on the current state of the art, the Exascale initiative, and the SciDAC initiatives.

1) *Emphasize importance of commitment to a national program*
2) *SciDAC 4 program is developing components for integrations*
3) *Identify current gaps, starting from [1], and update as progress is made, e.g., from SciDAC 4, and new gaps make themselves apparent*

References

[1] https://science.energy.gov/~/media/fes/pdf/workshop-reports/2016/ISFusionWorkshopReport_11-12-2015.pdf