

DOE Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences
Call for Whitepapers - Due by April 16, 2015

<https://www.burningplasma.org/activities/IntegratedSimulations2015>

In preparation for the upcoming DOE Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences, jointly sponsored by the offices of Fusion Energy Sciences (FES) and Advanced Scientific Computing Research (ASCR), the workshop chair Paul Bonoli and co-chair Lois Curfman McInnes invite all members of the FES and ASCR communities to submit whitepapers. The objectives of the whitepapers are to prepare topics for discussion at the workshop and to identify content to include in the workshop report.

The workshop goals are to review recent progress and identify gaps and challenges in fusion theory and computation directly relevant to the topic of disruption prevention, avoidance, and mitigation and that of plasma boundary physics, with whole device modeling as the long-term goal. In addition, the workshop will reassess these challenges and their concomitant opportunities and will adjust or broaden them appropriately by taking into consideration recent progress and using the criteria of urgency, extreme-scale computing benefit, readiness for progress within a ten-year time frame, and world-leading potential.

The workshop is organized into panels that broadly cover three fusion topics (A,B,C) and crosscutting issues in computational mathematics and computer science (D,E,F,G) in the context of integrated simulations for magnetic fusion energy sciences. The scope of each of these panels will build on prior workshop findings (as indicated in the resources listed at the end of this document) and will include recent advances in FES SciDAC Centers and ASCR SciDAC Institutes. Whitepapers should address one or more of the following specific panel topics:

- A. Disruption prevention, avoidance, and mitigation:** gaps and challenges in theory, guidance from experiment, status of simulation capabilities, status of validation and measurement capabilities.
- B. Plasma boundary, including the pedestal, scrape off layer, and plasma-materials interactions:** gaps and challenges in theory, guidance from experiment, status of simulation capabilities, status of validation and measurement capabilities.
- C. Whole device modeling:** software, status of integrated modeling, validation and measurement capabilities, the roles of first-principles models (e.g., requiring extreme-scale computing platforms) and reduced models.

- D. Multiphysics and multiscale coupling:** mathematical formulations (e.g., models, meshing, discretization), algorithms (e.g., solvers and time advancement, coupling between scales and domains), quantitative a posteriori error analysis, verification.
- E. Beyond interpretive simulations:** stochastic inverse problems for parameter determination, sensitivity analysis, uncertainty quantification, optimization, design, control (so-called ‘outer loop’ issues).
- F. Data management, analysis, and assimilation:** integrated data analysis and assimilation that support end-to-end scientific workflows; knowledge discovery methods in multi-modal, high-dimensional data (qualitative and quantitative); integrating data management and knowledge discovery software architectures and systems.
- White papers for this topic should include use cases that define the technology needs. It will be valuable to have use cases that describe an end-to-end problem scenario, complete with as much specific information as possible about science needs and resource utilization (e.g., amount of data moved/processed, over what period of time, lifetime/lifespan of data and data products, types of facilities used like centrally located SC centers or computing collocated with experimental facilities). Also valuable would be clear statements of desired/required analysis and “data mining” objectives with a brief description of the application area.
- G. Software integration and performance:** workflows and code coupling software, performance portability, software productivity and software engineering, governance models for the fusion integrated modeling community.

Instructions: Each whitepaper should indicate if an oral presentation is desired or not, specify a primary panel topic from the list A-G above and optionally secondary and/or crosscutting topics. The subtopics listed for panels A-G are intended for guidance and are not meant to be limiting. In formulating a whitepaper, please consider the following: (a) *motivation*: What specific challenge or opportunity facing the fusion community does the whitepaper address? (b) *approach*: What are the potential approaches to meeting that challenge or opportunity (optional)? and (c) *impact*: What would be the impact on the fusion community by meeting this challenge or opportunity (a positive impact) or not (a negative impact)?

Format and Submission Guidance for Whitepapers:

1. Whitepapers must be submitted in PDF format, maximum of 2 pages, inclusive of all text, tables, and figures. References are not included in the 2-page limit. Use no smaller than 11-point font and at least 1-inch margins. Each file’s size should not exceed 5 MB. There is no limit to the number of whitepapers that an individual or group of co-authors may

submit. Each whitepaper should provide contact information (name, institution, email address) for a single corresponding author.

2. Submit each whitepaper to the email address ISwhitepapers@burningplasma.org. In the subject header of the email, please specify the primary panel topic of the whitepaper (A-G listed above). Please send a separate email for each whitepaper submission rather than bundling multiple whitepapers in one email.
3. Whitepapers will be accepted through April 16, 2015.
4. Oral presentations will be given via teleconference on May 18-19, 2015 for those whitepaper submissions requesting orals. We will try to accommodate all requests for oral presentations but may have to limit speakers depending on final numbers.

All whitepapers received will be posted or linked, for public viewing, on the workshop website. This website is hosted by the US Burning Plasma Organization, a national organization of scientists involved in burning plasma research that is often used by the fusion community to collect and archive relevant material. Whitepapers will feed into the draft workshop report and will be used to help organize workshop discussions.

Resource Documents: This workshop will build on prior workshop findings as indicated in the following resource documents:

2014 FESAC Strategic Planning Panel: report, whitepapers, references:

<https://www.burningplasma.org/activities/?article=2014%20FESAC%20Strategic%20Planning%20Panel>

2011 FSP Planning Study:

Report: http://w3.pppl.gov/fsp/FSP_Summary_FILES/FSP_Program_Execution_Plan.pdf

General information: <http://w3.pppl.gov/fsp/Overview.html>

FSP Validation wiki: http://www.psfc.mit.edu/FSP-Validation/index.php/Main_Page

2011 FSP Project Definition Workshop: https://ice.txcorp.com/trac/2011_FspDefinitionWorkshop

FSP Science Drivers wiki:

http://fspscidri.sites.lehigh.edu/index.php?title=Main_Page#Integrated_Science_Application_Plans

2010 Report on the Workshop on Scientific Grand Challenges: Crosscutting Technologies for Computing at the Exascale:

http://science.energy.gov/%7E/media/ascr/pdf/program-documents/docs/Crosscutting_grand_challenges.pdf

2009 Report on Fusion Energy Sciences and the Role of Computing at the Extreme Scale (part of an ASCR-led workshop series):

http://science.energy.gov/~media/fes/pdf/workshop-reports/FES_Grand_Challenges_Report_final.pdf

2009 FES Research Needs Workshop (while simulations were just a part of this workshop, the report provides a good overview of magnetic fusion challenges): report, whitepapers, references:

<https://www.burningplasma.org/web/renew.html>

2007 FSP Workshop Report:

http://science.energy.gov/~media/fes/pdf/workshop-reports/Fsp_workshop_report_may_2007.pdf

2014 Workshop on Software Productivity for Extreme-scale Science: report, whitepapers, references:

<http://www.ornl.gov/swproductivity2014/>

2013 Workshop on Applied Mathematics Research for Exascale Computing: report, whitepapers, references:

<https://collab.mcs.anl.gov/display/examath/Exascale+Mathematics+Home>

2013 ASCAC Data Subcommittee Report on Synergistic Challenges in Data-Intensive Science and Computing:

http://science.energy.gov/~media/ascr/ascac/pdf/reports/2013/ASCAC_Data_Intensive_Computing_report_final.pdf

2012 Report on the Workshop on Extreme-Scale Solvers: Transitions to Future Architectures:

<http://science.energy.gov/~media/ascr/pdf/program-documents/docs/reportExtremeScaleSolvers2012.pdf>