Progress and Plans for Experimental Validation

by
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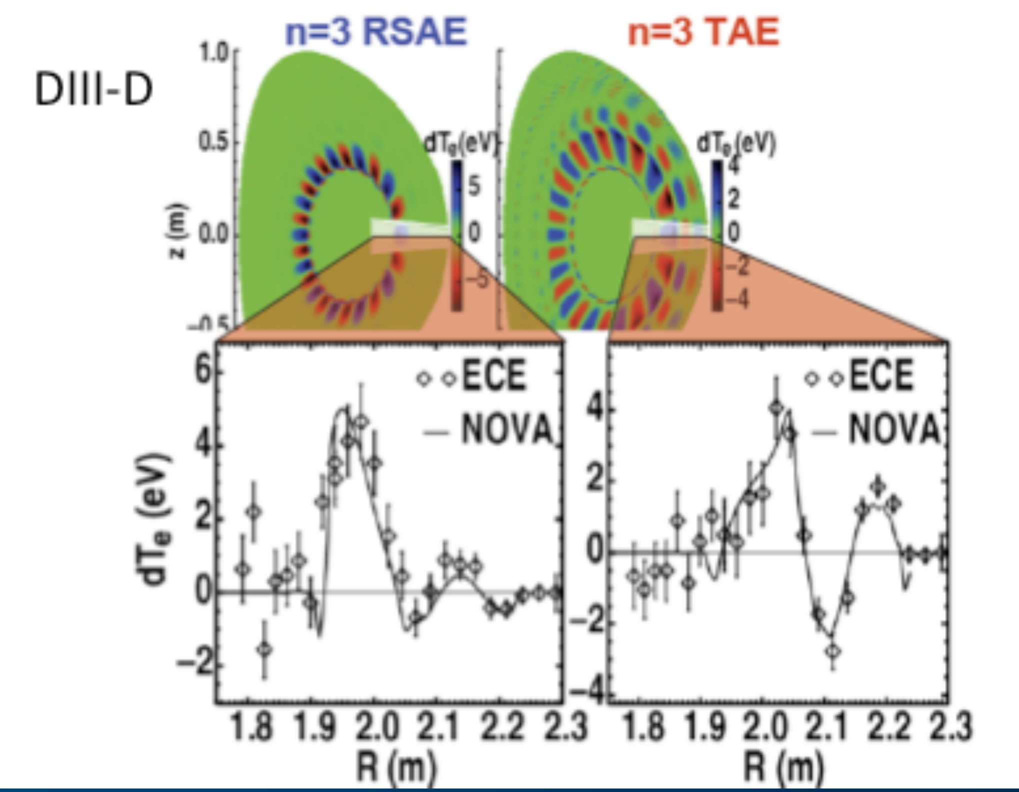
for FSP Validation Team



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PPPL

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FSP Experimental Validation: Mission

The mission of the FSP validation effort is to assess and improve physical and computation models by systematic, quantitative comparisons with experimental measurements.

Requirements for planning phase: A well-defined WBS, schedule and milestones leading to the following deliverables

- **"Best practices" guidelines**
- **Modes of collaboration with experimental groups**
- **Prioritized list of critical elements in scientific models for validation**
- **Strategy for data management and documentation**

WBS, Schedule and Milestones Developed for the Five Major Validation Tasks in Planning Phase

1. **Outreach: understand current practices in MFE and best practices in the wider scientific computing community**
2. **Gap analysis: identify critical missing elements, a strategy and resources to fill these gaps**
3. **Development of a best practices guide: including role of dedicated analysts**
4. **Definition of the mechanisms for coordination with experimental groups**
5. **Establishment of the requirements for data management and documentation**

Schedule and Progress in Outreach and Coordination

Q4 CY 2009: Gather outreach materials and identify contacts

1. Completed initial population of validation wiki site: www.psfc.mit.edu/FSP-Validation/
2. Prepared generic presentation material for fusion and non-fusion visits
3. Generated lists of fusion and non-fusion institutions to contact
4. Prepared website for community feedback

Q1 CY2010: Contact institutions

1. Scheduled
2. Carry out contacts (in progress)

Q2 CY2010: Summarize

1. Write report for each contact, web accessible (in progress)
2. Analyze and prioritize issues
3. Document high priority issues

A Wiki Site has Been Set Up to Facilitate Two-Way Communication

FSP-Validation

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

FSP-Validation | FSP-Validation | ReNeW Workshop :: USBPO | fspplan | Fusion Facili...el Directory | Linkup2.net...ss Numbers | TMobile Wireless | access2 | Apple | Amazon | .Mac

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Main Page

Fusion Simulation Program: Validation

The goal of the Fusion Simulation Program (FSP) is to enable scientific discovery of important new plasma phenomena with associated understanding that emerges only upon integration. This requires developing a predictive integrated simulation capability for magnetically-confined fusion plasmas that are properly validated against experiments in regimes relevant for producing practical fusion energy. This capability is needed to maximize exploitation of fusion experiments, especially ITER, and to establish the scientific basis for an economically and environmentally attractive source of energy. More details can be found at the main FSP site: http://www.pppl.gov/fsp. Wikis on other topics are available for Science Drivers, Frameworks and Components.

The mission of the FSP validation effort is to assess and improve physical and computational models by systematic, quantitative comparisons with experimental measurements.

Meeting this mission will require:

- An outreach to MFE and other scientific communities to develop a set of "best practices" and analytic techniques for carrying out validation of complex scientific codes.
- Strong interaction with experimental groups to define appropriate modes of collaboration, sharing of intellectual property and joint planning.
- A strategy for "documentation", which creates a single, universal view into all FSP data related to validation.
- Collaboration with theorists and computationalists to ensure that the validation focuses on critical elements in the models and that the results of validation are effectively used to guide development.

Contents

Work Plan: The outline and any drafts of the detailed work plan we are developing.

Outreach: Current best practices for validation, plus information on community feedback.

Additional resources

Outreach Discussions Targeted a Broad Range of Scientists Interested in Validation

- U. of Wisconsin, Madison: theorists, experimentalists
- PSFC-MIT: theorists, experimentalists, computer scientists (over 20)
- DIII-D: theorists, modelers, experimentalists (over 50)
- Joint US-Japan Workshop on Integrated Modeling and Simulation: computational scientists
- U. of Maryland: theorists, small experiments
- LLNL and LANL: ASCI and DOD program discussions
- FSP Workshop: Boulder, CO (over 50)

Sample Feedback on FSP in General

- What are the FSP near-term deliverables?

- How will FSP balance between a strong emphasis on high performance computing and support of experiments?

- Will FSP support small experiments?

- Large facilities utilize many experimental modeling tools, how will FSP include these?

- Concern about scaling up from current small development groups (with the past history of success)

- Maintain flexibility in framework

Sample Feedback on FSP Validation

- What is the appropriate management structure for FSP validation to be successful?

- Will funding be available to experimental facilities to support these FSP validation efforts?

- How can FSP provide incentive to engage a broad community in order to accomplish its mission? How is the career path of the analysts maintained?

- Need for overall transparency in V&V including sharing of source code, detailed results, etc.

- Strong interests in data storage, access, systemization, ease of use and documentation

Schedule and Progress in Gap Analysis

Q2 CY 2010: Document present practices in validating and multi-physics components

1. Prepare a representative description of physics component validation currently being practiced (in progress)

Q3 CY2010: Identify the strengths and weaknesses of present practices

1. Analyze strengths and weaknesses of present practices
2. Propose strategy to address critical issues and resource requirements
3. Propose future direction for validation
4. Prototyping

Q2 CY2010: Report finding and gather feedback from community

1. Revise gap analysis
2. Assess prototyping

List of Archived Current Practices is Growing

1 Existing validation efforts: Core Transport

- 1.1 Comparison of GYRO synthetic diagnostic results with DIII-D BES and CER data
- 1.2 Comparison of GYRO synthetic diagnostic results with C-Mod PCI data
- 1.3 Comparison of integrated simulation profile results with tokamak data

2 Existing validation efforts: Macroscopic Phenomena

- 2.1 Comparison of NIMROD simulations with DIII-D data for a major plasma disruption
- 2.2 Computed sawtooth oscillation periods compared with tokamak data
- 2.3 Status of Global Ideal MHD

3 Existing validation efforts: Heating and Current Drive

- 3.1 Validation of RF Theory and Simulation Codes in the Lower Hybrid and Ion Cyclotron Range
- 3.2 Validation of ECH Heating and Current Drive

4 Existing validation efforts: Pedestal Physics

- 4.1 Validation of the Peeling-Ballooning Model of ELMs
- 4.2 Development and validation of H-mode pedestal models

5 Existing validation efforts: Plasma-Wall Physics

6 Community Feedback: Suggestions and Proposals

Schedule and Progress for Best Practices Guide

Q4 CY 2009: Identify fields where predictive modeling has made an impact

1. Prepared a clear set of four or five application domains, with a high level understanding of the associated modes and codes which have been used to provide predictions

Q1 CY2010: Document the processes, procedures and outcomes of the predictive modeling efforts in these application domains

1. Domain areas documented: Reliability engineering and system safety, CFD, aerospace, astronautics and aeronautics (in progress)

Q2 CY2010: Carry out interviews with practitioners and incorporate insights

1. Chris Hill, Cecilia DeLuca (ESMF), Reagan Moore (Data Intensive Cyber Environment), ASCI centers (in progress)

Science and Best Practices in V&V- Tech Transfer from LLNL to FSP

- Uncertainty quantification (UQ) is an example of a “best practice” methodology used in the ASCI program. UQ provides a rigorous mathematical basis and specific methodologies for efficiently determining parameter dependences and analyzing error propagation in complex, multi-dimensional parameter spaces encountered in multi-physics simulations and experiments

- UQ gives guidance in a systematic way as to the most important parameter dependences and what modeling needs to target to resolve discrepancies with experimental data

- UQ is a maturing science and is a significant enterprise at LLNL
  - UQ is being applied in projects in the weapons program, ASCI, engineering, climate modeling, NIF, etc.
  - UQ is applied in both experiments, simulation, and verification/validation of theory and simulation against experiment
  - There is an LLNL LDRD Strategic Initiative in UQ with a diverse team from weapons, engineering, life sciences, applied math & comp.

- FSP effort at LLNL is consulting the LLNL UQ team to include advanced UQ strategies and other relevant ASCI best practices in the design of the verification and validation procedures and tools for the FSP

Schedule and Progress in Coordination with Experimental Groups

Q2 CY 2010: Describe proposed methods to jointly plan, manage and staff validation activities

1. Written plan jointly agreed by FSP management team and major experimental facilities (in progress)
2. Agree upon set of rules for sharing data, codes, publications and IP

Q3 CY2010: Approach for providing and supporting new simulation tools for experimental groups

1. Written description of FSP approach

Q4 CY2010: Method for effective joint planning

1. Written plan describing agreed-on approach for meshing FSP and experimental planning processes

A Collaboration with Major Facilities Document Has Been Drafted

The document outlines:

1. General principles for collaboration and IP sharing with major experimental facilities
2. Interactions with facilities on planning
3. Roles for the FSP and the experimental team
4. Lessons learned from experimental facilities for FSP in terms of organizing its own research effort

- Ideas drawn from existing collaboration agreement used by the three major facilities, and their governing and planning processes
- Draft reviewed by project managers, who are in general agreement. Detailed comments to be incorporated in next draft

Progress on Defining Roles and Responsibilities of Analysts

- **Draft set of principles outlining analyst roles, responsibilities, workflow and support mechanisms completed and circulated within FSP validation group**
  - Centered on science driver specific test cases
    - benchmark fidelity of existing FSP components and frameworks,
    - identify gaps which necessitate new research
  - Tests cases
    - based on typical predictive and interpretive modeling use cases
    - utilize measurements from a variety of experiments and operating conditions
    - assess model fidelity via suites of collaboratively designed metrics

- **FSP validation analysts are charged with**
  - Partnering with experimentalists, modelers, and theorists to identify, conduct, publicly document, and refine validation test case studies
  - Working with modelers and theorists (including those not supported by FSP) to test new and improved models/theories against current FSP capabilities

- **Propose separate class of production analysts responsible for supporting general predictive and interpretive FSP modeling activities**

Schedule and Progress in Documentation and Data Management

Q4 CY 2009: Outreach and coordination with rest of FSP

1. Assessment of needs based on contacts inside and outside of community (in progress)
2. Agreement on scope and strategy (in progress)

Q1 CY2010: Define functional and non-functional requirements and evaluate approaches

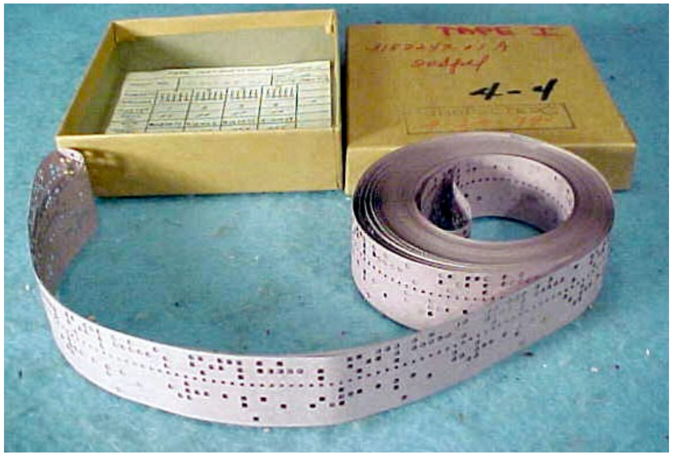
1. Drafted scope for FSP integrated data management

Q2-4 CY2010: Prototype and evaluate

1. Design/assemble/document "first best guess"
2. Test/evaluate using actual validation exercise
3. Assessment and recommendations

Integrated Data Management

Summary



Presented at FSP Workshop

3/17/2009 Boulder, Co.

M. Greenwald

Nature of FSP Drives Requirements

- **Multiple customers (developers, verifiers, validators, other users)**
  - Users have very different use-cases for data
- **Larger collaboration, longer duration**
  - Heterogeneous developer/user base drives requirement for consistent representation of all relevant physics and geometry, ease of use, etc.
- **Large, heterogeneous data sets, variety of sources, data types.**
  - Data from a wide range of codes, experiments, verification and validation activities, etc.
  - Wide array of applications which produce and/or consume data
    - Avoid n^2 problem
  - Need to create and present consistent, coherent data sets
  - Support/adapt for technology evolution

Vision for FSP Integrated Data Management

- **Scope includes all data produced or used by FSP activities (run preparation, simulation output, verification, validation)**
- **Does not include I/O carried out during high performance computing**
- **Support creation of unified, coherent, global data collections**
  - That is, we're not just talking about structured data within a file but a large collection of related information
- **Store everything that will be needed**
  - Build on strong abstractions and structures
  - It's all data (don't make unnecessary distinctions)
- **Maintain ease of use/access for non-specialists**
  - Name it and get it - wherever it is, whatever the source
  - On a project this large, we're all non-specialists
- **Ensure data retains its meaning over time**
  - Provide adequate self-description, metadata

Approach to Integrated Data Management

- **Global view supported by a global data catalog (metadata catalog)**
  - Entries for each FSP activity - simulations, verification exercises, experimental data used for inputs or for validation
  - Catalog contains everything about where the data came from (provenance), all data description and any information that would be useful for searching and browsing
  - Support standard logbook functions for human input
  - Anything that can be stored automatically should be
- **Bulk archive for long-term storage of "large" and "small" data**
  - Collection of data objects
  - All I/O through Universal Access Layer (UAL)
  - Data access by "name" so need naming service/data dictionary

Next Steps For Integrated Data Management

- **Draft workshop report, circulate and finalize.**
- **Begin draft of Integrated Data Management Report.**
  - Describe requirements and approaches
  - Identify major challenges
- **Gather candidate solutions, develop conceptual design.**
- **Assess and decide.**
- **Prototype, analyze and report as appropriate.**

Validation Planning Phase Deliverables

Q2 CY 2010:

1. Best practice document first draft (in progress)
2. Data management and requirement plan – draft completed

Q4 CY2010:

1. Validation plan
2. Experiment coordination plan

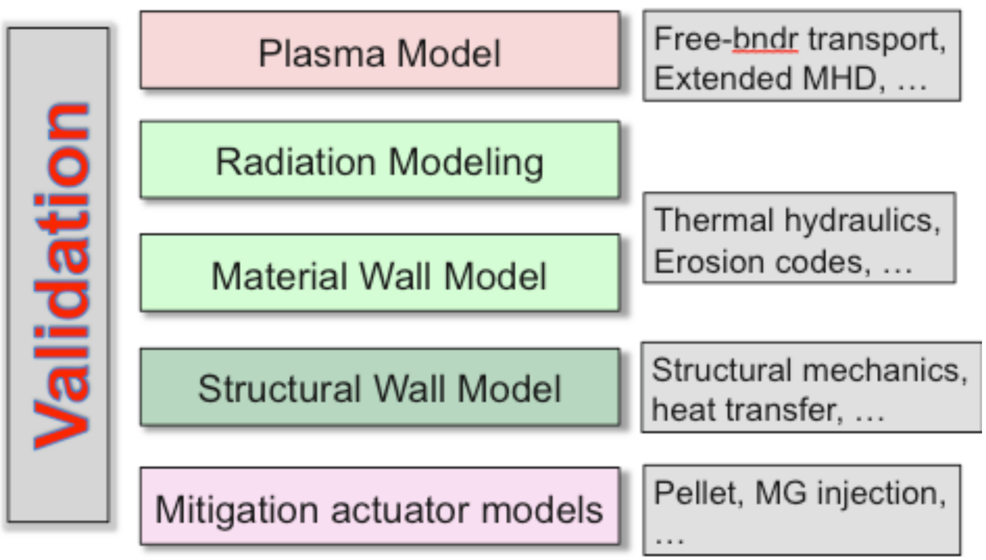
Q1 CY2011:

1. Submit final report

Strong Coordination with Other FSP Activities Needed to Develop Implementation Plan

Example: Disruption Validation

Needed elements of disruption modeling



Validation of initial phase of disruption is doable now- more systematic study of ideal MHD and VDE induced disruptions

Challenges:

- **Runaway electron modeling –** no computational model for coupling FP solutions with MHD self-consistently
- **Codes currently have difficulties solving through thermal and current quench –** need to work with reduced models
- **What level of fidelity is required for validating radiation model, material wall model, etc.?**

Summary

- Since the last PAC review, a validation WBS, schedule and milestones have been developed

- We are on schedule in meeting the intermediate milestones including extensive outreach activities

- Significant work ahead in gap analysis and developing implementation plan

- Continuing dialogue with the community will be needed to deliver the final report