FSP: Validation Program Planning

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FSP Program Advisory Committee

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FSP Validation: Mission

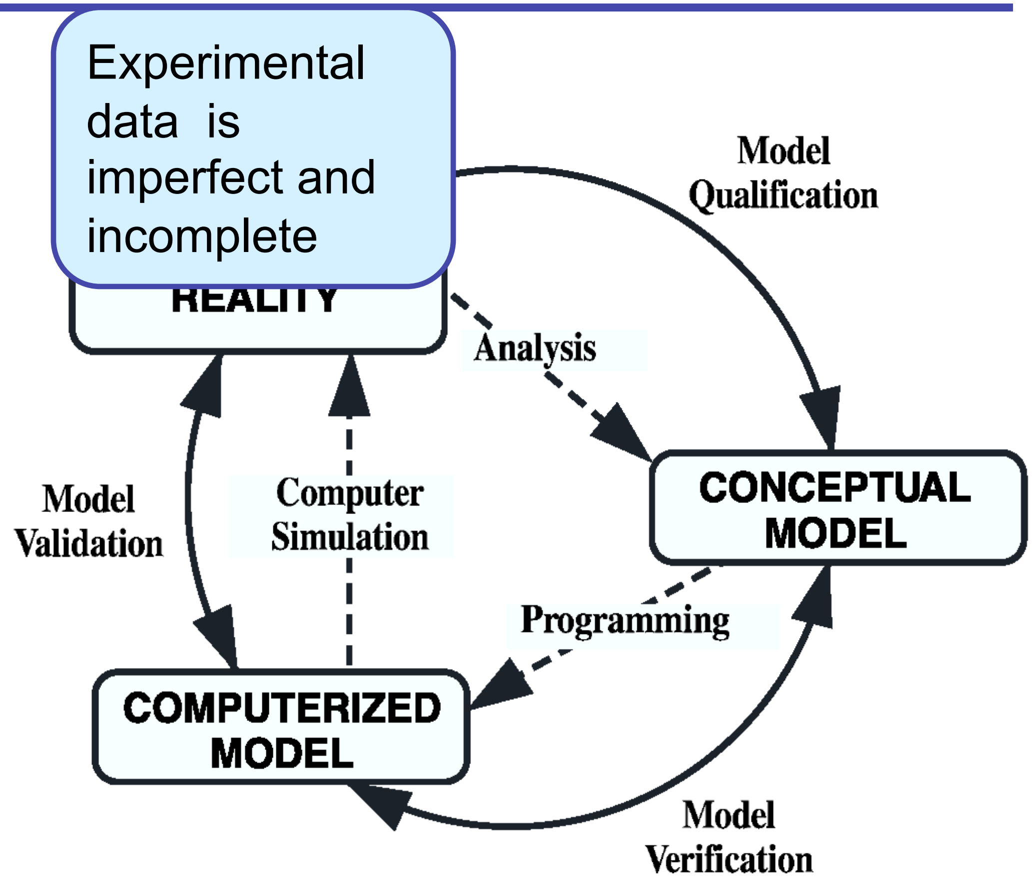
The mission of the FSP validation effort is to assess and improve physical and computational models by systematic, quantitative comparisons with experimental measurements:

Meeting this mission will require:

- Developing and implementing a set of “best practices” and analytic techniques for carrying out validation of complex scientific codes through outreach to the MFE and other scientific communities.
- 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 clear and unified 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 of those models.

Verification and Validation Will Be Critical Elements of the FSP

- Verification is an essentially mathematical process meant to test whether the computational model accurately represents the physical (conceptual) model
- Validation is a physical process which seeks to build confidence in the underlying physical model via detailed comparison between simulations and experiments



Schlesinger 1979

Together V&V seek to build confidence in the **utility** of the models they test.

Outline

- Overview on planning
- Details of tasks and deliverables
- Discussion of risks
- Notes on coordination within FSP

First Step: A Plan for a Plan

The current effort is focused on developing a detailed work plan **for the program definition phase**. We need to:

- Refine our concept of what needs to be done
- Enumerate a concrete set of tasks and deliverables
  - Who does which tasks?
  - How will they be carried out?
  - Estimate resource requirements (for FSP definition phase)
- Define a preliminary schedule

Status: Currently this detailed work plan is about 70-80% complete, including a first draft of quarter by quarter schedule of tasks and deliverables

Major Planning Tasks

Our work plan for the program development phase contains 5 basic elements:

1. Outreach: understand the needs of our project, current practices in the MFE community and best practices in the wider scientific computing community.
2. A gap analysis: identify critical missing elements requiring development or prototyping, a strategy and an estimate of resources required to fill these gaps.
3. Development of a best practices guide for validation including details on tasks and roles, especially the role of dedicated analysts.
4. Definition of the mechanisms for coordination with experimental groups.
5. Development of requirements and a prototype for validation documentation.

For each, we'll now describe the issues, subtasks and proposed deliverables

Outreach and Coordination: Issues

- We need to get input from inside and outside the MFE community to help plan the FSP validation program
  - Document best practices and lessons learned
  - Determine best modes for collaboration and coordination for a well functioning FSP validation program
  - How to support validation work carried out external to FSP
  - Assess community views of priorities – critical physics tests and methodologies
  - Identify critical gaps in tools or methodologies
  - Gather requirements and other feedback from community
- This task also requires that we inform and educate these communities about the goals and approach of the FSP

Outreach and Coordination : Subtasks

- Define set of issues and questions for discussion
  - Based on issues outlined on previous slide
  - Refined as we go
- Identify target communities and individuals
  - MFE
  - Climate
  - Combustion
  - ASC
  - Others?
- Identify best modes for communication and community feedback for each
  - Face to face meetings, telephone
  - Web forums and wiki
  - Literature searches
- Carry out, analyze and document outreach

Outreach and Coordination : Deliverables

- Prepare set of standard materials and presentations
  - One for fusion one for outside
  - Populate content on web sites
  - Include a web-based tool for feedback
- Schedule and carry out forums/discussions
- Analyze the data acquired
  - Priorities
  - Lessons learned
  - Requirements
  - Feedback on FSP and validation
- Document

Gap Analysis: Issues

- Can we identify critical gaps in methods or capabilities
- We're already thinking about:
  - Post-processing and visualization tools
  - Analysis and synthetic diagnostics and other software requirements
  - Statistical techniques, quantification of errors and uncertainties
  - Validation metrics
  - Experimental capabilities
  - Measurement capabilities
  - Dedicated analysts

Gap Analysis : Subtasks and Deliverables

- Analyze current practices for validation of physics components, including software infrastructure needs, statistical methods, uncertainty and error analysis
- Analyze practices for integrated multi-physics codes
  - What new problems do these present?
- Document the strengths and weaknesses of current practices
- Identify major gaps in methods or tools
- Propose approach for filling gaps
  - Developments carried out by FSP
  - Prototyping during program definition phase
  - Developments encouraged by FSP
- Estimate of resources requires

Best Practices: Issues

- "Validation" in the sense of comparisons between codes and experiments has long been part of our program
  - Most of this work is "opportunistic" and "bottoms up"
- In the future, what will be required, is a **more systematic, more quantitative, rigorous and better documented** approach
- We want to identify the best practices from work in our own field and other related fields
  - Identify methodologies, tasks and roles
  - Explore the role of dedicated analysts
  - Define means for coordination and management
- We need to document these practices in a living document that will serve as a guide across the entire FSP project.

Best Practices: Issues (2)

Elements that we expect to include:

- Roles and responsibilities
- Design of validation experiments – principles and practice
- Hierarchy of experimental tests
  - Complexity and coupling of physical systems (validation hierarchy)
  - Measurements (primacy hierarchy)
- Approach for assessing sensitivity, uniqueness
- Documentation of code predictions
- Measurement and documentation requirements for experiments
- Quantification of errors and uncertainties
- Quantification of comparisons - Metrics
- Documentation of methodologies and results

Best Practices : Subtasks and Deliverables

- Identify and document the best of current practices in our own and related fields
  - In particular, look for application domains where predictive modeling has had a major impact
  - Note extensive literature already exists
  - Take advantage of contacts made and data gathered during outreach
- Document processes, procedures and outcomes of these application domains
- Distill essential elements and prepare draft for best practices document
- Iterate with communities of interest

Coordination With Experimental Groups: Issues

- How to carry out joint planning?
  - Short-term – related to specific validation exercises
  - Long-term – plans for machine upgrades and diagnostics
    - How are FSP needs prioritized and communicated?
    - How are experimental capabilities identified and exploited?
- How to marshal resources and execute these plans?
- How to share intellectual property?
  - Experimental data, codes, etc
  - Rules for presentations, publications
- Approach for sharing and supporting new simulations tools for use by experimental groups?
- We've established contact with all the major facilities and some of the smaller ones

Coordination With Experiments : Subtasks and Deliverables

- Propose, agree and document methods for effective joint planning, including:
  - Collection and prioritization of FSP needs
  - Interaction with experimental run planning (existing processes quite mature and effective)
  - Input into long range planning (could interactions with ITPA be a model?)
- Describe proposed methods to jointly manage and staff validation activities
  - Particular concern is support for dedicated analysts – who need to be tightly coupled to experiment and code groups
- Define, agree and document rules and procedures for sharing intellectual property
  - Current rules on major devices are likely close to what is required
- Describe FSP approach for providing and supporting new simulation tools for experimental groups

Documentation: Issues

- Validation poses, perhaps, the greatest challenge for FSP documentation
  - distributed, collaborative effort - multiple experiments, analysts, code developers, computer systems
  - heterogeneous, probably distributed data
  - Inputs, complex methods and processes need to be well documented
  - results need to be clearly represented
- Goal: Create a simple, unified "view" into all FSP data
  - Link code inputs, runs, outputs, comments, experimental data, validation analysis, presentations, publications, etc
  - Well characterized, data structures
  - Well defined namespace
  - Single, simple API (IMHO - service oriented via "URI“)
  - Searchable, browsable (usable)

Documentation : Subtasks

- Outreach
  - Assess user needs based on outreach to fusion researchers and related communities
- Coordination with rest of FSP
  - Documentation strategy shared by entire FSP (!)
- Define functional and non-functional requirements
- Explore various approaches
- Prototype and evaluate
- Define standards
- Define access rules and implementation strategy - in coordination (inside and outside FSP)

Documentation : Deliverables

- Outreach - written report on user requirements
- Coordination with rest of FSP
  - assessment of common requirements
  - agreement on scope and strategy
- Define functional and non-functional requirements – written report
- Assessment of approaches currently in use within MFE program and by analogous outside groups
- Prototype and evaluate
  - design/assemble/document "best first guess"
  - test/evaluate using actual validation exercise
  - assessment and recommendations
- Written set of proposed rules for data access and IP sharing, for review by FSP management team and potential collaborators

Looking Ahead: V&V Related “Risks” for FSP

- V&V for integrated models
  - Are there mathematically tractable solution in any limit?
  - How to disentangle physical effects?
- Error quantification for computation models
- Diagnostic capabilities
  - Spatial coverage
  - Measurement of all important quantities (e.g. Ti fluctuations)
  - Measurement uncertainties
- Difficulty of recruiting, training and supporting dedicated analysts
- Difficulty in prioritizing tasks for V&V and influencing long-range plans for experiments (Consider the difficulty of adding turbulence diagnostics to ITER)

Need To Embody V & V Planning Within FSP

- As FSP plan solidifies, map out research needs and directions in detail
- Ask some important questions
  - How will model predictions be used?
  - Which applications?
  - What are the impacts of predictions? of errors in predictions?
- Define requirements for validation
  - When are models "ready"?
  - Which are the critical elements of each model? – **priorities for testing**
  - What are the experimental and diagnostic requirements?

Coordination with Code Groups Within FSP Will Be Essential

- Identify critical physics for testing
  - Validation requirements at various “levels” of physics integration
  - Define validation experiments and measurements required
- Coordinate with verification efforts
  - make sure this has sufficient priority and is carried out in timely manner
- Feed back into development process
  - Validation results should guide code development
  - Ensure adequate computational resources for verification and validation
- Common infrastructure
  - Standards!
  - Documentation – approach, schema
  - Data structures, API
  - Plans for post-processors, analysis tools, visualization tools and synthetic diagnostics

End