FESAC (FSP) PANEL FINAL REPORT: FINDINGS & RECOMMENDATIONS

FUSION ENERGY SCIENCE ADVISORY COMMITTEE (FESAC) MEETING

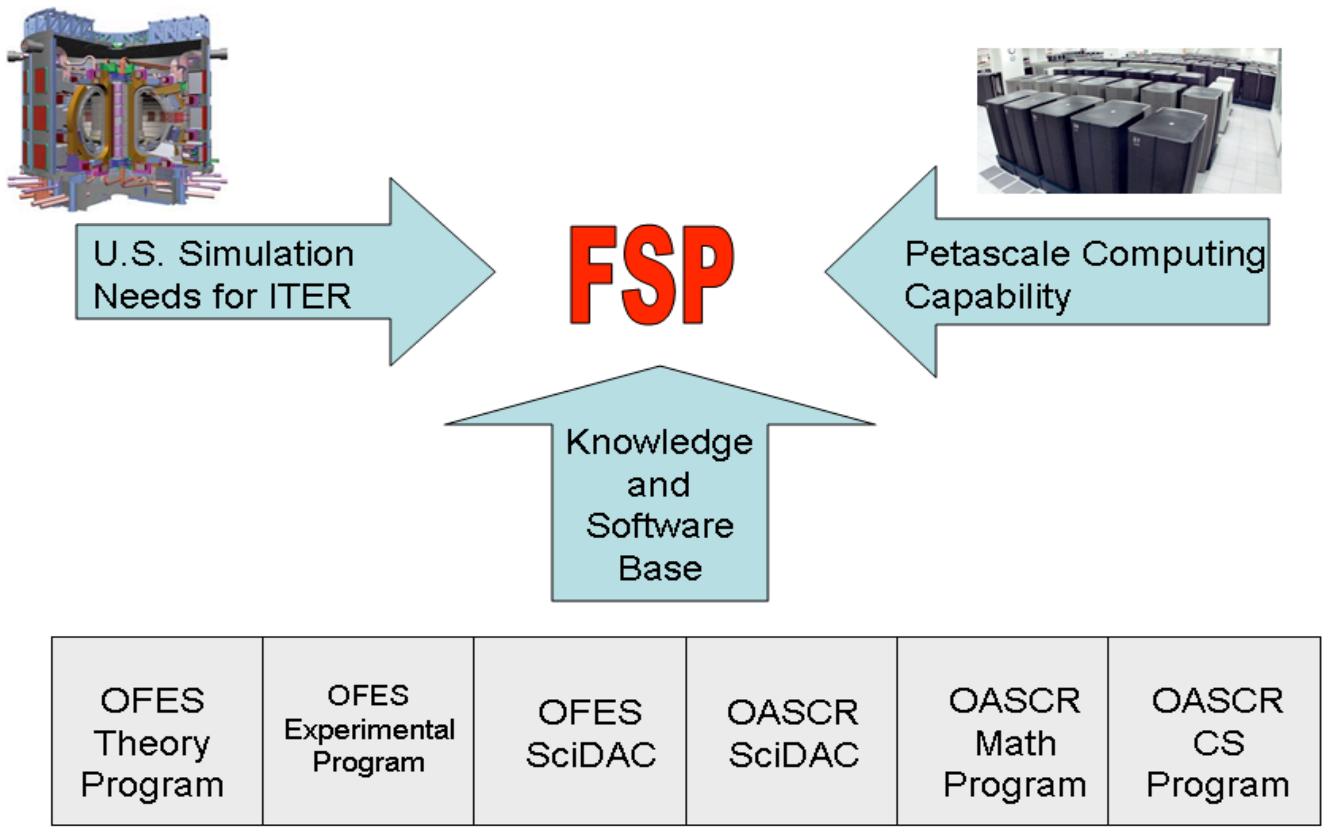
W. M. TANG
Princeton University

Gaithersburg, Maryland

23-24 October 2007

Unique Opportunity for US Leadership

- **Critical need for reliable predictive simulation capability for *ITER & DEMO***
- **Leadership Class Facilities moving rapidly toward petascale computing &beyond**
- **Knowledge and software assembled under truly interdisciplinary SciDAC Program & the OFES and OASCR base research programs**



SciDAC Goal: Creation of 21st Century Computing Infrastructure built on "real" interdisciplinary collaborations

- ***Codes:*** new scientific domain applications codes capable of taking full advantage of Leadership Class Facilities (LCF's) at the terascale, petascale, & beyond
- ***Software Tools:*** new mathematical algorithms & solvers together with advanced systems operations capabilities needed to achieve maximum efficiency on High-Performance Computing (HPC) platforms
- ***Data Analysis & Management Methods:*** new data analysis methodologies with advanced visualization for knowledge extraction and management of unprecedented growth in huge data sets from experiments and simulations
- ***Networks:*** new networking technologies & collaboration tools needed to link geographically separated researchers

FSP Charge Questions

Ref. FSP Workshop Report -- http://www.lehigh.edu/~infusion/FSP_report.pdf

- **Has the report identified key scientific issues and grand challenges that can be addressed by this approach to linking the scientific knowledge base for fusion energy?**

- **Have all the critical technical challenges been identified for which predictive integrated simulation modeling has a unique potential for providing answers in a timely fashion, in a way that traditional theory or experiment by themselves cannot?**

- **Is there a clear plan to establish the fidelity of the advanced physics modules, including a sound plan for validation and verification?**

- **Does the FSP Workshop clearly identify the critical areas of computational science and infrastructure in which investments would likely produce the tools required for the FSP to achieve its goals?**

- **Have the issues associated with project structure and management of the proposed FSP been properly addressed?**

FESAC FSP SUBCOMMITTEE

* **William Tang (PPPL and Princeton U.) Chair**: Chief Scientist, Princeton Plasma Physics Laboratory (PPPL) and Associate Director for Princeton Institute for Computational Science and Engineering at Princeton University

* **Riccardo Betti (U. Rochester)**: Professor of Mechanical Engineering & Physics at U. Rochester; *Member of FESAC*

* **Jeffrey Brooks (ANL)**: Senior Computational Nuclear Engineer at ANL; *Dr. Brooks is an expert on first-wall plasma boundary material science issues*

* **Vincent Chan (GA)**: Director of Theory and Computational Science at General Atomics; *Member of FESAC*

* **Thom Dunning (U. Illinois)**: Distinguished Professor of Computational Chemistry & Director of NSF's NCSA (National Center for Supercomputing Applications); *Prof. Dunning was the first Director of DOE's SciDAC Program*

FESAC FSP SUBCOMMITTEE

* **Charles Greenfield (GA)**: Deputy Director of Experimental Science Division at General Atomics; *Dr. Greenfield is Deputy Director of the national Burning Plasma Organization (BPO) with focus on ITER-relevant physics issues*

* **Brian Gross (GFDL)**: Deputy Director and Head of Computing at the Geophysical Fluid Dynamics Laboratory -- NOAA's National Laboratory for Climate Modelling

* **Michael Norman (UCSD)**: Professor of Physics and Center for Astrophysics & Space Sciences; *Prof. Norman is a world-renowned computational astrophysicist*

* **Miklos Porkolab (MIT)**: Professor of Physics and Director of Plasma Science & Fusion Center (PSFC) at MIT

* **Rick Stevens (U. Chicago & Argonne National Lab)**: Professor of Computer Science at U. Chicago and Associate Director for Computational and Life Sciences at Argonne National Laboratory; *Prof. Stevens is a member of DOE's Advanced Scientific Computing Advisory Committee (ASCAC)*

<u>TIMELINE of ACTIVITIES for FESAC FSP SUBCOMMITTEE</u>

- **MAY 16, 17 -- FSP Workshop -- Prospective FESAC Subcommittee members invited to attend as observers -- first meeting of this panel during Workshop**

- **JUNE 7, 8 -- Briefing on FSP Workshop to Plasma Science Advanced Computing Institute (PSACI) by A. Kritz -- significant numbr of prospective FESAC FSP Subcommittee members in attendance**

- **JUNE 8 -- Final Version of FSP Charge Letter to FESAC released & Full Membership of FESAC FSP Subcommittee announced the following week (June 15, '07)**

- **JULY 3 -- FSP Workshop Final Report distributed to FESAC FSP Subcommittee**

- **JULY 16 -- FESAC Meeting -- FESAC FSP Subcommittee Chair makes presentation on:** ***Discussion of Charge and Plans for FSP (<u>including delivery date of Final Report on October 19</u>***

- **JULY 23 through OCTOBER 12 -- Series of FESAC FSP Subcommittee Teleconferences**
-- Responsibility for development of written response to Charge Questions distributed among panel members with leads for each of the 5 questions assigned
-- Series of <u>8 full-panel Teleconferences</u> held over this time-frame (supplemented by significant number of additional discussions involving sub-sets of the panel membership)

- **OCTOBER 19 --** ***<u>FINAL REPORT from FESAC FSP Subcommittee submitted to full FESAC</u>***

- **OCTOBER 23 -- Discussion of FESAC FSP Subcommittee Final Report**
-- FESAC FSP Panel Chair presents: FESAC FSP Subcommittee Final Report: Findings & Recommendations
-- Associated discussion of formal final response of FESAC to Dr. Orbach's FSP Charge

<u>GENERAL IMPRESSIONS OF FSP INITIATIVE</u>

• **Primary Objective**: "produce a ***world-leading realistic predictive simulation capability*** that will be of major benefit to the overall science and mission goals of the US Fusion Energy Science Program" (R. Orbach)

- *important to ITER, relevant to major current and planned toroidal fusion devices, and strategically vital to US interests in developing DEMO*

• **Major Challenge:** development of ***advanced software designed to use leadership class computers*** for carrying out ***multi-scale physics simulations*** to provide information vital to delivering a ***realistic integrated fusion simulation model with unprecedented physics fidelity***

• **Budget Target:** ***15 year timeline with funding at around $25M per year*** primarily by OFES with significant support from OASCR

-- *$25M/yr over past decade for University Alliances Program within ASCI*

• **Roadmap:** FSP Workshop Report has deliverables targeted at end of 5, 10, and 15 years - should be ***both challenging and <u>achievable</u>***

-- V & V should be prominent

-- Need for clear connections to ongoing OFES base programs (theory & experiment) & SciDAC FES Centers (including CS & Applied Math expertise)

Charge Question 1: **Has the report identified key scientific issues and grand challenges that can be addressed by this approach to linking the scientific knowledge base for fusion energy?**

Response: **Conditional "YES"**

- **The five critical science issues identified as most urgent for burning plasmas/ITER are *important and compelling***

--- similar list from independent assessment by European community (Reference -- *A. Becoulet, et al. IAEA '06, Paper TH/P2-22*)

--- each is a computational "grand challenge" in own right requiring integrated simulation capability

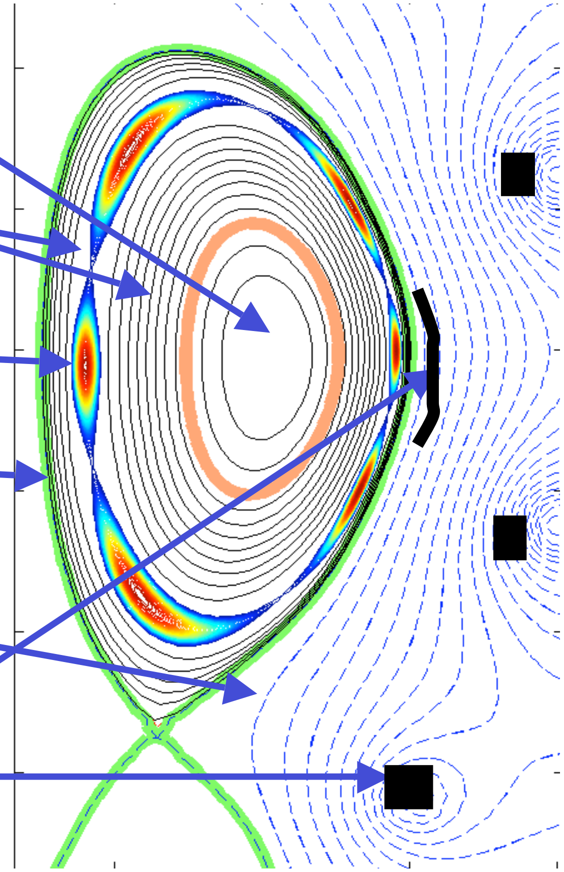
- **Fig. 2.2 (of Workshop Rpt.) captures *scientific complexity* of interacting physical processes within a tokamak discharge with *---- each topic in its own right requiring improved detailed physics understanding***

- **Table 2.1 (of Workshop Rpt.) illustrates how properties of tokamak plasmas depends on large variety of processes where "nearly everything depends on everything else" *---- makes case that an integrated approach is needed from a scientific perspective***

Elements of an Integrated Tokamak Modeling Code

[Fig. 2.2 from FSP Workshop Report]

- Sawtooth Region (q < 1)
- Core Confinement Region
- Magnetic Islands
- Edge Pedestal Region
- Scrape-off Layer
- Vacuum/Wall/ Conductors/Antenna



Core & Edge Transport

Plasma Turbulence

Large Scale Instabilities

MHD Equilibrium

Plasma-Wall Interactions

Atomic Physics

Radiative Transport

Energetic Particles

Heating Current Drive

Need for Integrated Approach: *"nearly everything depends on everything else"*

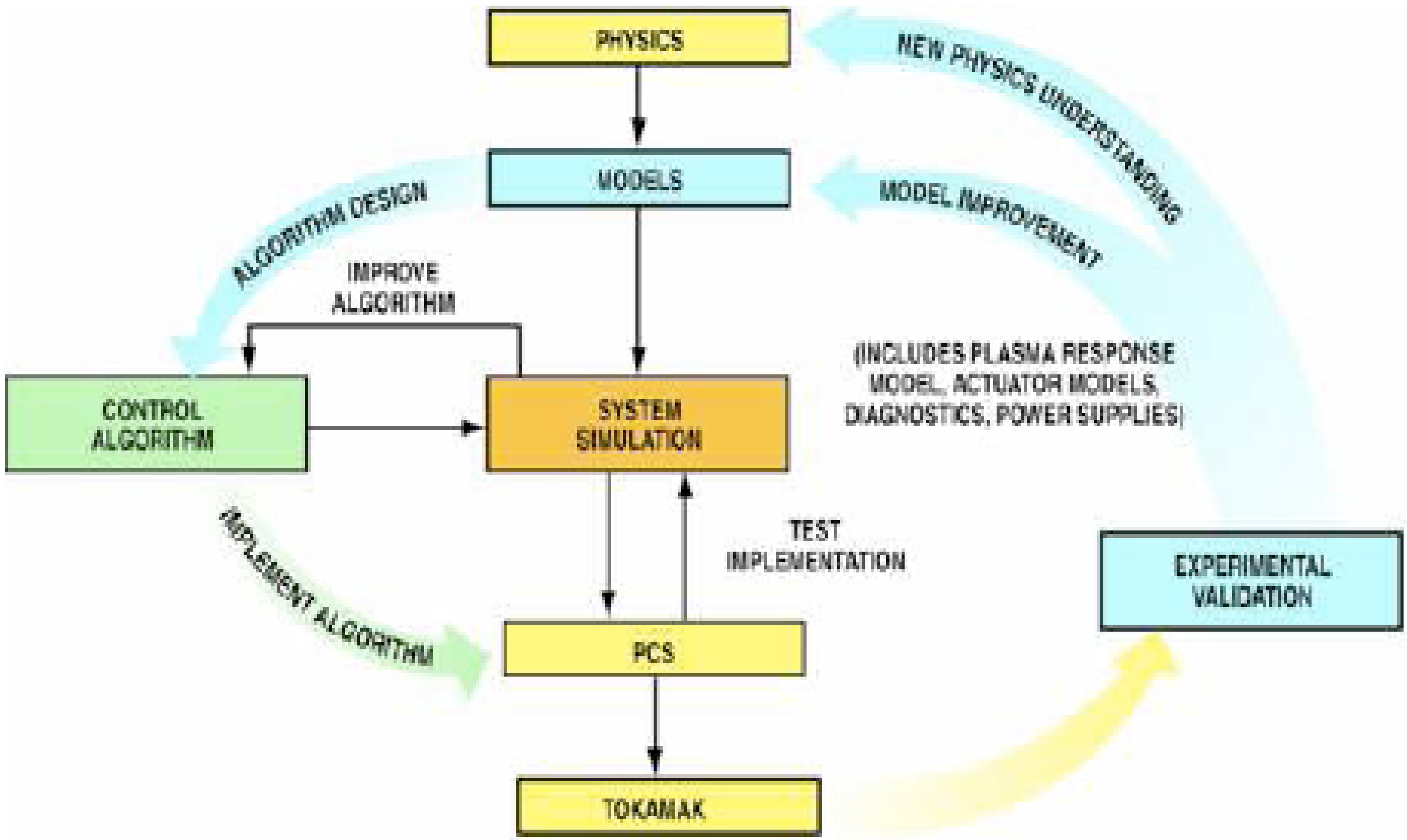
Table 2.1 (page 1 of 5) in Workshop Report: *Interactions of Physical Processes in Tokamaks*

Prediction and Control	Sources and Actuators (RF, NBI, fueling, coils)	Extended MHD and Instability Models	Transport and Turbulence	Energetic Particles	Edge Physics	Plasma-Wall Interactions
Pressure profile	Source of heat and particles affects pressure profile	Magnetic islands locally flatten pressure profile. Ideal no-wall beta-limit affected by pressure profile	Pressure profile determined by transport, together with sources and sinks	Co-resonant absorption with RF power deposition broadening by radial diffusion of fast particles	Boundary conditions affect pressure profile. RF power losses in edge due to nonlinear processes	Neutrals from wall affects density profile. RF power loss in vessel due to sheaths
Current profile	Noninductive currents; q-profile control	Stability determined by, and magnetic islands locally flatten, current density profile	Magnetic diffusion equation used to compute current profile	Current profile broadening due to radial diffusion of fast electrons	ELM crashes periodically remove edge current density	Eddy currents in wall affects plasma current profile
Plasma shaping	Controllability of plasma shape/ divertor	Controllability of ELMs and beta limit affected by plasma shape	Transport affects profiles that affect core plasma shaping	Profile of energetic particle pressure affects core plasma shaping	Shape at plasma edge affects core plasma shape	Coil currents and wall eddy currents affect plasma shape
Energetic particle profile	Co-resonant RF interactions modify velocity-space distribution	Effects of NTM on energetic particle profile	Effects of core turbulence on energetic particle profiles			

Schematic of Integrated Plasma Control System for ITER

(PCS stands for a real-time Plasma Control System)

Question: ***How will insights from 1st Principles approaches be folded into this kind of "Reduced Control-level Model"?***



Response to Charge Question 1: (continued)

• Readiness Issues:

(1) Which emerging or maturing simulation approaches appear most ready for integration within the next 5 years?

(2) How close are we to implementation of integrated model depicted in Fig. 2.2 in part or in whole?

(3) Similar question regarding FSP approach to Control Capabilities:

(i) feedback control: MHD foundation for progress is sound;

(ii) profile control: knowledge of particle & momentum transport is weak;

(iii) ELM (edge localized mode) control: edge-pedestal model inadequate

(4) Similar question regarding FSP approach to Plasma-Surface Interactions:

-- recommend a more general focus on this topic

e.g., sputtering erosion/re-deposition, dust formation, tritium trapping in tungsten, etc. are arguably just as critical as "tritium migration"

• Prioritization Issues:

(1) Need to identify effective strategy for FSP utilization of existing scientific knowledge in base program is essential

(2) In practical sense, cannot expect complete understanding of everything before proceeding with development of improved integrated models

(3) Most realistic approach ---- develop a reduced model based on current knowledge with understanding that this model will continuously improve as more knowledge is acquired & implemented

Charge Question 2: Have all the critical technical challenges been identified for which predictive integrated simulation modeling has a unique potential for providing answers in a timely fashion, in a way that traditional theory or experiment by themselves cannot?

Response: **Conditional "YES"**

- **The critical technical challenges identified are appropriate, and, as in the earlier reports from Dahlburg and Post, *at least first major phase of FSP should be on a subset of these issues* to ensure useful deliverables in a timely way**

- **Expectations of FSP productivity should be *realistic and commensurate with actual funding support***

  --- $3M in SciDAC FES for individual physics components, followed by $6M (3 yrs. later) for SciDAC "proto-FSP" integration projects (in "binary" sense)

- **Uniqueness aspect: *Simulation bridges gap between experiment and traditional theory via state-of-art advances in Applied Math, Computer Science, and HPC together with V&V for improved predictive capability***

  --- Experiment encompasses all realistic physics but limited in *scalability of predictions* by natural bounds of hardware

  --- Traditional Theory makes approximations to 1st-Principles equations to produce analytic and simplified numerical predictive solutions in *special limits of validity*

Charge Question 3: Is there a clear plan to establish the fidelity of the advanced physics modules, including a sound plan for validation and verification?

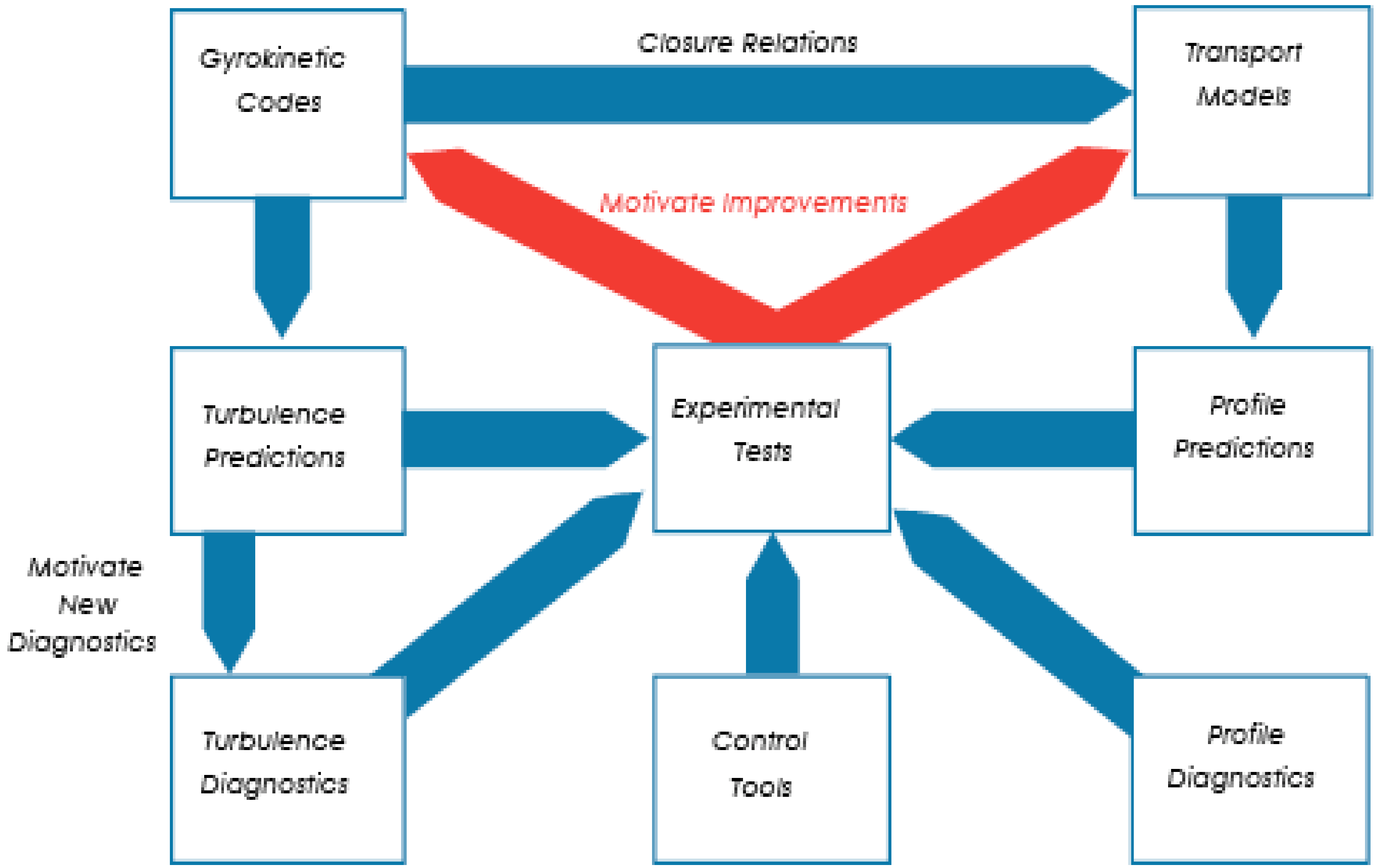
Response: **Conditional "YES" -- FSP Workshop Report clearly recognizes major importance of establishing the physics fidelity of advanced physics modules & associated essential role of Verification & Validation (V&V)**

- **While present vision for FSP provides reasonable framework and mechanism to move in right direction, it *needs a clear plan for V & V that benefits from/relies upon base programs for theory and experimental research***

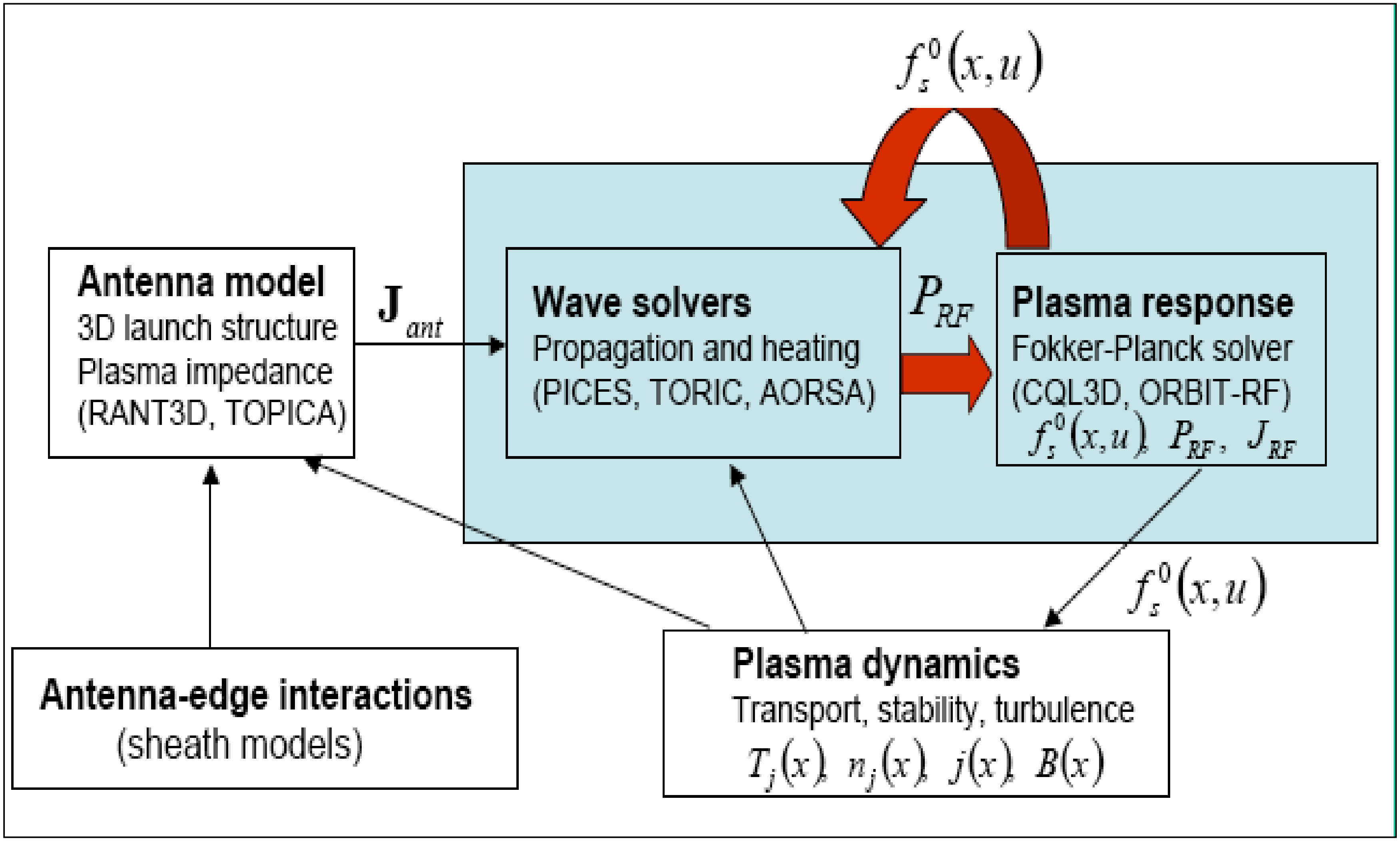
- **Verification** ***assesses degree to which a code correctly implements the chosen physical model***
--- FESAC FSP Panel believes that this is more than "essentially a mathematical problem" --- Special emphasis should be placed on code verification via cross-code benchmarking and comparisons with theoretical predictions

- **Validation** ***assesses degree to which a code describes the real world --- Report in need of more specificity; i.e., example "action items"***

Schematic: *Combined Efforts from Theory/Modeling/Experiment for Realistic Predictive Transport Capability in Plasma Core*



Schematic: *Combined Efforts from Theory/Modeling/Experiment for Realistic Predictive Capability in RF Wave-Particle Interactions*



Response to Charge Question 3: (continued)

• Summary Recommendations on Question 3:

1. **Code Comparisons with Theory & Experiment**: Code validation successful only to the degree to which a code describes the real world -- ***code needs to be flexible to accept advances made as a result of comparisons between experiment and new theoretical developments.***
--- ***Validation and model development should not be regarded as separate activities***

2. **Synthetic Diagnositics**: Value of *synthetic diagnostics* cannot be overlooked -- ***powerful tool for comparison between model and experiment***.
--- New area of research that has already produced impressive results in a few limited cases such as RF physics.

3. **Complementary Resources for Experiment & Theory**: Current devices are capable of performing experiments in all five of the critical scientific areas identified earlier
--- properly designed validation exercise may ***require resources not already available***, such as diagnostics and/or control actuators
--- FSP needs complementary ***development of experimental tools to validate models***
---FSP needs ***progress in some areas of fusion theory presently not well supported***

Charge Question 4: **Does the FSP Workshop clearly identify the critical areas of computational science and infrastructure in which investments would likely produce the tools required for the FSP to achieve its goals?**

Response: **Conditional "YES" -- FSP Workshop Report describes well the CS methodologies needed to produce needed tools including enabling mathematical techniques and infrastructure**

- **Chapters 3-6 of Report provide strong testimonial to *excellent working relationship between prominent researchers supported by OASCR and OFES***

- **More *specificity desirable on identifying most important software deliverables* and how they would be applied to FSP codes**
  --- specificity regarding code names & algorithms relevant to FSP more evident in earlier Dahlburg Report
  --- vision needed for how formidable *macro/micro-physics coupling* challenge will be addressed even if provided "infinitely powerful" compute power in future
  --- vision for *systems architecture & operational infrastructure* needed to address future "deadline-driven" data assimilation methods (for interpretation of shot-data for time-urgent experimental planning)

- **Dealing with programming strategies for the *multi-core architectures* expected to dominate future leadership class systems pose a huge challenge for FSP**

Response to Charge Question 4: (continued)

• Summary Recommendations on Question 3:

1. **Requirements & Risk Analysis**: One of first tasks of FSP should be to conduct a ***requirements and risk analysis associated with the computational tools and infrastructure*** to determine the appropriate ***level of direct investment*** and ***expected increase in capability due to normal developments in the field***

2. **New FSP-specific SciDAC-like Joint Partnerships**: FSP should engage in SciDAC-like ***joint partnerships to develop the FSP specific-capabilities for computational tools and infrastructure***.

--- build on ***existence of successful examples of joint work funded by ASCR and FES*** in the areas of mathematical techniques, computational libraries, collaboration technology, data analysis and advanced visualization tools

--- such efforts should be encouraged & resourced with ***support levels tightly coupled to the science and engineering goals of the FSP***

3. **Computational & Software Infrastructure Requirements**: These ***FSP requirements must be communicated early and often*** to those organizations providing computational and data capabilities for the Office of Science, such as the Leadership Computing Centers, ESnet and NERSC

Charge Question 5: Have the issues associated with project structure and management of the proposed FSP been properly addressed?

Response: **Conditional "YES" -- While the FSP Workshop Report does properly identify and address the issues associated with project structure and management, *prioritization with respect to the most critically important ones is needed***

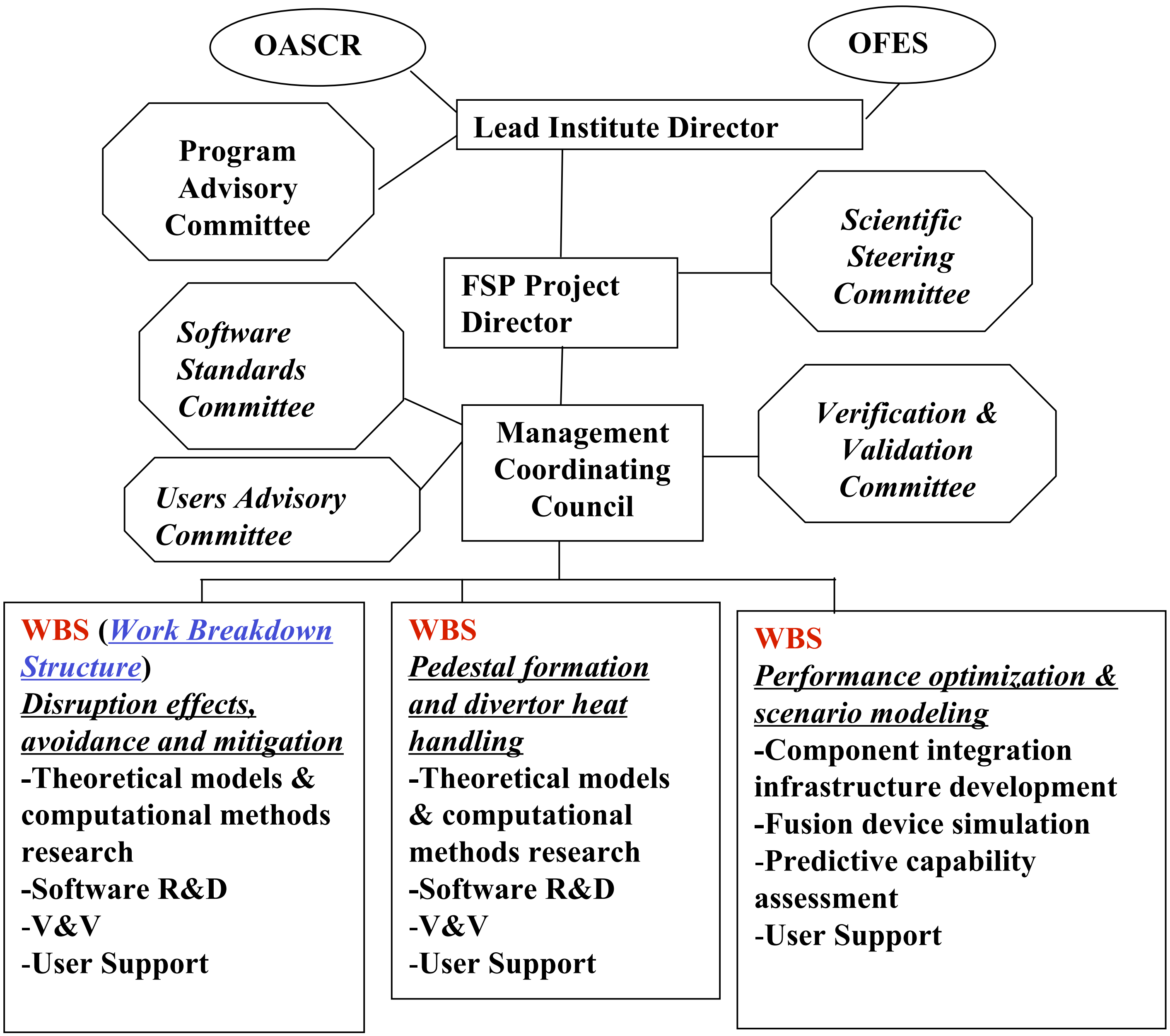
- **FSP needs to be able to quantify *Risk Assessment/Mitigation***
  -- needed for project of this magnitude (comparable to experiments) together with backup solutions/recovery methods identified

- **FSP should have a detailed *Work Breakdown Structure (WBS)* in line with best practices guidelines (Example from Combustion Systems Simulation)**
  -- needed for technical decisions for *integrated product in which scientific basis for some components still evolving*

- **FSP as a large, multi-institutional, geographically-distributed project, demands *crisp communications* on requirements, schedules, progress, & timely issues**

- **FSP's project management & structure need to ensure high motivation & reward system for participants *within project and also within home institution***

Schematic: Model FSP Organization Chart



Conclusions & Recommendations

• FSP Workshop Report represents impressive collaborative effort from a large segment of OFES and OASCR communities to help formulate an exciting project to produce realistic simulations of fusion systems with unprecedented physics fidelity

• Integrated modeling capability from FSP should be *embodiment of the state of theoretical & experimental understanding of confined thermonuclear plasmas*

-- provide reliable predictive capability with V & V to accelerate progress on answering outstanding scientific questions in field

• A successful FSP will better enable study of burning plasmas, aid the US role in operation of ITER, and help position the US for DEMO

--- powerful (peta- to exascale) platforms of future likely needed for effectively participating in ITER and for designing DEMO

• While the *Workshop Report is convincing on need for and benefits of FSP*, the associated *plan demands more specificity in a number of ways*

RECOMMENDATIONS

- **While it was felt that the FSP Workshop document came across as too generic and "all inclusive," the FESAC Subcommittee believes that it contains sufficient information for making the case that the *FSP can succeed in answering questions in a timely way that experiment and traditional theory by themselves cannot*.**

- **In order to be successful, the FSP should not be "everything to everyone." It must be *focused and project-driven with well-identified deliverables* that the stakeholders fully support.**

- **The FESAC FSP Subcommittee agrees with the five critical scientific issues identified in the Workshop Report as important areas of focus appropriate for the FSP. However, an integration effort encompassing all five of these challenging issues from the beginning looks to be too large a step. To be practically achievable, the *FSP should begin with more modest integration efforts that exhibit a compelling level of verification and validation*. This recommendation is in line with a similar position taken in the original FSP Report from Dahlburg, et al.**

RECOMMENDATIONS

- **The FSP should be a <u>repository of the latest physics as it evolves</u>. In this sense it cannot be a "stand-alone" project. It must be properly coordinated with theory, experiment and fundamental simulation. More specifically, a proper implementation of the *FSP will demand an effective plan for developing "advanced scientific modules" via utilization of results from the OFES base theory program, the SciDAC FES program, new insights from joint experiment-theory-modelling efforts, and the expertise residing in OASCR's computer science and applied math programs*.**

- **The FSP cannot succeed without a *viable validation and verification effort*, and this will imply expanding the diagnostic effort and linking it better to the FSP, for example through an *increased synthetic diagnostic development effort*. This will require special personnel with an appreciation of both diagnostic methods and code expertise.**

- **The management of the FSP should be organized with clear accountability and oversight and work out a *clear and compelling work-breakdown-structure (WBS).* It should also seek <u>advice and guidance from a broad community of stakeholders, experimentalists, analytic theorists, fusion engineering scientists, applied mathematicians and computer scientists</u>.**

RECOMMENDATIONS

- **The FSP should establish and maintain strong *connections with relevant international projects* and also draw on the large experience base from existing *scientific software development projects from other fields*.**

- **The DOE should properly launch a true FSP only if a *sufficient critical funding level can be realistically met and sustained*.**

Concluding Observation from FESAC FSP Subcommittee:

The effective "enfranchising" of more of the fusion community -- especially the experimentalists and technologists as well as analytic theorists -- into the Fusion Simulation Project (FSP) will require that this program produces <u>first-rate scientific capabilities that help advance the research</u> of a large user base of scientists working in these areas, <u>particularly as their work relates to ITER and burning plasmas</u>.