Report To Stewart Prager, Director, Princeton Plasma Physics Laboratory

Fusion Simulation Program Advisory Committee, March 25-26, 2010, PPPL
D. Post, chair, A. Boozer L. Greengard, B. Gross, G. Hammett, W. Houlberg, E. Marmar, M. Norman, C. Sovinec, T. Taylor, and J. Van Dam
(R. Stevens and D. Meiron were unable to attend)

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Charge to the FSP Program Advisory Committee (FSP PAC)
Dr. Stewart Prager, PPPL Director for the FSP PAC Meeting, March 25-26, PPPL

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(1) Science Drivers -- Regarding the current set of proposed science drivers and associated science development road-maps, please comment on:
a) Their appropriateness for the FSP;
b) Does the list of science drivers cover the important topics?
c) Do the roadmap items cover the high priority items in each science driver?

(2) Community Engagement -- Has the FSP program definition team defined and begun implementation of an effective community outreach plan?

(3) FSP Mission -- Regarding the FSP mission, please respond to the following questions:
a) Has the FSP mission been defined and articulated in a clear and compelling way?
b) Is the defined program scope (i.e., what will and will not be included in the program) appropriate and well focused?
c) Has the FSP been appropriately placed into the context of other MFE program elements and the relationship to them adequately defined?

Introduction

The Fusion Simulation Program (FSP) Planning Project (PP) has accomplished much since their last meeting with the FSP Advisory Committee (PAC) in September 17-18, 2009. With regard to the major charge areas, a vision for the needs and challenges and an initial list of capabilities for each of the six science drivers has been developed with input from the fusion community. An initial verification and validation approach has been defined in conjunction with the US experimental fusion community. The framework issues and a program strategy are becoming clearer. The DOE Office of Science fusion and computer science communities are becoming engaged in the FSP planning activities. While much remains to be done, a start has been made.

The detailed assessments of the progress in each of the three main charge issues (Science Drivers, Community Engagement, and the FSP Mission) and the recommendations for each charge follow.

Charge 1: Science Drivers and Roadmap Elements

The FSP PP has identified six major science drivers: 1) Integrated Boundary Layer; 2) Core Profiles; 3) Pedestal; 4) Wave Particle Interactions; 5) Disruption Avoidance and Mitigation; and 6) Whole Device Modeling. The last is not really a single science driver but rather the integration of combined effects of the other five science drivers. The FSP PP has identified candidates for the major capabilities needed for each science driver. Work has begun on defining the detailed approach needed for each driver to realize the needed capabilities. The PAC judges that the initial list of drivers and required capabilities is a good first step toward the development of a roadmap for each driver. However, this initial list is only a start, and the PAC agrees with the FSP PP that much remains to be done.

The degree to which the FSP will advance fusion science and is supported by its stakeholders within and outside the fusion program will largely depend on the development of a successful strategy or roadmap for each science driver and an approach for integrating their effects. The development of a strategy requires: (1) identifying the major gaps in our ability to predict the behavior of fusion plasmas, (2) determining which gaps could be significantly narrowed by better utilization of existing theoretical, computational, and experimental tools, and (3) determining which new computational capabilities would have the greatest benefits to the fusion program for a given commitment of resources. The formation of an appropriate FSP team to address each science driver can only be made when an adequate strategy for addressing that driver is in place. The time scale on which better predictive capabilities would have maximal benefit to the fusion program vary from driver to driver so priorities should be set.

The PAC recommends that the FSP continue to develop a strategy and prioritized plans for realizing the capabilities for each science driver through a transparent and documented process. This process should involve the fusion experimental and theoretical communities and the DOE computational science communities with participation from other communities (including communities outside DOE and outside the US). The adequacy and feasibility of the roadmap for covering the needs of the magnetic fusion program should be assessed by a focused review by these communities as part of the FSP PP deliverables. This strategy will be the basis for the formation of a team to address each driver. The success of the FSP planning process is in large part determined by the timely completion and review of the strategy.

The requirements and opportunities for verification and experimental validation should be key elements in the selection of science drivers and roadmaps, including outreach to US and international partners for long duration discharge data.

The presentations and discussions during the PAC meeting indicated that a good start on almost all issues has been made. The PAC would like to see the science driver outreach continue with a stronger effort to engage the experimental community in the selection and prioritization process.

The PAC endorses a staged software delivery model, with early and periodic releases, each with greater capability. This will be important for community support and feedback. In addition, the PAC recommends careful consideration of the early deployment of three-dimensional simulation capabilities. This can be begun by taking advantage of the existing 3D codes in community.

Finally, the organization of science driver topics should not compartmentalize thinking regarding FSP objectives. The FSP objectives encompass the goal of integrated predictive modeling.

Charge 2. Community Engagement -- Has the FSP program definition team defined and begun implementation of an effective community outreach plan?

The FSP program definition team has made significant strides in community outreach since the last Advisory Committee meeting, and the PAC commends the progress in this important activity. Among the highlights: briefings/site visits were conducted at seven major experimental facilities; two planning workshops were completed; technical requirements input through a broadly targeted questionnaire were collected; and a national website was created, incorporating FAQ and working group wikis which serve as a central information repository for the program, as well as a collaboration site for the working groups.

The PAC recommends a continuation of these activities, especially the site visits and workshops, which are productive avenues for community engagement. The PAC suggests that the project create a forum/blog and an email archive on the FSP website for soliciting additional input and feedback. More work is required to make sure that all FSP websites are linked from the homepage (http://www.pppl.gov/fsp/index.html). Finally, the PAC recommends collecting and publishing (on the national website) the raw input and process leading to consensus in roadmap definition, prioritization, and final program definition. Transparency is a key requirement for community buy-in.

Charge 3. FSP Mission

(a) Has the FSP mission been defined and articulated in a clear and compelling way?

We commend the progress toward an improved vision statement, but the mission statement is still somewhat long. A good set of vision and mission statements will be essential for DOE to gain the level of support needed for a program of the size of the FSP. We suggest something along the lines of:

VISION: The Fusion Simulation Program (FSP) will advance fusion science towards energy by providing validated predictive simulation capability.

MISSION: The Fusion Simulation Program (FSP) will develop advanced HPC-enabled tools to help accelerate understanding of magnetized toroidal plasmas via efficient integration of multiple, coupled physical processes. This task will engage theory, experiment, and advanced HPC resources to deliver unprecedented capability for harvesting information from experiments and designing new devices with improved performance.

(b) Is the defined program scope (i.e., what will and will not be included in the program) appropriate and well focused?

The PAC would like a clearer articulation of what is planned for the FSP scope. The de facto definition of the initial scientific scope of the program emerges from the list of the six science drivers and their concomitant roadmaps, each consisting of 8-10 items. As such, this is a very ambitious program. In the initial two years or so, the program should be more sharply focused on a limited number of specific deliverables. Achieving them will give a strong initial boost to the program. Specific Goals for the longer term program should be articulated. In particular, plans should be developed for assessing to what extent existing codes can be integrated into the FSP software distributions and to what extent the FSP should develop entirely new code libraries.

(c) Has the FSP been appropriately placed into the context of other MFE program elements and the relationship to them adequately defined?

The relationship of FSP to the MFE experimental program and the division of duties was spelled out. It would be helpful to identify the specific experiments worldwide that could be used during the next ten years to validate specific simulation capabilities. The FSP should use the validation process to recommend new experiments. OFES should maintain the flexibility to act on these recommendations. A description is needed for the relationship of FSP with the theory/simulation base program. A clearly articulated statement of the latter would help with community support of the FSP. The FSP will clearly need contributions from the theory/simulation base program and, in turn, the theory/simulation base program is one of the potential "customers" for the FSP software products.

Summary

The Fusion Simulation Program Planning Project offers the fusion community the opportunity (resources and time) to develop and deploy software that enables the fusion program to address its most compelling challenges. The 10^{15} exponential growth in computing power over the last sixty years can provide a new, powerful problem-solving capability to achieve a better understanding of magnetized plasmas for the fusion program. Success will require development of required applications, validation campaigns with the experimental community and new models from the theory community.

Exploiting this opportunity will require explicit funding to develop large-scale software products that can provide accurate calculations of the many important competing physics effects using complex computers. This requires sustained funding for multi-disciplinary teams just as it does for the construction and operation of fusion experiments. Just as fusion moved from small-scale experiments in the 1950s to large scale experiments such as TFTR and JET and now ITER, code development must move beyond the "cottage-industry" stage. The base theory/simulation community doesn't have the resources to develop and deploy these codes. Yet, even with the limited resources available, many important contributions have been made using computational tools, and the fusion community is one of the larger users of the DOE leadership class computing facilities. With explicit support to develop a range of software products that can exploit the next generation of computers, the fusion community can make major advances in its ability to understand and predict the complex behavior of fusion experiments and concepts. The leadership in DOE is aligned to support the FSP if a good plan is developed. The FSP is a large and potentially unique opportunity for the fusion community.

The FSP PP has made good progress since the last meeting in September, 2009, as noted in the body of the report. For the next meeting in September, 2010, the PAC is looking forward to seeing a description of the priorities and other progress, especially management and organizational structure, at the next advisory panel meeting

Appendix 1 Recommendations and comments for the six science drivers

The PAC didn't have adequate time to assess the six science drivers in detail, both because there wasn't much information available about the drivers before the PAC meeting, and because there wasn't adequate time during the meeting to develop a detailed assessment even if the material had been available earlier. A key responsibility of the FSP PAC is to provide advice that will help ensure that the FSP PP is following a process that will lead to a viable plan for the FSP. That advice is given in the main body of the report. However, a part of that role involves providing detailed technical advice about the approaches being developed for each science driver.

Charge 1.1 Integrated Boundary Layer (SOL), Divertor, Plasma Wall Interactions

The Boundary Layer is a high priority research area that requires advanced computational techniques for realistic numerical modeling.

The relevant unresolved scientific issues for fusion include: the effects of heat and particle loads; erosion and/or melting of the first wall; impurity contamination of the core plasma; and tritium retention. The SOL plasma also provides the boundary conditions for the pedestal, including temperature, density and flows. The science challenges include: coupled turbulence, stability, neutrals, atomic and molecular physics, and chemistry and materials morphology, across a wide range of overlapping spatial scales. Modeling of parallel and perpendicular transport effects on open field lines, combined with the presence of non-axisymmetric fields and boundary surfaces, needs to be treated in a fully 3-D manner. The FSP PP covers these issues.

The draft "roadmap" appears to cover the key issues. However, the PAC has the following recommendations for modification and/or clarification of the plans:

1) Restriction to the "first few microns" of the wall should be relaxed. Diffusion farther into the wall can play an important role in retention. Melting leads to much larger distortions.
2) Rotation and momentum transport should be explicitly included.
3) Non-ideal wall topologies (gaps, misalignment) should be explicitly incorporated.
4) ELM avoidance and/or control should be highlighted. We note that this topic will have strong overlap with the Pedestal science driver.

Charge 1.2 Core Profiles

The science driver on core profiles is of undoubted importance to the program. Self-consistent coupling of turbulence and transport to predict core plasma performance in MHD-quiescent plasmas is a good candidate for an early FSP deliverable. One issue that is crucial for understanding error field shielding and the precursors to disruptions is the interaction of islands with plasmas when islands have opened to a gyroradius scale.

Charge 1.3 Pedestal

The pedestal region is critical to predicting the overall performance of a fusion reactor. It is a challenging problem that requires a significant computational initiative to solve, and so it is appropriate for the FSP. The accurate calculation of 3-D effects (RMP coils) is a high priority item for the fusion program, but it is also a challenging calculation. The ability to model other

ELM control techniques, like pellet pacing, should be included as part of the FSP plan. Development of nonlinear electromagnetic gyrokinetic simulations of turbulent transport for the pedestal and edge will require a large amount of work, but the scale of that challenge is not adequately reflected in the emphasis in the roadmap.

Charge 1.4 Wave-Particle Interactions (fusion products and RF)

Both RF and energetic particle physics are appropriate for FSP: (1) these areas will require a high level of integrated simulation; and (2) both areas for highly relevant to ITER. We recommend that RF be given a higher priority than indicated in the list of scientific issues, key challenges, and payoffs for wave-particle interactions. The roadmap commendably includes two items, out of eight, that combine RF physics and energetic particle physics. RF is important for heating, and for current drive and current profile control. The roadmap for this science driver is appropriate as a provisional list.

Charge 1.5 Disruption Avoidance, Detection & Mitigation

The topics of disruption avoidance, mitigation, and effects are critical for ITER and for the development of the tokamak reactor concept. Unmitigated disruptions in ITER would significantly increase maintenance and repair costs and hamper scientific productivity. At future energy-producing reactor facilities, even fully mitigated disruptions would temporarily interrupt service. It is therefore appropriate to make the topic of disruptions one of the primary science drivers for the Fusion Simulation Project.

One of the question posed to the FSP team by the PAC is "Why is disruption avoidance not listed in the roadmap elements for the disruption science driver?" Summarizing the response, the team acknowledges that this is an apparent oversight. Accurate predictions of core profiles, the interaction of RF control for NTMs and sawteeth, and integration through whole-device modeling are essential elements of avoidance, and they are part of other science driver topics. The PAC is generally satisfied with the team's response, provided that the topical connections for disruption avoidance are made explicit and recognized by contributors who are responsible for all relevant science drivers.

Other comments relate to the 'roadmap' elements that have been listed for the disruption science driver:

- Most, if not all, modeling of runaway electron confinement during disruption has been conducted for the thermal quench phase of a disruption. From experimental results, we know that the critical phase is during the current quench. Capabilities and gaps for modeling runaway electrons during the current quench phase need assessment. If development is required, it should receive relatively high priority.
- Improved modeling of gas jet and pellets for disruption mitigation is one of the last items listed in the roadmap elements. At present, these techniques are the most promising approaches to reduce runaway electron confinement and thereby avoid damaging effects. This programmatic priority deserves early attention, possibly in parallel with other development, within the science driver.
- One of the roadmap elements lists 3D mechanical interactions through eddy and halo currents. While the structural response is important, the plasma's response to 3D interactions with external components needs to be emphasized. Perturbations from imposed fields and

asymmetric responses to non-uniform wall conductivity and shaping influence plasma rotation and locking.

Charge 1.6 Whole Device Modeling

The proposed science driver issues for whole device modeling and the associated science development roadmaps are appropriate and reasonable. An issue that needs additional focus is development of reduced fidelity models that capture the major important effects of a set of phenomena in an algorithm that is fast and compact and suitable for inclusion in a multi-physics whole device code. It is a major missing aspect with respect to priorities. Reduced models will always be the first step in design studies (scoping) and the basis for algorithms in control systems. They are also an essential part of many codes for data analysis and interpretation. All science drivers must consider model reduction as a fundamental process that will facilitate whole device modeling (from design scoping to control). This is as much a data analysis challenge as a physics challenge. Model reduction should be considered at each stage of the development process in the roadmap, but gets more and more critical as model complexity increases.

Appendix 2 Meeting Agenda

FSP PROGRAM ADVISORY COMMITTEE MEETING
March 25-26, 2010 Room LSB-318, PPPL

THURSDAY, March 25, 2010

8:00 AM – 8:45 AM: PAC CLOSED SESSION (I) Intro. Session with new PAC Chair (D. Post) , Meet and greet, assign responsibilities…..
8:45 AM – 9:00 AM: Welcome & PAC Charge (S. Prager)
9:00 AM – 10:15 AM: FSP Progress Overview & Management Plans (W. Tang)
10:15 AM -- 10:30 AM: Coffee Break
10:30 AM -- 11:15 AM -- Progress & Associated Roadmaps for Science Drivers (M. Greenwald)
11:15 AM -- 12:00 PM – Progress & Plans for Physics Integration/Frameworks (J. Cary)

12:00 PM -- 2:00 PM LUNCH -- PAC CLOSED SESSION (II)
(with Lunch) in DCR (Director's Conference Room)

2:00 PM – 2:45 PM – Progress & Plans for Advanced Components (X. Tang)
2:45 PM – 3:00 PM -- Coffee Break
3:00 PM – 3:45 PM – Progress & Plans for Experimental Validation (V. Chan)
3:45 PM – 4:30 PM – Progress & Plans for FSP ASCR Activities (D. Kothe)
4:30 PM -- 5:30 PM -- PAC CLOSED SESSION – (III)
5:30 PM – 6:00 PM -- CLARIFYING QUESTIONS FROM PAC TO FSP TEAM
7:00 PM – FSP PAC DINNER (at Wyndham Hotel)

FRIDAY, March 26, 2010

9:00 AM – 10:00 AM – RESPONSE OF FSP TEAM TO PAC QUESTIONS & ASSOCIATED DISCUSSIONS
10:00 AM – 1:00 PM – PAC FINAL CLOSED SESSION (with Lunch) in DCR (Director's Conference Room)
1:00 – 2:00 PM -- PAC Outbrief
2:00 PM – PAC Meeting Adjournment

Appendix 3 Attendees:

Ricardo Betti
Allen Boozer*
Vincent Chan
John Cary
Ron Davidson
Lori Diachin
Eliott Fibush
Leslie Greengard*
Martin Greenwald
Brian Gross*
Gregory Hammett*
Rich Hawryluk
Wayne Houlberg*
Doug Hudson
Arnold Kritz
Douglas Kothe
John Mandrekas
Earl Marmar*
Doug McCune
Michael Norman*
Walt Polansky
Douglass Post*
Stewart Prager
Alan Reiman
Ravi Samitani
Andrew Siegel
Carl Sovinec*
William Tang
Xianzhu Tang
Tony Taylor*
George Tynan
James Van Dam*
Leonid Zakharov
Michael Zarnstorff

*PAC members