Fusion Simulation Program (FSP) Progress Overview and Management Plans

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Charge to the FSP Program Advisory Committee (FSP PAC)

[Relevant Aspects addressed in all presentations to follow]

(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) the priorities for addressing them; and (c) whether they adequately cover the key areas needed for progress in MFE.

(M. Greenwald's Talk)

(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?

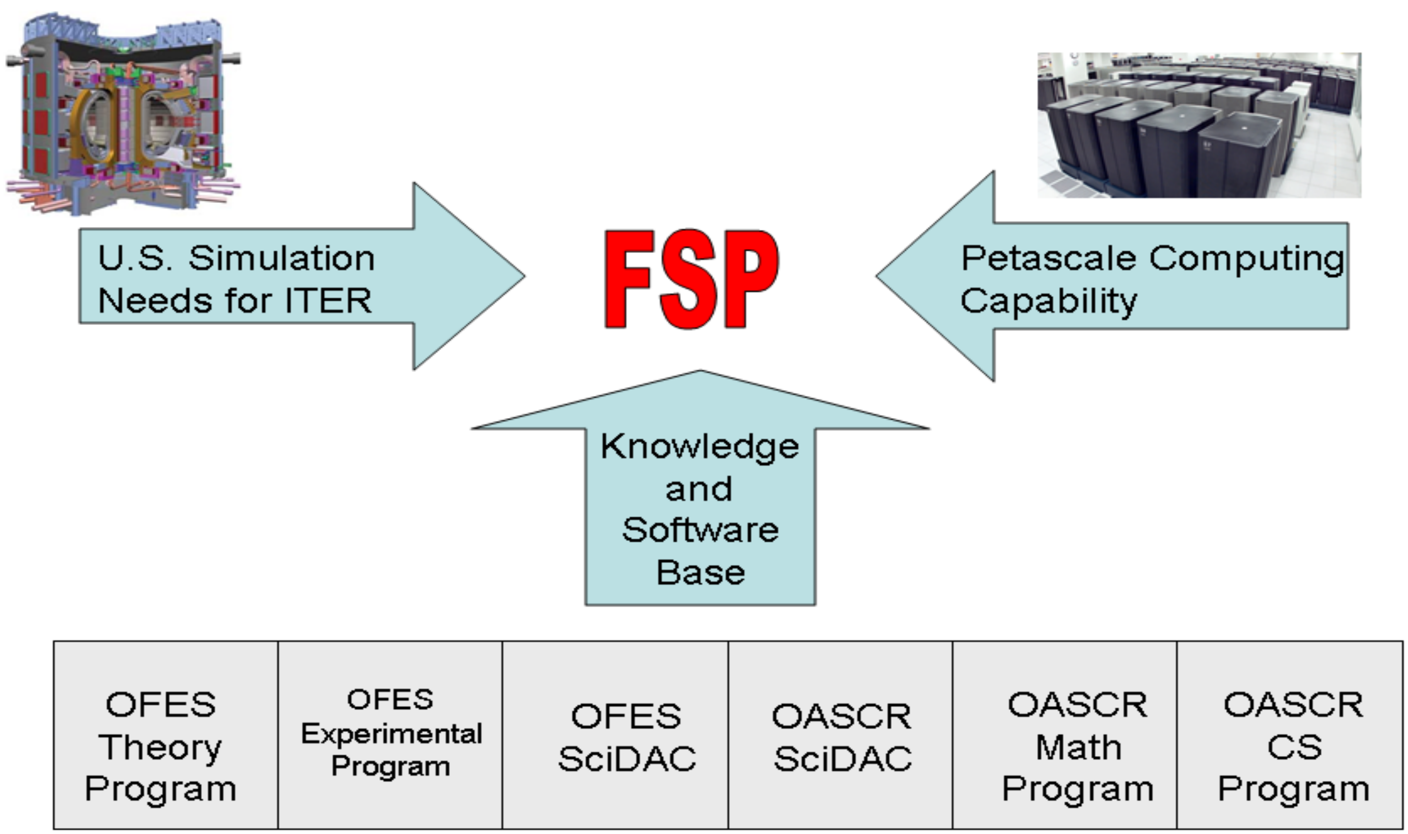
FUSION SIMULATION PROGRAM (FSP) PROGRESS OVERVIEW & MANAGEMENT PLANS

Outline:

I. Motivation, Mission, & Vision
II. Situation Analysis
III. Materials Challenges & FSP
IV. Milestones & Deliverables
V. Planning Elements
  -- cross-coordination between groups
VI. Risks
VII. Concluding Comments

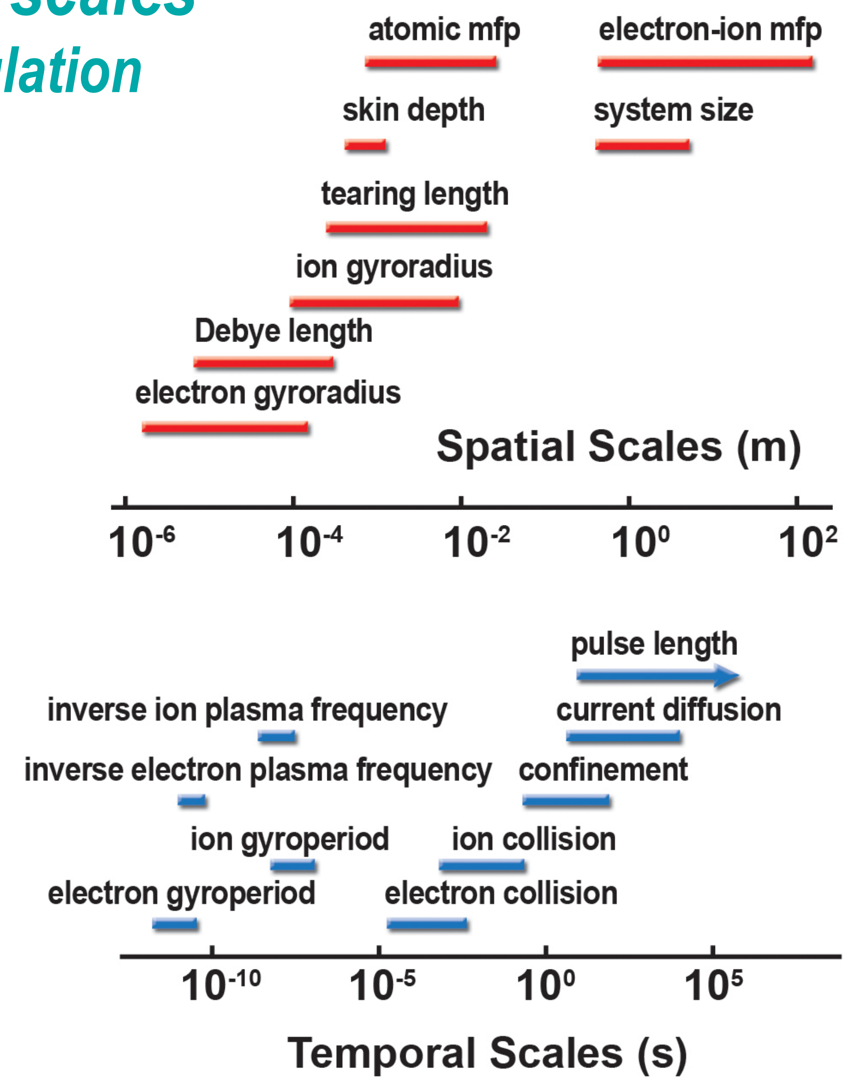
FSP -- A Strategic *Opportunity* to Accelerate Scientific Progress in FES

- Need for reliable predictive simulation capability for *BP/ITER (especially in the US)*
- Powerful ("Leadership Class") Computational Facilities moving rapidly toward petascale & beyond
- Interdisciplinary *collaborative experience*, knowledge, & software assembled over the course of nearly a decade under SciDAC plus OFES and OASCR base research programs in the US



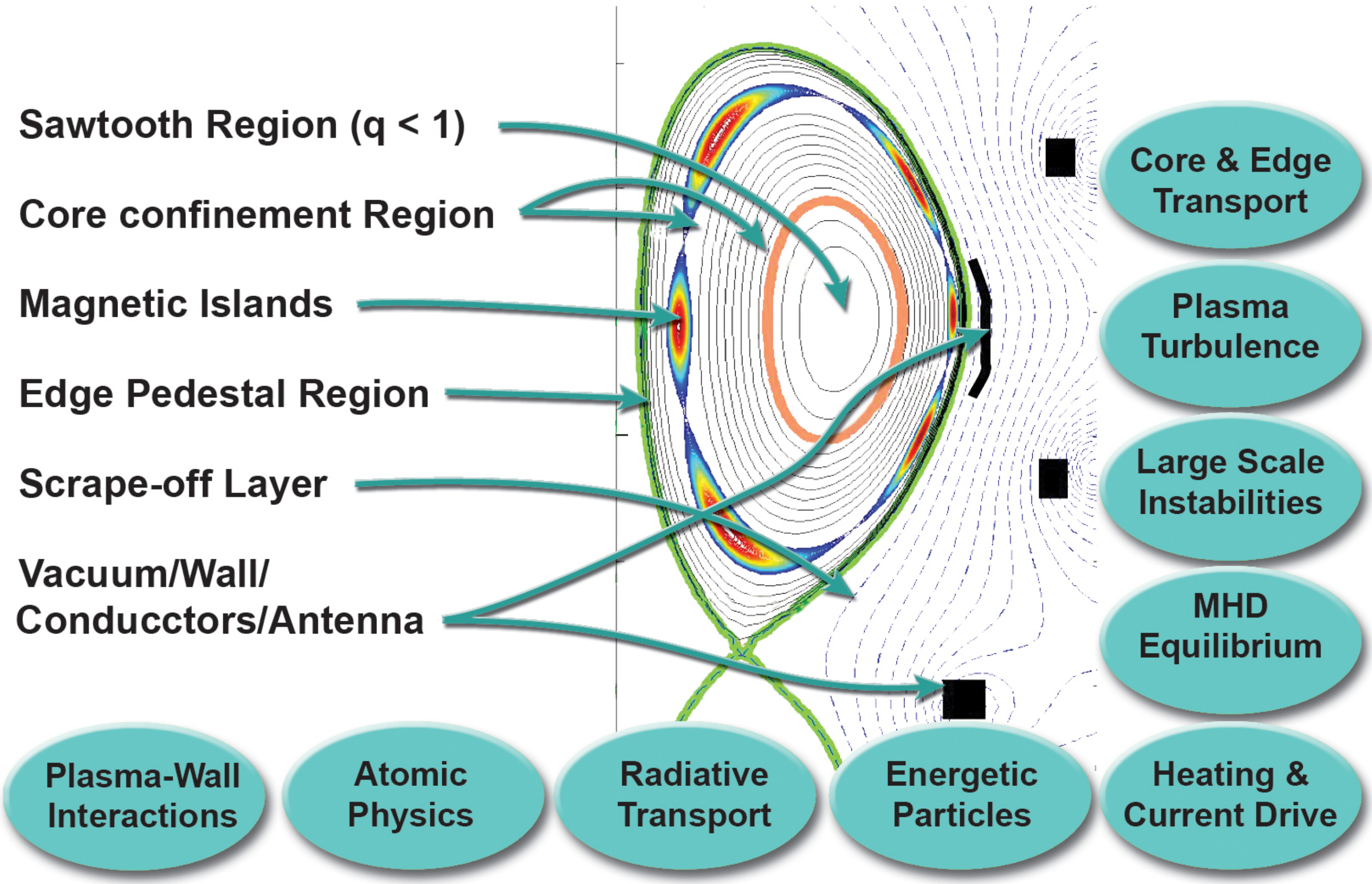
Integrated predictive models must span huge range of spatial & temporal scales
-- major challenges to theory and simulation

- **Overlap in scales often means strong (simplified) ordering is not possible**
- **Needed to effectively harvest insights from ITER and to plan for DEMO**
- **Effective simulations at the petascale** *(10^{15} floating point operations per second)* **and beyond are required to address grand challenges in plasma science**

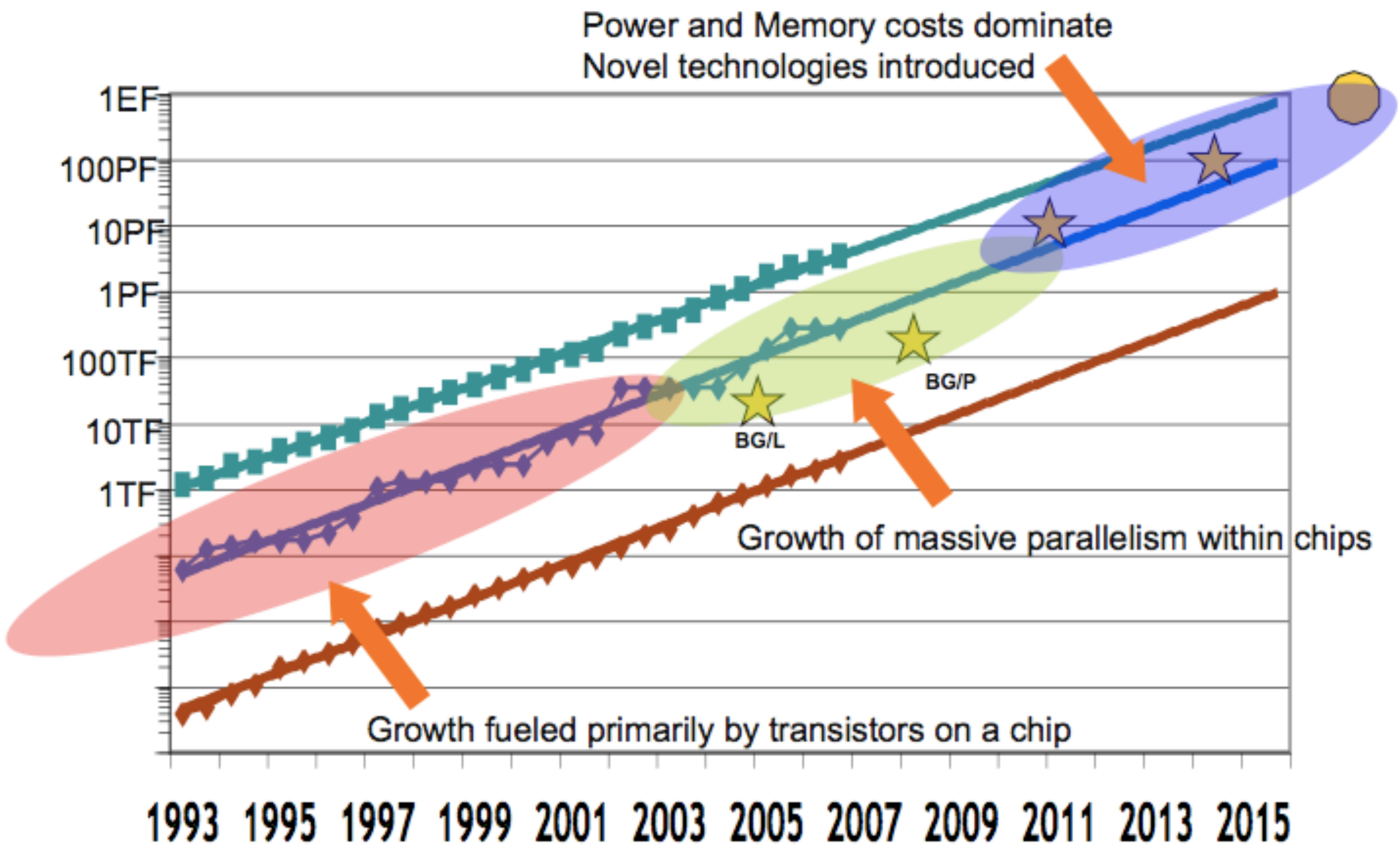


FSP Integrated Model of Many Effects

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



Future Computational Challenges: “Exascale”



Slide courtesy Argonne Leadership Computing Facility (ALCF)/Argonne National Laboratory

Advanced Computing can Transform Fusion Energy Science

- ***FSP Considerations:*** [achieving "buy-in" from general FES community]
  - Need to distinguish between ***"voracious"*** (*more of same - just bigger & faster*) vs. ***"transformational"*** (*achievement of major new levels of scientific understanding*)
  - Need to improve ***significantly*** on ***experimental validation*** and ***theoretical verification*** to enhance realistic predictive capability

- ***Associated Extreme Scale Computing Challenges:***
- ***Hardware complexity***: Heterogenous multicore (*e.g., cpu+gpu -- LANL, ORNL, …*), power management, memory, communications, storage, …
- ***Software challenges***: Operating systems, I/O and file systems, and coding/ algorithmic needs in the face of ***increased computer architecture complexity*** … ***"parallelism doubles every two years" (as a new form of Moore's Law)***

  (*MPI + threads; CUDA; rewriting code focused on data movement over arithmetic; …..*)

  People: ***Training the next generation of simulation/modeling-oriented CS, Applied Math and applications-oriented computational scientists and engineers ….***

FSP MISSION & VISION

VISION: *The Fusion Simulation Program (FSP) will enable scientific discovery of important new plasma phenomena with associated understanding that emerges only upon integration. It will provide a predictive integrated simulation capability for magnetically-confined fusion plasmas that are properly validated against experiments in regimes relevant for producing practical fusion energy.*

MISSION: *The Fusion Simulation Program (FSP) will provide the capability to confidently predict toroidal magnetic confinement fusion device behavior with comprehensive and targeted science-based simulations of nonlinearly-coupled phenomena in the core plasma, edge plasma, and wall region on time and space scales required for fusion energy production.*

SCOPE: *WHAT FSP WILL AS WELL AS WHAT IT WILL NOT DO*

- **General approach is to focus on achieving validated predictive capability for addressing integrated modeling challenges for advanced toroidal systems with special attention to burning plasmas and future DEMO issues – broader alternative configuration topics will not be addressed early.**

- **FSP coverage of 3D physics will naturally focus on nonlinear evolution of instabilities (naturally non-axisymmetric) and on non-axisymmetric equilibrium modifications possibly capable of controlling ELM's [i.e., involving RMP's (resonant magnetic perturbations)].**

- **Materials Challenges & FSP:** *The FSP will be a key customer for emerging models of plasma-wall interactions and will address this challenge as a component of its strategic vision (i.e., focusing on first few microns in PMI studies).*

-- A broad initiative on first wall and structural materials, including simulation, , experimental validation, and materials development would be a very important companion activity for the FSP.

-- E. Synakowski @ FESAC: " ..... launching of a vigorous materials and nuclear science program that will be part of defining and constructing a fusion nuclear science facility, and will fill gaps en route to a DEMO."

The FSP Will Make Unique Contributions to the Fusion Program

- Addresses multi-physics and multi-scale problems that are now treated in isolation -- scientific discovery of new phenomena which *emerge only with integration*.
- Carries out a rigorous and systematic validation program, *in collaboration with experiments*, to put models on firmest and most realistic possible foundation.
- The FSP Science Drivers (SD) have been identified as forefront scientific problems in FES that can be aided by computing at the extreme scale *in collaboration with ASCR* over the next decade
- Develops predictive models which improve our capabilities for *reliable scenario modeling*, especially for ITER, and for design of future machines such as DEMO.
- Incorporates *powerful HPC capabilities to help accelerate scientific understanding* and modern software engineering approaches to ensure the reliability, robustness and ease-of-use of the new tools that are developed.
- Leverages ongoing activities (theory, experiment, modeling in FES and applied math, computer science in ASCR) to develop unprecedented simulation capabilities.
- Embodies our state of knowledge in a suite of advanced codes under a unified framework and made widely available to the FES community.

The FSP Will Make Unique Contributions to the ASCR Program

- The FES community is well-positioned to be a major applications area for demonstrating the benefits of exascale computing. (ref. D. Kothe's presentation):

  "Computational fusion science projects on the ASCR LCF platforms are demonstrably leading the overall computational science community"

- FES advances in models, algorithms, and software have and will continue to demonstrate "applications readiness" of benefit to the ASCR mission to *"to develop the algorithms, computer programs and hardware that advance scientific research."*

- FES can "show the way" for other applications domains by its prominent role in cross-cutting ASCR-led HPC programs such as *SciDAC (Scientific Discovery through Advanced Computing) and INCITE (Innovative and Novel Computational Impact on Experiment).*

- Positive impact of availability of impressive suite of well-diagnosed FES experimental facilities & associated large foundational data sets aligned with FSP to *help drive UQ (Uncertainty Quantification) R&D involving sensitivity analysis.*

FSP OVERVIEW: Significant Past, Present, Future Events

- **PAST**: 2007 FSP Workshop Report (A. Kritz/D. Keyes) – major FES-ASCR meeting

-- FESAC FSP panel report (recommendation for OFES to proceed with the "Project Definition" phase of the FSP) - October 2007

-- ASCAC FSP panel report (recommendation for OASCR to partner with OFES in the FSP) -- July 2008

-- PPPL-led Proposal submitted (December 2008) in response to DOE RFP http://www.sc.doe.gov/grants/FAPN09-04.html

-- DOE-SC Workshop on "Grand Challenges in FES (March 2009) – major international meeting of over 110 experts in FES and ASCR

-- FES ReNeW – extensive and detailed community planning activity (June 2009)

- **PRESENT**: The FSP team* funded to carry out a detailed "planning study" over two years (8/09-7/11) – with requirements as specified in the DoE RFP.

*Team of 6 national labs (PPPL, ORNL, LANL, LBNL, LLNL, ANL), 2 companies (GA, Tech-X), and 9 universities (MIT, Princeton, Columbia, NYU, UCSD, Chicago, Lehigh, Purdue, Texas)

-- Current "program definition" phase *managed as a project*

- Includes *FSP program scope & deliverables* and *FSP planning scope with WBS*
- Targeted goals, schedules, milestones, responsible working groups with wikis on FSP web-site
- Build on "lessons learned" from other major scientific software development projects such as ASC [e.g. -- FY06 ASC Program Plan & more recent interactions @ LLNL and LANL]

FSP OVERVIEW: Significant Past, Present, Future Events

- **PRESENT**:

-- The FSP planning effort has an *active outreach* to the theory, modeling and experimental *national & international communities in FES* and the applied math and computer science *communities in ASCR* to help define scientific priorities and establish mechanisms for *productive collaborations* – e.g., visits to GA, MIT, Maryland, LLNL, ANL, LANL, ….. & *FSP PLANNING WORKSHOP (March, 2010)*

-- The FSP planning team has posted on its national web-site [*http://www.pppl.gov/fsp/*] an *FAQ section* and generally welcomes input, comments and suggestions from the FES and ASCR communities.

- **FUTURE**:

-- Series of conceptual design reviews of FSP elements; assessment of proto-FSP's; organizational review of overall FSP plan; follow-on FSP Planning Workshop (like Exp. Facilities Research Forum); and external "red team" assessment of FSP Plan

-- A DOE-Office of Science review will be held at the end of the 2-year planning study (shortly after July 2011)

• *The Final Plan for the FSP will include a PEP (Program Execution Plan) to enable prompt ramp-up in late 2011 in the event of final DoE approval.*

FSP Program Definition Process

- Science Drivers: *identification of initial 6 science drivers for which reliable predictive simulation capabilities are demanded to enable accelerated progress toward delivering magnetic fusion energy*
- Perform *gaps analysis* of computational capabilities required to address associated physics challenges, including *development of plans for*:
    - Advanced Physics Components
    - Physics Integration/Frameworks
    - Verification & Validation + UQ (quantitative characterization and reduction of uncertainty including sensitivity analysis)
    - Data Management
    - FSP Production Services (address user-community challenges)
- Develop associated "living roadmap" with both *near-term* and longer-range milestones.
- Estimate resources (manpower, computing resources, …)
- Define an effective management structure (addressing *multi-institutional, multi-disciplinary challenges*) , and recommend *risk mitigation* strategies
- Produce a *compelling program plan* – including "lessons learned" from NNSA-ASC, climate, DoD programs, …

FSP Program Definition Milestones

- Identification of science drivers with associated <u>"gaps analysis"</u>
  - Scientific roadmaps with strategies for addressing both science and software gaps – major progress, e.g., in recent community planning workshop (Boulder, CO – March 15-18, 2010)

- Program and management plans for FSP
  - -- FSP plans that emphasize strategic importance of delivering some nearer-term software capabilities to the user community as well as connection to longer-term development of those capturing the needed science.

- FSP plans for Proto-FSP assessments (*with external expertise engaged*)
  - -- These evaluations include "lessons learned," transition process incorporating best elements from each approach, and flexibility of design to address *future path to exascale challenges.*

- FSP plans for coupling to requisite <u>expertise from FES & ASCR communities</u>

FSP Community Engagement Activities

- **Develop plan for coupling to requisite expertise from FES & ASCR communities needed to address FSP goals**
  - FSP information briefings/site visits began in July '09 and are continuing -- to discuss proposed plan with larger community [e.g., at ANL (7/09), PPPL (9/09), GA (2/10), MIT (2/10), U. Maryland (2/10), LLNL (2/10), LANL (3/10) & planned visits at ORNL (5/10), IFS, U. Wisconsin, NYU, Columbia U., …….)]
  - Public meetings (e.g., DoE OFES Budget Planning Meeting, etc.)
  - FSP Workshops (Proto-FSP Workshop @ ORNL (Jan. '10); FSP Planning Workshop @ Boulder, CO (March '10), …..
  - National web-site (http://www.pppl.gov/fsp/) and working group "wikis" up and operating with continuing improvements including posting of information from PAC meetings, DoE presentations, information from Workshops, etc.
  - Frequently Asked Questions (FAQ's) & Answers: "living document" requesting further community input on additional questions; posted on the national FSP web-site
  - Active participation in and contributions to International Integrated Modeling Workshops & Meetings (e.g., US-Japan Workshop on Integrated Modeling at MIT – P. Bonoli (US), A. Fukuyama (Japan), co-chairs with P. Strand (EU), M. Greenwald, A. Kritz, …. (Feb. 2010) – *more formal bilateral collaborations proposed by EU*

FSP Planning Workshop Summary (March, 2010)

- Coordinates: Boulder Co., 3/15-3/18 ~45 participants from broad range of institutions and disciplines
- Goal: *identify scope, requirements, approaches, gaps, and software architectures for*
  - Physics components
  - Physics composition designs
  - Task composition (or workflow)
  - Integrated data management
  - Production computing
  - Software development infrastructure
- Outcome: *significant progress toward FSP definition*
  - Component factorization and coupling scheme with requirements and gaps for each science driver in the near term and long term.
  - Agreement on need to support programmable workflows; multiple visualization tools expected
  - Agreement on principles and approach for Integrated data management
  - Enumeration of requirements for software development infrastructure
  - Agreement that support of and assistance to non-developer users crucial for scientific success with pipeline from research codes to production codes; capacity computing support needed
  - Enumeration of requirements for software development infrastructure and identification of candidate solutions

FSP Planning Activity Milestones & Deliverables

Fiscal Year Quarter	Q409	Q110	Q210	Q310
Deliverables	✓FSP Kickoff meeting held on July, '09 ✓Communication logistics (web-site, wikis) ✓FSP PAC organized and first meeting held (Sept.'09) ✓FSP Mission and Vision statements	✓FSP FAQ's with Answers on web-site ✓Draft FSP Program Scope Document ✓Draft FSP Program Deliverables ✓FSP Briefing with DOE-SC Leadership ✓Draft FSP Production/ Customer Interface Plan	✓Draft Outreach Schedule ✓Draft FSP Planning Project Plan with Deliverables & Dates ✓Draft WBS for Planning Project with resource allocations ✓Proto-FSP Workshop * FSP Planning Meeting 2nd FSP PAC Meeting (Mar.'10)	Charge & Chair for Proto-FSP Assessments Report Validation Best Practices Data Management and Requirements Plan Community Input on Science Drivers & Applications collected 1st Draft – time estimates for initial Frameworks tasks & analysis of 2 science drivers 1st Draft – Components gaps analysis & process for selection and prioritization of new components development
Fiscal Year Quarter	**Q410**	**Q111**	**Q211**	**Q311**
Deliverables	Proto-FSP Assessments Report 3rd FSP PAC Meeting (Sept.'10) Final Drafts: (1) Components gaps analysis & process for selecting/ prioritizing new components to address SD's; (2) Frameworks analysis of needs/prioritization for components integration to address SD's; (3) Validation gaps analysis and remediation	Infrastructure Plan 1st Drafts: (1) Overall Implementation Plan; (2) Framework Implementation Plan; (3) Validation Plan; (4) Experimental Coordination Plan; (5) Components Execution Plan; and (6) Prioritizing and sequencing of Science Drivers	Implementation Plan 1st Draft - Project Execution Plan (PEP) Frameworks Community Input Workshop Report Reports on Validation Metrics for Data Mgt. Prototypes Components Program Plan Report on why FSP is required by each targeted Science Driver 4th FSP PAC Meeting (Mar.'11)	Project Execution Plan Final FSP Planning Package Frameworks Section of FSP Plan Validation Section of FSP Plan Components Section of FSP Plan Science Drivers Section of FSP Plan

Collaboration With Experimental Facilities

- **The FSP will need strong collaboration with experimental facilities for validation of the physics codes produced**
  - ***FSP codes expected to be of significant value to the facilities for planning and interpretation of experiments.***

- **Discussions have begun with the major facilities to define:**
  - ***General principles for collaboration and intellectual property (IP) sharing***
  - ***Proposed mechanisms for short-term and long-term planning***
  - ***Roles & Responsibilities for the FSP and for experimental teams in their collaboration***
  - ***Lessons learned from the major experimental facilities that would be useful in planning the FSP research program– e.g. open community research forums***

- **The existing collaboration agreements for and approaches to research governance used by the facilities provide a proven model for the FSP.**

- ***A draft document has been circulated and generally agreed on by project managers at each facility.***

- ***Experience suggests that success will require ongoing partnerships and mutual interactions, institutionalized through formal agreements, regular participation in planning and reporting activities, and cross-membership in planning groups as appropriate.***

FSP Risks

- ***Science Drivers**: (1) underlying physics models not sufficiently complete to adequately resolve scientific issues consistent with experimental reality; and (2) major challenge of reaching agreement on importance of any given science driver due to varying needs in different parts of FES community*
- ***Frameworks**: (1) chosen framework technologies may prove incompatible with future computational architectures; and (2) existing components found to be insufficiently engineered and/or robust for use in the more demanding framework environment*
- ***Components**: balancing the needs of delivering advanced physics code software products and the exploratory research needs for producing the physics capabilities required to resolve the FSP science drivers' challenges*
- ***Validation**: even with premier plasma diagnostics, there are practical limitations of experimental measurement to comprehensively measure all important parameters with the needed spatial coverage and resolution*
- ***Verification**: dealing with challenges associated with integrated vs. single physics – especially "model uncertainty quantification"*
- ***Production:** lack of necessary experience with objective software product testing ("alpha," "beta," …) and with customer support for large user community*
- ***General Risk**:*
  - *Managing a major software R&D project of the scale of FSP is unprecedented in DOE-SC*

Current Perspectives on FSP

- A credible base of component capabilities and framework approaches can produce valuable integrated software tools within the next 5 years to enable significant progress on each of the science drivers (SD).
  - Initial “gaps analysis” of needed science & simulation tools indicate significant improvements in fidelity beyond current integrated modeling capabilities in each addressing each SD area likely
  - Strong Verification and Experimental Validation critically needed to ensure progress noted
  - Limitations are identifiable and identified.
- The diversity of potential components/integration approaches for the same SD indicate significant gaps remain between current capability and a more realistic first-principle-based predictive capability.
- Within 10-15 year time-frame common component R&D capabilities emerge to address SD’s in key areas.
- Within 10-15 year time-frame, R&D thrusts in the physics integration area are on converging paths: (e.g., integration of core & edge turbulent transport; and integration of kinetic & MHD descriptions of core profiles; etc.)

FSP Team Response to Charges 2 and 3

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

Yes – elements include site visits, international collaborations, community workshops, public meetings (e.g., BPM, FESAC, …), and informative national web-site with FAQ's and wiki's for planning groups

- *FES and ASCR communities engagement via Site Visits -- GA, LLNL, MIT, U. Maryland, PPPL, ANL, LANL, ... – with planned visits to IFS, ORNL, U. Wisconsin, NYU, ….*
- *International collaborations activities have included US-Japan International Workshop on Tokamak Integrated Modeling involving US, EU, & Japan (MIT, Feb. 2010)*
- *Successful FSP Planning Workshop (Boulder, CO) – 45 participants from FES & ASCR*

Charge 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?

Yes – FSP Mission and Vision statements have been vetted with DoE-SC at direct briefings, discussed with community at numerous outreach visits, and posted on FSP web-site

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

Yes – FSP scope will first focus on major advanced tokamak challenges moving forward to burning plasmas with extensions to 3D dynamics (e.g., RMP for ELM control; and first few microns for PMI studies)

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

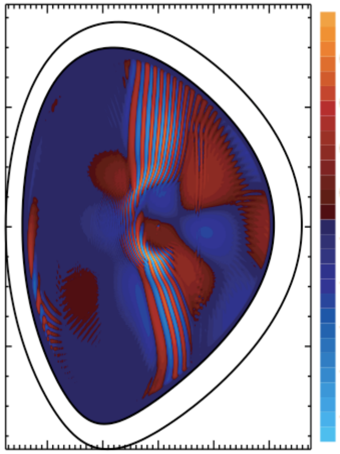
Yes – FSP will collaborate in mutually beneficial way with FES experimental program, FES theory program, SciDAC Program with strong ASCR participation, & FES international programs

Steve Koonin (DoE Energy Undersecretary):

"Advancing fusion science towards energy"

3 November 2009 – APS-DPP Meeting, Atlanta, GA

- *Validated predictive simulation capability is key*
  - Our confidence in validated simulation has to take a major step up
    - moving from description to prediction
    - use simulation to explore regimes beyond current experimental capabilities
    - close integration of theory, modeling and simulations, and experiments



  - *Fusion Simulation Program is a start along this path*