FSP FAQ's & ANSWERS: January 8, 2010

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Role of the FSP

- What is the mission (purpose) and vision (goals) for the FSP?

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.

VISION: The Fusion Simulation Program (FSP) will enable scientific discovery of important new plasma insights 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.

- What is the main contribution to the overall fusion program expected from the FSP?

The FSP should lead to deeper understanding and improved predictive models by integrating phenomena which are now treated in isolation. This will entail engagement of large-scale HPC in an unprecedented way to enable higher physics-fidelity integrated modeling capabilities. These will advance the fusion program's overall scientific mission, improving interpretation of experimental results and embodying our state of knowledge. This should also result in more reliable scenario modeling for existing and future machines – especially ITER and reliable extrapolation to DEMO.

- What are the expected product(s) of the FSP and how will they be different from the current modeling and simulation activities currently supported in the FES and ASCR Program Offices?

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There will be a number of basic “products," including: (1) an FSP simulation suite; i.e., a set of new scientific software tools and environments that embodies the community’s latest understanding of relevant fusion science and plasma physics in tokamak plasmas; (2) Direct guidance and support of current and planned fusion tokamak experiments, with ITER being the highest priority focus; and (3) Contribute to the education, training, and team building of the current and next generation of fusion scientists and computer and computational scientists needed to support, develop, and use the FSP simulation suite of HPC tools. The major difference from current R & D emphasized in the FES & ASCR programs is the focus on new insights gained from integration (as noted in the mission statement). FSP codes – both in its advanced components and its integrated tools are expected to engage experimental validation at an unprecedented level of emphasis and also to help enable efficient use of cutting-edge HPC capabilities.

- What are the unique aspects of the FSP relative to current modeling activities?

The Fusion Simulation Program (FSP) will enable scientific discovery of important new plasma phenomena with associated understanding that ***emerges only upon integration***. A realistic simulation capability that would allow fusion researchers to predict with confidence the performance of magnetically confined fusion plasmas and explore regimes unattainable in current experiments, will require an unprecedented degree of integration of all relevant physical processes across different regions and spanning a tremendous range of spatial and temporal scales. Computational hardware and software resources extending from the petascale to the exascale are expected to enable the delivery of associated advanced software tools in a timely manner. In addition, a systematic verification and validation (V&V) effort requiring unprecedented coordination and cooperation among theory, computation, and experiment will be necessary to establish the scientific credibility of this advanced suite of simulation tools.

- Will the FSP be focused only on tokamaks, or will it be able to model other magnetic configurations?

While the tokamak configuration will be the focus of the FSP during its foundation phase over at least the first several years, the infrastructure and framework for the program is expected to be sufficiently extensible to allow implementation of alternate configurations in the future.

- Is materials modeling within the scope of the FSP?

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The currently envisioned region for materials modeling in the FSP will encompass roughly a few microns of the first wall boundary region. More generally, materials modeling is of course recognized as a major area of importance for FES, and it is expected that close ties and coordination will be established with future FES materials science initiatives.

- What is the expected duration of the FSP?

The FSP plan requested by FES is to cover a 15-year period with major deliverables expected within 5-year segments. If proven to be successful, the FSP would likely extend beyond this period and continue to deliver increasingly realistic predictive simulation software with higher physics fidelity.

Planning

- What is the purpose of the FSP definition activity now underway?

The FSP definition effort is being carried out as a formal project with the goal of producing a plan for the implementation of the FSP that is sufficiently detailed and compelling to allow large scale development work to begin in earnest at the conclusion of the planning phase. Five specific deliverables are envisioned: 1. The identification of an initial set of science applications/drivers best suited for development. 2. The definition of the software architecture and infrastructure required and a plan for its development. 3. The identification of the initial set of required physics components and a plan for their development and integration. 4. The definition of the requirements and a plan for verification and validation 5. The definition of the management structure and a program plan for the FSP

- How is the FSP planning activity being organized and managed?

The project team is organized into five groups, covering planning areas for the FSP itself: 1) science applications; 2) software architecture, frameworks and integration, 3) advanced modules and code verification, applied math and advanced algorithms; 4) experimental validation; and 5) management. Overall management for the project definition phase is led by the director (W.Tang) and the deputies for plasma science (M. Greenwald) and for advanced scientific computer research (D. Kothe). The management team is rounded out by the heads of the planning groups including A. Kritz, J. Cary, X. Tang, L. Diachin, and V. Chan. Altogether, personnel from 6 national

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labs, 2 private companies and 9 universities are directly funded for the planning activity.

- Who is involved in the FSP planning activity?

After a competitive peer-review in 2009, FES selected a national multi-institutional and multidisciplinary team of six national laboratories, nine universities, and two private companies to carry out a two-year detailed planning study for the FSP. The planning team (individuals listed on the FSP web-site (http//www.pppl.gov/fsp) is composed of scientists with a broad range of expertise in fusion plasma science (including theorists, computationalists, experimentalists, and material scientists) and also in applied mathematics, computer and computational science, and software engineering. The FSP PLANNING TEAM (6 national labs, 2 companies, & 9 universities) includes: W. Tang (PPPL/PU), D. Batchelor (ORNL), H. Berk (IFS), J. Brooks (Purdue U.), J. Cary (Tech-X/U. Colorado), V. Chan (GA), C.S. Chang (NYU), P. Colella (LBNL), L. Diachin (LLNL), P. Diamond (UCSD), M. Greenwald (MIT), D. Keyes (Columbia U.), D. Kothe (ORNL), A. Kritz (Lehigh U.), W. Nevins (LLNL), A. Siegel (ANL/U.Chicago), X. Tang (LANL), and G. Tynan (UCSD). In addition, strong input and contributions from the community are expected and currently being received.

- What is the schedule with expected deliverables for the FSP planning activity?

Beginning with the FSP Kickoff Meeting in July, 2009, information on this and all subsequent activities including FSP Program Advisory Committee (PAC) meetings will be posted on the FSP web-site at (http//www.pppl.gov/fsp). A first draft of the FSP conceptual design plan together with an associated program execution plan and other supporting draft documents is expected to be completed by January, 2011 with the final version delivered by July, 2011.

- Once the planning process is completed, how is the FSP expected to proceed?

The results of this careful planning study will help DOE-SC in its decision to launch the full FSP.

- What will the FSP planning activity produce?

A plan for the charter and execution the FSP in a way that ensures its goals and strategies are aligned with the needs of the DOE FES program and the fusion community at large -- including ITER. Specifically, the FSP “plan” will consist of a number of documents that will be constructed by and vetted with

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the broader fusion community. These will include a strategic plan, containing the FSP mission and vision; a validation plan, an experimental coordination plan, a management plan; an integration and outreach plan; a risk management plan; a requirements management plan; a program tracking plan; a data management and requirements plan; a change management plan; a quality management plan; an infrastructure plan; an implementation plan, and a project execution plan. This comprises the set of documents within the “FSP plan.” In addition, other written documentation is planned that will address, e.g., a proto-FSP assessment and possible other areas such as outreach, education, and training.

- How will the full FSP be managed?

The development of a sound management plan for the FSP is part of the ongoing planning study; a strong management structure based on project management principles is envisioned to ensure the success of a multi-institutional, geographically dispersed, large-scale research program with focused and prioritized deliverables that engages diverse scientific communities.

- How can I get involved in and contribute to the FSP planning activity?

Input, comments, and suggestions are actively sought on all aspects of the planning activity. The best way to get involved is by contacting one of the team members listed on the FSP web-site (http//www.pppl.gov/fsp). In addition there is a set of wikis, linked from the main FSP web page, for each of the planning groups. Follow links to request an account, which will allow you to add your own content to these sites.

Program

- How will the FSP collaborate with the FES theory program?

The FSP is expected to be a new program in FES that is independent of but strongly collaborating with the FES theory program, specifically in the areas of Science Drivers and Advanced Components. The FSP and the Theory program are jointly developing a list of key science drivers to meet FSP’s mission. Theory will help provide a firm scientific foundation and rigorous formulation of the physics models and identify limitations to approaches. Computational models developed by Theory, either reduced models or fundamental simulations, which meet established metrics would be candidates for adoption by FSP. The FSP will draw on resources in Theory for independent physics verification of code components. Physics capabilities

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will be continuously enhanced during the FSP under the Advanced Components team. The enhancements will be carried out in partnership with the current Theory program. In particular, the Theory program will be depended upon to explore alternate strategies that might eventually become part of the FSP.

- How will the FSP partner with FES experiments in order to validate simulation/modeling capabilities?

The FSP is expected to be a new program in FES that will strongly collaborate with but not provide direct funding for experiments or diagnostics development. More specifically, we anticipate strong interactions with experimental programs – both large and small – as essential elements for model validation. Discussions are underway to define mechanisms for joint planning of experiments and long-term strategic development of both code and experimental capabilities. We expect that the relationship between the FSP and the experiments would be on a basis similar to those defined by existing collaboration agreements that all of the major facilities maintain. We expect that the experiments will be important customers of FSP production codes.

- How will the FSP partner with ongoing FES simulation efforts (such as the FES SciDAC centers)?

The FSP will partner with the ongoing FES simulation efforts and especially the FES SciDAC centers in a complementary way with respect to physics component development and integration techniques. During the planning phase, these interactions will help identify the associated gaps in capabilities needed. It will also rely on these parallel efforts for continuing innovation to meet the evolving scientific and computational challenges of the FSP. The FSP will provide assistance in adapting appropriate existing physics components to the FSP framework.

- How will the FSP collaborate with the Advanced Scientific Computing Research (ASCR) program?

The FSP will collaborate with ASCR programs in three primary ways. First, the FSP planning exercise will identify existing ASCR math and computer science technologies (developed by either the SciDAC or base research program) that can be leveraged by the FSP program in the execution phase. Second, there are opportunities for longer-term research collaborations between ASCR and FES scientists to develop new algorithms, methodologies, or techniques that could be funded directly by

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the FSP or jointly by the ASCR base program and FES theory program. Third, FSP will establish connections to the ASCR facilities division including leadership class computing facilities (LCFs) and NERSC, to leverage expertise in developing and deploying advanced simulation codes on next generation high-performance computer platforms.

- How are the Science Drivers being selected and how will they relate to the Frameworks Advanced Modules, and Validation efforts in the FSP?

The science drivers are a set of compelling scientific problems chosen to focus FSP's initial research along with the development of physics modules and software architecture. These further serve to define and exercise the needed wide range of capabilities and to produce useful tools to the broader fusion community. Criteria for selecting problems would include: 1. A clear need for multi-scale, multi-physics integration; 2. Importance and urgency for the fusion program; 3. Readiness and Tractability; and 4. Opportunities to open up new lines of research or to develop new techniques for high-performance computing. To help in the selection, development roadmaps are being prepared for each potential science topic.

- What will the expected balance be between the Production and the physics R&D efforts within the FSP?

The FSP will carry out a multi-disciplinary research program in plasma physics, applied math and computer science required for integrated, multi-scale, multi-physics fusion simulation. At the same time, the FSP will release production versions of codes, software architecture, and services to the broader community. The resource balance between these activities is a subject of the current planning activity.

- Who will have access to the FSP products?

All members of the FSP program team and official collaborators will have full access to FSP software and data. We expect that all codes released for production can be used by members of the fusion community to the maximum extent possible within the constraints of any sensitive data (proprietary, export control, etc.) regulations. The products are expected to be released as open source with a liberal license (e.g., BSD, Eclipse, GPL).

Operations

- How will new FSP components be developed?

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FSP will develop its components in two ways. The first is to adapt/upgrade existing physics component codes developed by the SciDAC and base programs. The second is to fund new component development based on promising new approaches from ongoing exploratory research in the SciDAC and base programs.

- How will existing FES physics components be integrated and how would they be made ready for the FSP?

The design of the physics composition and task composition software suites will determine how physics codes will be integrated, with different kinds of coupling being used depending on the needs. In any case, a few standards are likely to emerge for integration: documentation, usability on LCFs, robustness, and ability to name input and output files.

- What are the options/approaches envisioned for physics and code integration in the FSP?

Task composition couplings (e.g. diagnostic to data analysis and visualization tools) could be done through scripting languages or more complex workflow tools. Data could be transferred through files when that is appropriate. More intensive couplings or those relying on complex communication patterns could be done through method invocations and MPI-style communicators. Certainly more methods will be considered as we go through the FSP planning process.

- What is the vision for the kinds of FSP infrastructure that might be required?

It is anticipated that the FSP will build and support infrastructure including some level of hardware, software, and cyber security (authentication and authorization).

- How will the Verification & Validation (V&V) and associated Uncertainty Quantification (UQ) program be carried out in the FSP?

<u>Verification</u>: The verification process assesses the degree to which a code (both in the advanced direct numerical simulation [DNS] and reduced models categories) correctly implements the chosen physical model. Mathematically, this includes dealing with the accuracy of numerical approximations, mesh/space and temporal discretization, statistical sampling errors, etc. Code verification also involves: (1) comparisons with theoretical predictions (e.g., threshold/onset conditions for instabilities, weakly nonlinear evolution, nonlinear saturation estimates, etc.); (2) cross-code benchmarking (codes based on different mathematical formulations/algorithms but targeting the

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same generic physics (e.g. -- finite difference, finite elements, spectral methods, implicit schemes, etc. and/or models such as Particle-in-Cell, Vlasov/Continuum, Hybrid PIC-Fluid, etc.); and (3) use of the method of manufactured solutions to test more complicated coupling of terms in the mathematical model . In particular, components and the framework are expected to be verified by their developer teams, who will embody the verification runs in regression tests.
Validation: The validation program will be carried out as a joint effort by the FSP and major experimental facilities. Potential contributions from smaller experiments at universities will also be encouraged. The FSP would not fund machine operations or diagnostic development but would support dedicated analysts and development of analysis tools such as synthetic diagnostics. We are in the process of gathering input for a collaboration plan, to be jointly agreed with the experimental facilities; a best practices document, which will serve as a technical guide for validation activities and a strategy for data management and documentation for all validation activities.

Uncertainty Quantification: Uncertainty quantification (UQ) is the quantitative characterization and reduction of uncertainty in applications related to variability of input data/model parameters and uncertainties due to unknown processes or mechanisms. UQ encompasses uncertainty analysis, sensitivity analysis, and design validation and calibration, among other activities. This is a broad and active area of research, and uncertainty quantification will take place in several parts of the FSP. Verification related uncertainties (e.g., discretization related uncertainties) will be quantified by the component and framework teams in broad sense, and validation related uncertainties (e.g., suitability of the mathematical model to capture the physics of interest) will be quantified by the validation team analysts, but it is also expected that publishers of computational results will carry out basic uncertainty studies. Efforts will be made in the FSP to provide a set of tools and techniques to help in carrying out these studies.

- How will the FSP interact with similar efforts and initiatives carried out by our international partners?

It is expected that the FSP will continue to interact with integrated modeling efforts in the EU and Japan where the focus has been on significantly extending the capabilities of currently operating production models. Future validation opportunities offered by relatively new international facilities in Asia (e.g., superconducting long-pulse facilities such as

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KSTAR in Korea and EAST in China) will be actively explored by the FSP.

- What are the plans for maintaining and supporting the FSP suite of codes after 15 years -- the nominal “official completion” of this Program?

While DOE has funded a number of code development efforts in the past, it is important to note that after the funding of these efforts was discontinued, the resulting codes were not supported or upgraded on a regular basis. As a result, many have fallen into a state of very limited use or even obsolescence. As noted earlier, the FSP has a longer-term vision extending 15 years into the future. If the FSP proves able to meet its mission and is adopted/productively utilized by the FES community to deliver valuable new scientific insights resulting from integration, a compelling case would be made for continuing support to extend even beyond this horizon – recognizing the fact that there will always be room for improvement on science-based predictive models of complex whole-device systems.