Science Drivers for FSP
Plans and Action Items

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Science Driver Issues for FSP

- What kinds of physics problems should drive FSP architecture and plans?
  - To what extent should FSP focus on serving existing experiments?
    - Should the goals be driven only by tokamaks?
  - To what extent should FSP focus on critical issues for burning plasma experiments?
    - Should the primary focus be ITER?
  - To what extent should the scope include more basic science issues?
    - Need for balance?
- How should we transition from existing capability to long term goals?
  - The most relevant existing computational capability includes
    - SciDAC prototype projects (CPES, FACETS and SWIM)
    - Integrated modeling codes (PTRANSP, ONETWO, TSC, and CORSICA)
    - NTCC Module Library
    - Basic SciDAC projects (turbulence, RF, MHD, energetic particles, …)
    - Are there other computational capabilities that should be considered, for example those developed outside the US, in establishing the science drivers for FSP?
  - What other capabilities affect the science drivers, e.g., theory, diagnostics…?
- Which physics problems should we focus on during first year or two?
  - How should we sequence longer term physics problem goals?

Evolution of Science Drivers for FSP

- The committees that led to the establishment of FSP considered these questions at various levels
  - In particular the FSP workshop committees discussed in 2007 the issue of FSP science drivers in significant detail
- The vision for FSP was well stated in the 2002 Integrated Simulation of Fusion Systems Report [http://www.isofs.info/FSP_Final_Report.pdf]:

  The ultimate goals of the Fusion Simulation Project are to predict reliably the behavior of plasma discharges in a toroidal magnetic fusion device on all relevant time and space scales. The FSP must bring together into one framework a large number of codes and models that presently constitute separate disciplines within plasma science …

- FSP panels sought to establish well defined, realizable visions for five, ten and fifteen years keyed to needs of ITER and DEMO projects
- One of our tasks is to review and to determine if the science drivers previously considered are the most appropriate and if so, how can FSP facilitate the advancement of these science drivers

Critical Scientific Issues for FSP

- To initiate an expanded FSP, it was determined at the 2007 FSP workshop that answers to the following questions are required:
  - What are the critical compelling scientific and technical issues that the fusion program faces for which computation is required?
    - What substantial contribution can computer simulation make that traditional theory or experiment, by themselves, cannot?
  - For each critical issue, what is the current state of the art and what is missing from the current capability?
    - What are the underlying models and algorithms that are used in computer simulations relating to the critical issues?
      - Modules that are required are often scattered among a variety of codes and are not consistent in level of sophistication
  - For each critical issue, what new capabilities are needed in order to produce simulations that will aid in addressing critical issues?
    - What investments in fusion science as well as computational science and infrastructure must be made to obtain solutions for the critical issue?
- At the FSP workshop it was recognized that there are many critical issues for which the solution requires advanced simulation capability
- Five critical issues were selected for more detailed consideration

Critical Issues for Burning Plasma Experiments to be Addressed by FSP

- **Disruption effects and mitigation**
  - ITER can sustain only a limited number of full-current disruptions
  - Important to predict the onset of a disruption and to take actions that minimize damage when a disruption occurs
- **Pedestal formation and transient heat loads on the divertor**
  - Pedestal height controls confinement
    - Simulation of onset and growth of pedestal needed to predict confinement
  - Large ELM crashes can damage the divertor
    - Require prediction of frequency and size of ELMs as well as the effect of stabilization techniques
- **Tritium migration and impurity transport**
  - Since tritium can migrate through the edge plasma to locations where it is hard to remove, we must predict the transport of tritium
  - Since impurities can dilute the deuterium-tritium fuel and degrade fusion power production, we must predict impurity influx and transport

Critical Issues for Burning Plasma Experiments to be Addressed by FSP

- **Performance optimization and scenario modeling**
  - Performance includes sustaining maximum fusion power production
    - Since each ITER discharge will cost about $1M, it is important to plan each discharge and to evaluate the results of each discharge carefully
  - Scenario modeling is used to plan new experiments
    - Since multiple experimental teams will be competing for ITER running time, teams with best scenario modeling capability may obtain more running time
  - Scenario modeling is used in data analysis
    - Validated simulations provide a way to embody our knowledge of fusion plasmas
- **Plasma feedback control**
  - Burning plasma regime is fundamentally new, with stronger self-coupling and weaker external control than ever before
    - Burning plasma experiments are designed to operate near parameter limits but must avoid damaging disruptions
  - Real-time feedback control essential to avoid disruptions and to optimize the performance of burning plasma experiments
    - Instability control includes the use of modulated heating and current drive, as well as the application of non-axisymmetric fields

Disruption Effects and Mitigation

- **Disruptions are initiated by large-scale instabilities**
  - **Conditions for disruptive instabilities determined by evolution of plasma profiles, which are a consequence of sources and sinks and transport**
- **Disruption simulation capability is scattered across many codes that are not seamlessly integrated together into a coherent framework**
  - **Complete nonlinear evolution disruptions extremely difficult to compute**
- **Comprehensive analysis of disruptions and mitigation approaches require new and integrated physics elements, which include:**
  - **Plasma-wall interaction, impurity transport, atomic radiation physics**
  - **Equilibrium and kinetic profile evolution**
  - **Nonlinear evolution of large scale instabilities**
  - **Runaway electron production**
  - **Effects of axisymmetric control actuators such as poloidal field coils**
  - **Effects of non-axisymmetric control actuators such as resonant magnetic field perturbation coils**

Pedestal Formation and Transient Divertor Heat Loads

- First-principles gyrokinetic simulations of the pedestal and scrape-off-layer are being developed by:
  - Center for Plasma Edge Simulation and the Edge Simulation Laboratory
- Gyrokinetic codes used to simulate pedestal formation and growth
  - Spatially axisymmetric gyrokinetic codes simulate neoclassical effects
  - Full 5-D turbulence simulation codes have been developed
    - Need to develop fully electromagnetic edge gyrokinetic simulations
- Two-fluid codes have been applied to modeling of the pedestal on transport and turbulence timescales
- Monte Carlo and fluid formulations used to model neutral transport
- Linear and nonlinear extended MHD codes used to model ELM triggering and ELM crash evolution
  - Kinetic effects on ELMs may well play a significant role
- Require multi-scale integration between plasma phenomena operating on turbulence, neoclassical, large-scale MHD, various atomic physics, and transport timescales, as well as coupling to core plasma

Tritium Migration

- Modeling of deuterium and tritium recycling involves wall material simulations, presently performed by simple 1D diffusion codes
  - Present experimental results indicate D/T penetrates much deeper into the material than simple models indicate
  - Impact of energy pulses from ELMs is believed important
- Plasma tritium transport modeled by 3D Monte Carlo ion/neutral codes
  - Rates for the large number of molecular and surface processes often have a large number of adjustable coefficients to fit complex experimental results
    - Adjusted to values substantially larger than expected from simple theory
- Time-dependent diffusion simulations of tritium retention within first few microns of wall materials must be coupled to edge transport codes
  - Multi-species, 2D, two-velocity kinetic ion transport codes need to evaluate collisional, neoclassical impurity transport in edge region, coupled to core
- Inter-atomic potentials need to be developed for ITER mixed materials
  - For use in 3D molecular dynamics simulations of sputtering
- Molecular dynamics results need to be supplemented by 2D kinetic Monte Carlo simulations of slower wall surface chemistry processes that also generate hydrocarbons

Impurity Production and Transport

- **Impurities produced by plasma-wall interactions and fusion products**
  - **Physical and chemical sputtering and evaporative release contribute**
    - **Impurity influx complicated by the presence of various wall materials, such as beryllium, carbon, tungsten, in different locations of the wall**
    - **Further complicated by impact of heat fluctuations during ELM cycles**
  - **Sufficiently high impurity influx can rapidly degrade fusion performance**
- **Chemical sputtering is not well understood, particularly for carbon wall**
  - **Empirically parameterized models, which utilize experimental data on material composition, surface conditions, wall temperature, incident plasma flux, and sometimes long-time exposure history**
  - **Extensions of the molecular dynamic sputtering database, mixed material simulation, and kinetic Monte Carlo simulations are needed**
- **Impurity transport simulations in scrape-off-layer need improvements:**
  - **Need to include 3D turbulence impact on multi-species impurities and coupling to kinetic transport**
  - **Gyrokinetic simulations of core, pedestal and scrape-off-layer are needed to predict impurity concentration and resulting effects on fusion performance**

Performance Optimization and Scenario Modeling

- **Full-featured integrated modeling codes such as TRANSP or ONETWO are large codes that were started 30 years ago**
  - They consist of a patchwork of contributions from a large number of people who were often working on isolated tasks under time pressure
  - The required models are often scattered among a variety of codes and are not consistent in their level of sophistication
  - Most of the codes are not modular, they do not use modern software engineering methods, and the programming practices do not always conform to accepted standards for reliability, efficiency, and documentation
  - As a result, these codes are difficult to learn, to run correctly, and to maintain
- **A new comprehensive whole device integrated modeling code framework is needed for scenario modeling**
  - In addition to a comprehensive collection of physics modules, the framework should include synthetic diagnostics and the tools needed to make quantitative comparisons between simulation results and experimental data
  - Tight coupling is needed for strongly interacting physical processes
  - Integrated framework should have options for first-principles computations
  - Simulations can make a substantial contribution in a way that traditional theory and experiment, by themselves, cannot

Plasma Feedback Control

- **Owing to its role as first burning plasma experiment, its nuclear mission, and its stringent licensing requirements, at time of its commissioning, ITER will be the most control-demanding tokamak ever built**
  - **Feedback control used to avoid disruptions and optimize performance**
  - **The need to certify high confidence control performance will place extreme demands on the physics simulation community**
    - **Will require an unprecedented amount of integration between frontier physics understanding and mission-critical control solutions**
- **Currently, 1-1/2D simulation codes include feedback actuator modules**
  - **Connection between these simulations and real-time control platforms has been demonstrate and used routinely on some devices**
  - **However, currently, there is minimal integration with other physical effects**
  - **Varying levels of accuracy, completeness, and validation, which are often insufficient for ITER requirements**
- **Needed for ITER Control Data Access and Communications system:**
  - **Control design models derivable from more detailed physics models**
  - **Full or partial shot integrated control scenario simulation capability**
  - **Modular infrastructure for flexibly using these products**

FSP Involves Interactive Physics

- A common feature of all the FSP physics science drivers is their interactive nature
  - Combination and coordination of multiple physics tools are needed
- The 2007 FSP workshop focused on the interaction of physical processes in tokamaks
  - Plasma phenomena are controlled by plasma properties and, in turn, plasma properties evolve as a result of physical processes -- for example
    - Flow shear affects transport which then affects rotation velocity, which then produces flow shear
    - Transport causes profiles to peak which can lead to the triggering of MHD instabilities, such as a sawtooth crash, which abruptly change the central profiles which results in a change in transport
- Numerous additional examples of the interactive nature physical phenomena are illustrated in a table that was developed for the report of the 2007 FSP workshop

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			
Neutrals	Gas puffing, wall recycling and NBI affect neutrals profile			Neutrals charge exchange with energetic particles	Influx of neutrals strongly affects pedestal density formation	Neutrals recycle at first wall

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
Neoclassical Tearing Modes	ECCD, LHCD for stabilization, rotation control	Bootstrap current model, threshold, intrinsic rotation, island seeding by sawtooth crashes	Anisotropic transport on onset threshold and saturation, effect on neoclassical polarization currents	Alpha loss due to magnetic island and stochastic; energetic particle effects on NTM	Helical B (via poloidal coupling with NTM) on pedestal	Remnant alphas
Resistive Wall Modes	Rotation, physics of the rotation stabilization; controllability with non-axisymmetric coils	Beta limit, intrinsic rotation, error field locking, error field amplification; RWM triggering by ELM	Rotation damping, nature of anomalous viscosity	Energetic particle beta on stability	Finite pressure and current in the edge need to be accounted for, helical B on pedestal	Disruption mitigation, currents in the SOL
$m = 1$ helical instability	$q(0)$ and rotation control	Instability onset, fast reconnection, saturation amplitude, global q evolution, NTM seed	Impact of topology on turbulence and back reaction on $m = 1$	Alpha stabilization, monster sawteeth, fishbones, alpha loss and redistribution	Impact of transient heat/ particle/ alpha's and helical B on pedestal transport and stability	Load to the wall and impurity production
Rotation and Flow Shear	RF/NBI are primary sources	Neoclassical transport-induced intrinsic rotation, error field damping, MHD continuum damping	Momentum transport and self-generated zonal flow	Rotation damping, NBI-induced toroidal rotation in the presence of Alfvén modes and MHD modes	Self-generated radial electric field in pedestal	Boundary conditions at first wall and tokamak structure

	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
Pedestal	Localized heating and current drive	Pedestal bootstrap current	L/H transition, connection to core, pedestal electron and ion transport, shear flow generation and sustenance	Energetic particle and ash transport; effects of energetic particle re-distribution on pedestal	L/H transition	Impurity flux
Edge Localized Modes	Localized CF, ELM affects ICRF and LHRF coupling; suppression of ELMs: RMP, pellet, shaping	Ballooning-peeling, bootstrap current, intrinsic and induced rotation, interaction with $m = 1$, NTM, RWM	Connection to core non-diffusive transport, self organized criticallity avalanches, inward impurity transport	Poloidal coupling to AE, induced transient alpha loss	Relaxation events, control by helical B, impurity and ash transport, interaction with pedestal zonal flow	Heat/ particle/ ash to wall, impurity and transport, radiation coupling
Internal Transport Barriers (ITBs)	ICRF and ECCD — local shear control for triggering and controlling ITB	Minimum q profile manipulation, island as ITB trigger, intrinsic rotation	Formation threshold and structure, all transport channels	Energetic particle interaction with ITB in the presence of Alfvén modes	Correlation between ITB and pedestal structure	
Field Error Penetration	Rotation control	NTV, layer physics, resistive wall mode, suppression of ELMs	Nature of viscosity in resistive layer			
Disruptions	Efficiency of mitigation by impurity injection; use of other actuators	Halo currents, runaway electrons; reconnection and impurity transport	Thermal / current quench; impurity transport	Runaway electron production/ confinement		Mitigation techniques (gas jet, pellets, *etc.*)

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
Wall Flux Out and Impurity Flux in	RF sheath-induced erosion	Sawtooth, NTM, RWM induced transient heat/ particle/ alpha pulse	Nature of particle and impurity transport in the core	Alfvén Eigenmodes, cascade, fishbone, EF-induced EP, and its loss	Transport channels throughout pedestal, ELM-induced transport pulse, helical field-induced transport	Plasma/ materials interaction, SOL connection to pedestal
Discharge Scenario	Full discharge controllability; burn control	Role of NTM in hybrid scenario; NTM control; effects of ELM control on scenario	Full discharge achievability and performance prediction	Alpha-heated discharge prediction; burn control	Heat and particle flux due to 2nd X-point; divertor control	Wall equilibration effects

Advances in Physics Components Essential if FSP is to Contribute to Advancing Plasma Science

- Many physics components are important in addressing critical issues in the integrated modeling of plasmas
- In order to optimize burning plasma performance, many of these components require substantial physics and computational advances
- To illustrate the advances required, four components required in an integrated simulation of a burning plasma were identified at the FSP Workshop but it was recognized that other components might have been chosen to illustrate the advances required
- Problems where FSP can contribute during its first and second years
  - Predict intrinsic rotation, L-H transition, density limit, suppression of ELMs, sawtooth period and effects, onset, location and height of internal transport barriers
- Through the interaction of SciDAC teams, as well as other research teams, FSP may advance the solution of problems like these
  - This effort would also help clarify how the existing SciDAC and integrated modeling activities will contribute to the goals of FSP
- New physics results are needed to build confidence in FSP

Examples of First Year Science Driver

- 2010 and 2011 DoE milestones provide examples of problems where FSP can contribute during its first and second years
  - One goal of the FSP effort would be the development of a predictive model for toroidal and poloidal momentum transport that could be used in the FSP integrated modeling code
- Through FSP, work on the milestones can be extended to a broader community effort by bringing several SciDAC teams and other research group together
  - SciDAC CPES, CEMM and FACETS projects can contribute to this research
- FSP can coordinate the interactions of the simulations of the individual processes
  - For example, disruptions involve transport to predict the profiles, which trigger the MHD instabilities, that result in disruption
  - The disruption, in turn, affects the disposition of energetic particles

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  - To what extent should FSP focus on critical issues for burning plasma experiments?
    - Should the primary focus be ITER?
  - To what extent should the scope include more basic science issues?
    - Need for balance?
- How should we transition from existing capability to long term goals?
  - What additional capabilities are required for the science drivers, including computational, theory, and diagnostic capabilities?
- Which physics problems should we focus on during first year or two?
  - How should we sequence longer term physics problem goals?