# **Science Drivers for FSP**

#### Arnold H. Kritz

Lehigh University

#### **On behalf of the Science Drivers Team**

Glenn Bateman Herb Berk John Cary Pat Diamond Martin Greenwald Scott Kruger Doug McCune Raffi Nazikian Phil Snyder Harold Weitzner Lehigh University University of Texas Tech-X Corp., University of Colorado University of California, San Diego Massachusetts Institute of Technology Tech-X Corp. Princeton Plasma Physics Laboratory Princeton Plasma Physics Laboratory General Atomic New York University

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### Outline

- FSP Science Drivers Objectives and Goals
- Vision for FSP Science Drivers
- Tasks for Science Drivers Team
- Example Questions to be Addressed by FSP ReNeW
- Examples of Gaps
- FSP Science Drivers Selection Criteria
- Provisional Science Drivers
- Examples of Application of Science Driver Criteria
- Work Plan During Definition Phase
- Definition Phase Work Breakdown Structures (WBS)



## FSP Science Drivers Objectives and Goals

- Science drivers are a set of compelling scientific problems chosen to focus FSP development
- Science drivers serve to
  - Motivate & prioritize production of useful tools for broader fusion community
  - Define and exercise the needed wide range of capabilities
- Key objective of FSP
  - Accelerate the predictive understanding and control of magnetic fusion experiments through the integrated modeling of multi-scale physics
    - By exploiting the computational power of emerging peta-scale, and eventually exa-scale, computers
  - Stakeholders major facilities, small experiments, ITER, advanced design projects, analytic theory, modelers, advanced simulation
- Goal of the FSP science drivers team
  - Articulate key issues that must be addressed through integration of multi-scale physical phenomena in fusion experiments
- Science objectives can be achieved only through close interaction between the plasma theory and experimental communities
  - Collaboration will ensure the fidelity of each physics module and the validity and relevance of the simulation results



### Vision for FSP Science Drivers

- Ultimately, the Fusion Simulation Project is expected to produce a kind of "numerical tokamak" or "fusion system simulation" to compute:
  - All relevant physical phenomena, e.g., particle distribution functions, turbulence spectra, large-scale instabilities, ...
    - From the magnetic axis to the plasma-facing wall
    - Bridging the gap from microsecond to whole discharge time scales
- It is expected that different researchers will use FSP in different ways:
  - A few heroic simulations will be carried out for whole-device modeling at the highest level of physics fidelity
  - Validated reduced models will be used for more rapid whole-device scenario simulations including start-up, shut-down and performance optimization
  - Some users will focus on particular parts of the plasma, such as the scrape-off layer, or particular physical phenomena, such as turbulence
    - FSP will enable focused research to be carried out in the context of self-consistent whole-device simulations
  - Some researchers will use FSP simulations to analyze and understand existing tokamak discharges and to improve design of new fusion experiments and facilities



### **Tasks for Science Drivers Team**

- Examine ReNeW, Exoscale, FESAC (Priorities, Gaps and Opportunities) and past FSP workshop reports and generate a list of science drivers
- Establish and apply criteria to prioritize and sequence science drivers
  - Evaluate component and framework plans in order to determine criteria and prioritization for both near term and longer term science drivers
- Get feedback from the community and get buy-in
  - Presentations and fact finding at fusion facilities and other research groups
  - Interact and iterate with other FSP activities (e.g., framework and components) to get feed back
    - Identify plans to acquire, develop and complete required physics modules
- Science drivers team will need to develop a plan and mechanism to monitor FSP progress in advancing science
- Document and disseminate science driver planning
- Establish independent review process for components and framework
- Science Drivers Team Activities
  - Minutes of conference calls available on Science Drivers Wiki

http://fspscidri.web.lehigh.edu/index.php/Main\_Page



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#### **Example Questions to be Addressed by FSP-ReNeW**

- How rapidly will large reactor plasmas rotate, and what effect does rotation have on performance limits?
- How will a fully steady-state reactor-relevant wall affect the core plasma performance, and what approaches can be used to control the erosion, transport, and redeposition of wall material?
- How do we adequately fuel the plasma and remove fusion reaction byproducts and how do we manage and control the tritium inventory in a steady-state reactor?
- How do the energetic particles and/or the background plasma turbulent transport, MHD equilibrium and RF driven currents respond to energetic particle modes and/or turbulence?
- Can we successfully and accurately predict the approach to a disruption event and initiate control techniques to avoid the disruption or, if a disruption becomes unavoidable, can we mitigate the consequences?



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#### **Example Questions to be Addressed by FSP-ReNeW**

- Can we accurately identify the physics trigger(s) for L-H transition, onset of edge and internal transport barriers, and the control of ELM crashes?
- Can we predict the coupling of radiofrequency, beam and pellet sources across the pedestal?
- How do alpha particles affect radiofrequency wave propagation and absorption and what possible transport effects from radiofrequency waves on alphas may be expected?
- How can modeling bridge disparate spatio-temporal scales that link different aspects of high-performance, steady-state burning plasma physics?
- Can the reliability of each component, as well as the framework connecting components, be improved to the point where integrated models can be used routinely to plan and analyze burning plasma experiments in ITER?



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### **Examples of Gaps**

- Structure, size and stability of H-mode pedestal
  - Need to fill gap in the spectrum between fine scaled turbulence and large scale instabilities
- Core turbulence and transport on transport time scales
  - Bridge turbulence and transport time scales
  - Turbulence in the presence of magnetic islands
  - Full electromagnetic treatment of turbulence and transport
- Integrated whole-device modeling
  - Tight coupling among heterogeneous components with high physics fidelity
    - From magnetic axis to first wall, from startup to shutdown
- Integrated scrape-off layer divertor plasma-wall interaction
  - Lack of reduced models for cross field transport
  - Coupling of atomic physics, plasma-wall interactions together with turbulence
- Onset, consequences and mitigation of disruptions
  - Full non-linear treatment of disruptions and their effects on plasma profiles
- Wave particle resonances
  - Self consistent coupling of alpha particle power and plasma transport in a burning plasma
  - Interaction of flow shear and energetic particle induced perturbations on the radial electric field due to the action of fast ion driven instabilities



## **FSP Science Drivers Selection Criteria**

- Criteria for selecting FSP scientific problems would include:
  - Clear need for multi-scale, multi-physics integration:
    - Topic should require the capabilities envisioned for the FSP beyond scope of the current modeling programs
    - Solving the scientific problem should demonstrate that FSP "is more than the sum of its parts"
  - Importance and urgency:
    - Importance measured against the OFES mission to create knowledge base needed for an economically and environmentally attractive fusion energy source
    - Should answer questions or address scientific issues integral to knowledge base
    - Urgency should take into consideration schedules, dependencies and critical paths for program elements that the FSP would support

#### - Readiness and Tractability:

- Underlying physics along with the required applied math, computer science and computing platforms should be sufficient to initiate work at outset of FSP
- Need for the FSP to impact ongoing research at an early date should also be considered
- Some reasonably clear path toward solving the research problem, posed by the topic, should be envisioned
- Opportunity to open up new lines of research:
  - Attacking the problem should offer possibility of new insights or potential breakthroughs, particularly those not accessible by other means



## **Provisional Science Drivers**

- Integrated Scrape-off Layer, Divertor, Plasma Wall Interactions
  - Turbulent perpendicular transport, classical parallel transport physics, atomic physics and plasma wall interactions
  - Issues include:
    - Power and particle loads on divertor plates and first wall impurity generation, erosion, redeposition and transport;
    - Fuel deposition/tritium retention; fueling and density limit;
    - Choice of material; temperature for Plasma Facing Components;
    - Effects of off-normal events;
    - First wall conditioning dust generation; transport and effects;
    - Recycling and pumping, flow boundary conditions;
    - Boundary conditions for temperatures, density and flow at last closed flux surface including turbulence spreading between sol and pedestal

#### • Structure, Size and Stability of H-mode Pedestal

- Nonlinear MHD, turbulence, ELMs and other relaxation mechanisms
- Issues include:
  - Long-time solutions to turbulence problem
  - Scale separation between nonlinear MHD and nonlinear electromagnetic turbulence
  - Finite Larmor radius effects in narrow pedestal region



## **Provisional Science Drivers**

- Nonlinear Turbulence and MHD on Transport Time Scales
  - Electron and ion channels, particle and momentum transport using gyro-kinetic transport physics extended to transport time scales
  - Issues include:
    - Evolution of equilibrium profiles of temperature, density and rotation frequency
    - Self-generated and driven rotation
    - Interaction between turbulence and magnetic islands or MHD modes
    - Local versus non-local turbulence and transport
- Integrated Whole-Device Modeling
  - Multi-physics, multi-scale integration to compute turbulence spectra, onset and consequences of large-scale instabilities, and particle distributions as a function of space and time
  - Issues include:
    - Strong interactions between the different physical processes that occur on a wide range of different time and space scales
    - Used for scenario modeling (including start-up and shut down), optimization of discharge parameters (such as maximizing fusion power production) and the development of discharge control techniques
    - Self-consistent simulations are also used for testing theoretical predictions and validation of models by comparison with experimental data



## **Provisional Science Drivers**

- Detection Avoidance and Mitigation of Disruptions
  - Mitigation requires integration of MHD instability modeling, atomic and radiation physics, plasma wall interactions, and relativistic electron physics
  - Issues include:
    - Reliable predictions of triggering conditions leading to onset of disruption
    - Reliable predictions of nonlinear evolution of disruptions including rapid evolution of temperature, current density, fast particle and density profiles
    - Interaction with plasma facing wall

#### Wave-Particle Resonances

- Wave coupling and propagation, wave-particle interactions, nonlinear plasma responses, generation of waves from non-Maxwellian distributions
- Issues include:
  - Antenna or launcher coupling; wave propagation and damping; RF sheaths
  - Plasma response heating, current drive; flow drive; loss or redistribution of fast particles;
  - Nonlinear stability of energetic particle modes
  - Computation of saturated mode amplitudes
  - Anomalous velocity space diffusion; impact on alpha heating
  - Effects of background turbulence



### **Science Driver Questions**

- What is need for integration or what is the integration aspect?
- What is the physics challenge?
- Why is the science driver important and urgent?
- To what extent is science driver ready to be addressed and tractable?
- Will the science driver provide an opportunity to open up new lines of research?
- What are examples of issues to be addressed?
- Why can existing SciDAC projects not address the questions associated with the science driver?
- Why will it be possible to address these questions can by FSP?



### Integrated SOL-Divertor-PWI

#### • Scope

- Simulations span collisional plasma at bottom of pedestal, scrape-off-layer (SOL), the divertor, and the front surface of the first wall
  - At material boundary, include only the first few microns of the first wall
  - Modeling includes phenomena such as recycling, sputtering, and fuel retention
- Importance and urgency
  - Fusion reactors represent a tremendous extrapolation in power loading and pulse length
  - Simultaneous matching of SOL and core dimensionless parameters requires integrated edge modeling
  - Improved understanding and predictability will affect operating limits, choice of materials, geometry, and operating temperature for reactors
    - Power and particle loads on divertor plates and first wall
    - Impurity generation, erosion, redeposition and impurity transport
    - Fuel deposition/tritium retention
    - Effects of off-normal events
    - Dust generation
    - Fueling and density limit
    - Recycling and pumping
    - Production and effects of RF sheaths



### Integrated SOL-Divertor-PWI

- Physics Challenges
  - Anomalous cross-field transport has a dominant influence
  - Lack of clear spatial scale separation; large amplitude of fluctuations high degree of intermittency; coupling to atomic and material physics
  - Missing physics includes
    - Turbulent transport in scrape off layer
      - More complete fluid (short mean-free-path) codes especially with correct vorticity equations
      - Matching fluid and gyrokinetic results at appropriate limits (especially vorticity)
      - Proper calculation of self-consistent E field and self-generated flows (requires keeping higher order terms)
      - Proper treatment of open field lines (no flux surface averaging)
    - Issues with ordering: scale separation and large fluctuations
    - Fully integrated divertor physics including private flux region and X-point
    - Sheath physics including transmission factor for heat loads, also RF sheaths
    - Plasma-wall interactions
    - Multi-scale material physics including chemistry and morphology
    - Self-consistent solution in realistic 3D geometry



## Integrated SOL-Divertor-PWI

#### • Tractability

- Current research is yielding better sets of equations, which begin to address the shortcomings
- Experimental measurements are quite good in the region of the plasma (and could be significantly improved without enormous expense)
- In situ diagnostics for surface analysis will be coming on line in a few years
  - More parameters can be measured and spatial coverage is better than in core

#### New lines of research

- Success will provide greatly improved models for the plasma at the boundary between open and closed field lines
  - Temperature, density and flow profiles
  - Viscosity and turbulence spreading
  - Fueling and density limit
- Necessary for understanding the behavior of the core plasma and for whole device modeling
- Integration
  - Multi-physics phenomena including collisional and turbulent transport, neutral transport, atomic physics and material physics
  - Generation of impurities via sputtering through RF-produced sheaths broadens the integration still farther
  - Wide range of spatial and temporal scales are involved



#### Integrated Whole-Device Modeling

#### • Need for integration:

 Simulation of plasma evolution requires self-consistent combinations of all relevant physical phenomena in tokamak discharges

#### Physics and computational challenge

- Compute turbulence spectra, onset and consequences of large-scale instabilities, and particle distributions as a function of space and time using self-consistent combinations of all of the relevant physical phenomena
- Strong interactions occur between the different physical processes that occur on a wide range of different time and space scales
  - All relevant modes of turbulence and channels of transport must be included along with relevant large-scale instabilities for self-consistent whole-device simulations
    - Transport (driven by turbulence, charged particle drifts and collisions) affects plasma profile evolution, which, in turn, impacts large-scale instabilities, which then alter plasma profiles, which then alter transport
  - All interacting physical phenomena must be included in order to make stand-alone predictions that go beyond limited extrapolations from existing experimental data



### **Integrated Whole-Device Modeling**

#### Importance and urgency

- Clear and compelling need for modern whole-device integrated modeling code
  - Span entire plasma from magnetic axis to first wall
  - Bridge gap between the microsecond time scale of basic physics phenomena and hundreds of seconds time scale for duration of plasma discharges

#### Readiness and tractability

- Recent FSP prototype SciDAC projects focus on combining pairs of regions or physical phenomena in high-performance computations
- Given progress in FSP prototype projects, as well as the mature capability developed for comprehensive integrated modeling using reduced models
  - Integration of all of the physics components is tractable in a comprehensive framework for high performance, whole-device modeling

#### Opportunities for new lines of research

- Provides opportunity to investigate the physics of transport, computed self-consistently with turbulence, sources and sinks
  - In all regions of the plasma including the scrape-off layer
- Investigate the interactions between turbulence, MHD instabilities and fast particles driven by radio-frequency and neutral beam injection
- Scenario modeling and detailed comparisons with experimental data using comprehensive whole-device simulations with high-fidelity physics
  - Significant improvements to our basic understanding of physical phenomena



### **Integrated Whole-Device Modeling**

#### Examples of issues to be addressed

- Reliable, validated, self-consistent predictions of evolution of plasma profiles from magnetic axis to the plasma-facing wall in variety of tokamak discharges
  - Include predictions of height and width of internal and edge transport barriers
  - Include turbulence spectra and the distributions of all particle species
- Complete, reliable scenario modeling from discharge start up to shut down
  - Include free-boundary evolution of plasma shape, evolution and coil currents
- Prediction, control and mitigation of the onset and consequences of large-scale instabilities (such as sawteeth, ELMs, NTMs, and RWMs)
  - Include interactions with turbulence, transport, sources, sinks and fast particle distributions
- Why these questions cannot be addressed by existing SciDAC projects
  - Required capabilities involve strong interaction among different physical phenomena and different parts of the plasma
    - Consequently, these issues cannot be addressed by focusing on only one or few physical phenomena or one region of the plasma.
- Why these questions can be addressed by FSP
  - Capabilities require integration of high-performance components central to FSP in order to investigate the strong interaction among different physical phenomena and different parts of the plasma with high physics fidelity



## Work Plan

- July 2009 through September 2009
  - Established plan of action at the FSP planning meeting, 15 16 July 2009
  - Regularly scheduled conference calls
  - Established an FSP Science Driver Wiki web page
    - Place minutes of Conference calls on Wiki
    - Populate Wiki with work and discussions of Science Driver Committee
  - Drafted and agreed on statement of FSP science drivers and goals
  - Drafted and agreed on statement of FSP science drivers selection criteria
    - These selection criteria will be used to evaluate FSP science drivers
  - Initial Gap analysis
  - Developed an initial draft of six FSP science drivers
    - Discussed application of selection criteria for each science driver
    - Initial description of FSP science drivers will be used
      - As the starting point for obtaining community input and
      - For guiding the FSP components and framework
- October 2009 through December 2009
  - Develop and refine presentations of science drivers to community
  - Finalize evaluation criteria for science drivers
  - Establish a preliminary prioritization of science drivers
    - Prioritization is based primarily on importance and urgency



## Work Plan cont.

- October 2009 through December 2009 continued
  - Establish preliminary sequencing of drivers based on considerations of
    - Logical chain of dependence (e.g., equilibrium needed before determining stability)
    - Readiness and tractability
    - Importance and urgency
  - Present status of science drivers to Components and Framework committees
  - Continue to document and disseminate results through Wiki and e-mail
- January 2010 through March 2010
  - Joint Workshop with Framework and Components Committees
  - Establish metrics for evaluation of community input
  - Inform community of criteria used to prioritize science drivers and metrics for evaluating community input
  - Gather input from community on FSP science drivers
    - Carry out evaluation of community input
    - Continue Gap analysis
  - Modify evaluation criteria as needed to address community needs
  - Modify prioritization of science drivers in response to community input
  - Modify sequencing of science drivers in response to community input
  - FSP Science Drivers Committee meeting at end of quarter
    - Finalize draft of prioritized and sequenced science drivers
    - Document reasons for the choices that were made



## Work Plan cont.

- April 2010 through June 2010
  - Establish draft of procedures and standards for independent testing and evaluation of
    - FSP components, FSP framework and FSP validation
  - Develop draft of use cases for FSP software
  - Modify selection, prioritization and sequencing of science drivers as needed
  - Describe independent testing and evaluation procedures and standards to FSP Components, Framework and Validation committees
    - Respond, as needed, to feedback from those committees
  - Document and disseminate results of committee

#### • July 2010 through September 2010

- Establish plan for FSP Science Drivers team to manage independent testing and evaluation of FSP components, framework and validation
- Develop sample cases to illustrate the application of procedures, standards and plan for independent testing and evaluation of FSP components, framework and validation
- Make presentations to the community on procedures, standards and plan for independent testing and evaluation of FSP components, framework and validation
  - Respond to input from the community and make modifications, as appropriate
- Document and disseminate results of committee



### Work Plan cont.

- October 2010 through December 2010
  - Finalize selection, prioritization and sequencing of FSP science drivers
    - Establish systematic way to evolve and modify prioritization and sequencing of FSP science drivers as needed throughout the FSP
  - Finalize procedures and standards for independent testing and evaluation of FSP components, framework and validation
    - Establish systematic way to modify procedures and the standards as needed throughout the FSP
  - Finalize plan for FSP Science Drivers team to manage independent testing and evaluation of FSP components, framework and validation during the FSP
  - Finalize documentation of work carried out by the FSP Science Drivers team
  - Present the work done by the FSP Science Drivers team to fusion community

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#### Definition Phase Work Breakdown Structures (WBS)

- **1. Prioritized and sequenced descriptions of FSP Science Drivers** 
  - 1.1 Description of evaluation criteria for science drivers
    - **1.1.1 Metrics for evaluation of community input**
  - **1.2 Gaps analysis for FSP science drivers**
  - 1.3 Annotated list of science drivers with description for how each science driver addresses the selection criteria
  - 1.4 Modification of science drivers in response to community input
    - **1.4.1 Input from community on annotated list of science drivers**
  - 1.5 Documentation of prioritized and sequenced descriptions of science drivers
  - 1.6 Dissemination of prioritized and sequenced descriptions of science drivers
- 2. Procedures and standards for independent testing and evaluation of FSP components, framework and validation
  - 2.1 Description of use cases for FSP software
  - 2.2 Input from community on procedures and standards for independent testing and evaluation of FSP components, framework and validation
  - 2.3 Documentation of procedures and standards for independent testing and evaluation of FSP components, framework and validation
  - 2.4 Dissemination of procedures and standards for independent testing and evaluation of FSP components, framework and validation



