Fusion Simulation Project

(Whole Tokamak Plasma Modeling)

FSP Committee and Panels

Presented by

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FSP Objective and Motivation

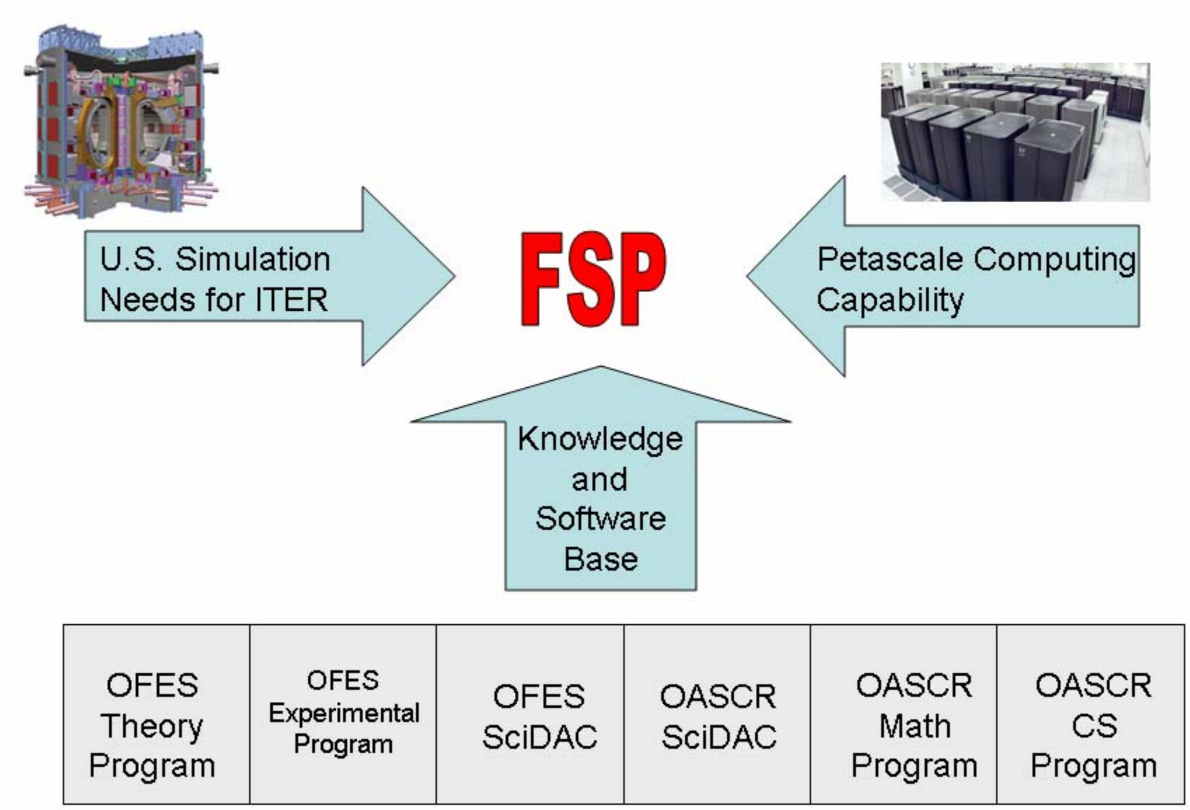
- Primary objective of Fusion Simulation Project (FSP)
  - Create high-performance software to carry out comprehensive predictive integrated modeling simulations, with high physics fidelity, relevant to ITER and other tokamaks
    - Leadership class computers are necessary to achieve this objective
- Urgent need for FSP motivated by fact that there are significant physics problems associated with ITER discharge scenario planning and control
  - Each discharge in ITER is expected to cost about a million dollars
    - Whole device computer simulations needed to optimize discharge scenarios
    - Experimental team with best scenario modeling will have a competitive advantage
  - Prior to completion of ITER construction, controls must be developed to suppress large scale instabilities that can adversely affect confinement
    - These instabilities include giant sawteeth and neoclassical tearing modes
  - Accurate predictions are needed for
    - Edge transport barrier that enhances the core plasma confinement
    - Edge instabilities that cause fluctuations in power to the divertor and first wall
    - Turbulence that leads to core and edge transport
- Verified and validated comprehensive integrated modeling capability is essential to support burning plasma experiments
  - Requires well supported theory and experimental fusion programs

FSP Background

- Previous Fusion Simulation Project (FSP) to address questions outlined in charge letter, February 22, 2002
  - Develop 5-6 year initiative the goal of which is develop an improved capacity for Integrated Simulation and Optimization of Fusion Systems
- FESAC appointed committee to develop a roadmap
  - Final FESAC Report December 2002
    - http://www.isofs.info/ FSP_Final_Report.pdf http://www.isofs.info/FSP_Appendix.pdf
  - Fusion Simulation Project (FSP) envisioned as a 15 year, $25M/year multi-institutional project
    - Develop a comprehensive simulation capability for magnetic fusion experiments with a focus on ITER
  - Recommended an approach through Focused Integration Initiatives
    - Coupling pairs of components before moving to whole device modeling
- OFES formed an FSP Steering Committee in 2003
  - Develop project vision, governance concept, and roadmap for the FSP
  - Recommends that the FSP consist of three elements:
    - Production component, a research and integration component, and a software infrastructure component
  - Final report in Journal of Fusion Energy, Vol. 23, No. 1, March 2004

Driving Forces for FSP

- **There are three driving forces for FSP:**
  - **Urgent need for a burning plasma simulation capability**
  - **Emergence of petascale computing capability**
  - **Knowledge and software that has been assembled under OFES and OASCR research programs**



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Context for FSP

- Computer plasma physics simulations have become significantly more sophisticated in recent decades
  - The first round of SciDAC projects concentrated on simulations of individual physical phenomena
    - Development of high fidelity physics models for individual physical processes needs to continue
  - The second round of SciDAC projects combined pairs of processes
    - RF + MHD, edge turbulence + MHD, edge + core
  - FSP is intended, after 15 years, to combine all relevant physical phenomena in comprehensive tokamak plasma simulations
    - In the first 5 years, there will be focus on a limited number of problems for which advanced simulation capability can provide exciting scientific deliverables that substantially impact realistic predictive capabilities
- Computer hardware is evolving at a very rapid rate
  - Within the next five years, we will be in age of petascale computing (10^{15} FLOPS) with massively parallel computers
  - Integrated modeling is particularly challenging because of the diverse physics and algorithmic modules
- FSP will develop comprehensive modeling of whole tokamak plasma
  - With simultaneous interactions of multiple physical processes treated in a self-consistent manner
  - Use modules with much improved physics fidelity

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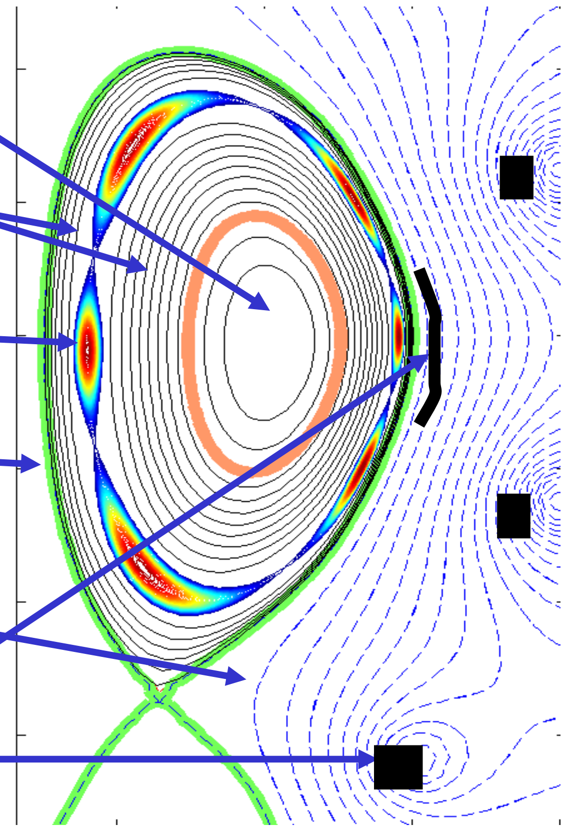
Elements of an Integrated Tokamak Modeling Code

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



Core & Edge Transport

Plasma Turbulence

Large Scale Instabilities

MHD Equilibrium

Heating Current Drive

Plasma-Wall Interactions

Atomic Physics

Radiative Transport

Energetic Particles

Physics is Interactive

- Many physical processes in tokamaks interact strongly
  - Whole device integrated modeling codes are needed to simulate strongly interacting physical processes observed in experiments
- Examples of interacting processes:
  - Large scale instabilities can interact and can strongly modify plasma profiles which in turn can affect the driving mechanisms producing instabilities
    - Sawtooth oscillations (internal kink/tearing modes) redistribute current density, thermal particles and fast particle species and seed neoclassical tearing modes
    - Neoclassical tearing modes (NTMs) are very sensitive to current and pressure profiles and produce flat spots in those profiles
    - Energetic alpha particles (fusion products) can excite global instabilities that can redistribute or remove these particles before they deposit their energy
  - Boundary conditions strongly affect core plasma profiles
    - H-mode pedestal height, normally limited by ELM crashes, controls core temperature profiles since anomalous transport is “stiff”
    - Wall conditioning has a strong effect on discharge performance
  - Distortion of velocity distribution due to slowing down of fast ions from NBI, RF and fusion reactions need to be included in gyrokinetic turbulence codes
    - Fast ions are redistributed by large scale instabilities and slowing down time is affected by plasma profile changes caused by sawtooth crashes

Questions and Plan for FSP

- Current funding of simulation efforts clearly insufficient to achieve FSP requirements
  - Dramatic increase in funding is required if FSP goals are to be achieved
- To initiate FSP, it is necessary to answer the questions:
  - What are critical technical issues facing the fusion program?
    - How can high performance computer simulations contribute to the resolution of these issues?
  - What substantial contribution can computer simulation make that traditional theory or experiment, by themselves, cannot?
  - What new contributions can result from advances in physics models, algorithms, software, and computer hardware?
    - What investments in fusion science as well as computational science and infrastructure must be made to obtain the needed answers?
  - How should the Fusion Simulation Project be organized and managed to address these critical technical issues?
- To obtain required answers, OFES and OASCR formed a Fusion Simulation Project committee in January 2007

http://www.lehigh.edu/~infusion

Possible FSP Budget Scenario

Provided by Steve Eckstrand at FSP Workshop

OFES and OASCR Fusion SciDAC Funding (Million FY2008 $)					
	Core SciDAC Funding		FSP Funding		
Fiscal Year	Collaboratory (OASCR)	SciDAC R&D (OFES)	Proto-FSP/ FSP (OFES)	Proto-FSP/ FSP (OASCR)	Total SciDAC Funding
2007	0	3	3/0	3/0	9
2008	0	3	3/0	3/0	9
2009	0	3	TBD	TBD	~11
2010	0	3	TBD	TBD	~16
2011	0	3	TBD	TBD	~22
2012	0	3	TBD	TBD	~25
2013	0	3	TBD	TBD	~28
2014	0	3	TBD	TBD	~28
2015	0	3	TBD	TBD	~28
2016	0	3	TBD	TBD	~28
2017	0	3	TBD	TBD	~28
2018	0	3	TBD	TBD	~28

FSP Committee

- **Co-Chairs: Arnold Kritz (Lehigh Univ.)**
  David Keyes (Columbia Univ.)
- **Phil Colella (LBNL)**
- **Martin Greenwald (MIT)**
- **Dan Meiron (Cal Tech)**
- **Scott Parker (Univ. Colorado)**
- **Cynthia Phillips (PPPL)**
- **Tom Rognlien (LLNL)**
- **Andrew Siegel (Univ. Chicago/ANL)**
- **Xianzhu Tang (LANL)**
- **Pat Worley (ORNL)**
- **Workshop was held May 16-17, 2007**
  - **FSP Committee members (and scribes) continued on Friday, May 18, to work on a draft of workshop report**
  - **Draft of FSP report will be available to FESAC sub-panel by June 30**

FSP Panels

Project Structure and Management

- Phil Colella – LBNL
- Martin Greenwald – MIT
- David Keyes – Columbia
- Arnold Kritz – Lehigh
- Don Batchelor – ORNL
- Vincent Chan – GA
- Bruce Cohen – LLNL
- Steve Jardin – PPPL
- David Schissel – GA
- Dalton Schnack – Wisconsin
- Frank Waelbroeck – Texas
- Michael Zarnstorff – PPPL

Integration and Management Code Components

- Dan Meiron – Cal Tech
- Tom Rognlien – LLNL
- Andrew Siegel – ANL/U. Chicago
- Michael Aivazis – CalTech
- Rob Armstrong – Sandia
- David Brown – LLNL
- John Cary – Tech-X
- Lang Lao – GA
- Jay Larson – ANL
- Wei-Li Lee – PPPL
- Doug McCune – PPPL
- Ron Prater – GA
- Mark Shepherd – RPI

FSP Panels

Status of Physics Components

Scott Parker – U. Colorado
Cynthia Phillips – PPPL
Xianzhu Tang – LANL

Glenn Bateman – Lehigh
Paul Bonoli – MIT
CS Chang – NYU
Ron Cohen – LLNL
Pat Diamond – UCSD
Guo-Yong Fu – PPPL
Chris Hegna – Wisconsin
Dave Humphreys – GA
George Tynan – UCSD

Required Computational and Applied Math Tools

Phil Colella – LBNL
David Keyes – Columbia
Pat Worley – ORNL

Jeff Candy – GA
Luis Chacon – LANL
George Fann – ORNL
Bill Gropp – ANL
Chandrika Kamath – LLNL
Valerio Pascucci – LLNL
Ravi Samtaney – PPPL
John Shalf – LBNL

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Questions Addressed for Critical Issues

- What are the compelling scientific issues for which computation is required?
  - Five issues are identified that can significantly impact success of ITER and burning plasma experiments
- What is the current state of the art and what is missing from the current capability?
  - Underlying models and algorithms that are used in computer simulations relating to the critical issues are identified
    - Modules that are required are often scattered among a variety of codes and are not consistent in level of sophistication
- What new capabilities are needed?
  - Capabilities needed to carry out simulations that will aid in addressing critical issues
  - Deliverables needed to produce these new capabilities are described for 5, 10 and 15 year time frames

Critical Issues for Burning Plasma Experiments to be Addressed by FSP - 1

- **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 heat fluctuations to 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 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, must predict the transport of tritium
  - Since impurities can dilute the deuterium-tritium fuel and degrade fusion power production, must predict impurity influx and transport

Critical Issues for Burning Plasma Experiments to be Addressed by FSP - 2

- 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 likely to get most 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
  - 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

Physics Components Essential for Integrated Burning Plasma Simulations

- **Core and Edge Turbulence and transport**
  - **Turbulence simulated with nonlinear gyrokinetic codes**
  - **Must link turbulence with transport on a much longer time scale**
- **Large-scale instabilities**
  - **Includes neoclassical tearing modes, edge localized modes, sawtooth oscillations, resistive wall modes, and toroidal Alfven eigenmodes**
  - **Simulated using nonlinear extended MHD codes**
- **Sources and sinks of heat, momentum and particles**
  - **Includes neutral beam injection, radio frequency and nuclear fusion**
- **Energetic particle effects**
  - **Produced by fusion reactions, neutral beam injection, radio frequency**
  - **Can drive instabilities which, in turn, can eject energetic particles**
- **Other components include edge physics, equilibrium, atomic physics …**
- **Physics components are important in addressing critical issues**

Integration and Management of Code Components

- In fusion research, FSP represents a new level of large scale integration of high performance simulation codes
  - Very large project, which requires geographically distributed collaboration because expertise is distributed
- Advances in component architecture are critical
  - To facilitate large number of people working simultaneously on a large code
- FSP will require different levels of integration across:
  - Time scales, spatial regions, different physical phenomena
- Legacy and recently written codes will play a role in early stages of FSP
  - FSP should make use of the expertise embodied in existing codes
  - FSP must satisfy the large user base of currently used codes
- In managing codes, there is trade-off between rapid development and code stability
  - Software tools will help manage code development and maintenance
  - Investments are needed for software design, repository management, release management, regression suites and documentation
- Software tools needed to enhance connection between simulations and experiments

Applied Mathematics in FSP - Research Areas

The list below is not an exhaustive list but rather a list of most likely research topics in applied mathematics within the scope of the FSP

- **Fully implicit Newton-Krylov methods**
  - For research codes (*e.g.* extended MHD)
  - For coupled systems ("implicit" coupling)
  - Physics-based preconditioners
- **Adaptive Mesh Refinement methods**
  - Higher order spatial and temporal
  - Time implicit AMR methods
- **Scalable solvers**
  - Iterative
  - Sparse but special structures (block-dense)
- **Adaptive fast-transform and pseudo-spectral methods**
- **Applied math issues in multi-physics coupling**
  - General applied math issues concerning consistency of coupled formulation, convergence, accuracy
  - Methods such as projective integration (a la Kevrekidis' "Equation-Free" approach) may be useful for linking disparate time scales

Computer Science Areas in FSP

- Scientific data management and mining
  - Transparent sharing of data
  - Exploit scientific data mining for predictive simulations and to interpret experiments
    - Utilize modern database-like file storage approaches
- Scientific data analysis and visualization
  - Develop reliable quantitative scientific insight from raw data
- Software engineering
  - Trusted, maintainable, extensible, flexible, predictive integrated simulation model
- Performance engineering
  - Performance portability, performance instrumentation, frequent performance assessment and regression studies, performance characterization
- Successful exploitation of high performance computing resources
  - Identify achievable performance and suitability for massively parallel computing, for code, for algorithm, and for problem instance
- User interface to make complex FSP code usable

Verification and Validation

- **Verification assesses the degree to which a code correctly implements the chosen physical models**
  - Sources of error include algorithms, spatial or temporal gridding, numerics, coding errors, compiler bugs, or convergence difficulties
  - Code verification activities include:
    - Software quality assurance, which is particularly difficult on massively parallel computers
    - Removing deficiencies in numerical algorithms, which involves comparing computational solutions with benchmark solutions, analytical solutions, manufactured solutions, and heroically resolved numerical solutions
  - Solution verification is referred to as numerical error estimation
- **Validation assesses the degree to which a code describes the real world**
  - Model validation emphasizes the quantitative comparison with dedicated high-quality validation experiments
  - Predictive estimation is characterization of errors from all steps in sequence of modeling process
    - Leads to probabilistic description of possible future outcomes based on all recognized errors and uncertainties

Five-year Deliverables

- New powerful integrated whole device modeling framework that uses high performance computing resources to include the most up-to-date:
  - Global nonlinear extended MHD simulations of large scale instabilities, including effects of energetic particle modes
  - Turbulence and transport modeling (core and edge)
  - Radio frequency, neutral beam, and fusion product sources of heating, current, momentum and particles
  - Edge physics, including H-mode pedestal, edge localized modes, atomic physics, and plasma-wall interactions
  - Range of models that include fundamental computations
  - Stringent verification methods and validation capabilities
  - Synthetic diagnostics and experimental data reconstruction to facilitate comparison with experiment
- State-of-the-art data archiving and data mining capabilities
- Production system to provide wide accessibility to a large user base
  - Verification and Validation achieved through widespread use of code
  - State-of-the-art visualization capabilities
- Provide capability to address critical burning plasma issues using high fidelity physics models and a flexible framework on petaflop computers

Ten and Fifteen-year Deliverables

10-year goal: Develop advanced and thoroughly tested simulation facility for initial years of ITER operation

- **Use high performance computations to couple turbulence, transport, large scale instabilities, radio frequency, and energetic particles for core, edge and wall domains across different time and spatial scales**
  - **Pair-wise coupling will evolve to comprehensive integrated modeling**
- **Ability to simulate active control of fusion heated discharges using heating, fueling, current drive, and 3-D magnetic field systems**

15-year goal: Unique world-class simulation capability that bridges the gap between first principles computations on microsecond time scales and whole device modeling on the time scales of hundreds of seconds

- **Provide integrated high fidelity physics simulations of burning plasma devices that include interactions of large scale instabilities, turbulence, transport, energetic particles, neutral beam and radio frequency heating and current drive, edge physics and plasma-wall interactions**

FSP Management

- FSP - a scientific development and focused research effort of unprecedented size and scope in U.S. fusion theory and supporting computational science and applied mathematics research programs
  - A strong and well-coordinated management structure is required
    - OFES and OASCR will specify the requirements in the request for proposals
    - Submitted proposals will provide detail on how the project will be structured and managed to achieve its goals
- Sample FSP Structure
  - Lead institution for FSP that is chosen by an open, competitive process
    - Responsible to DOE for meeting the project goals and milestones
    - Assemble management team that will coordinate and insure the success of the elements of the project
  - Management Coordinating Committee
    - Project Manager, and additional members chosen from the institutions participating in the project, to represent the broad community and institutional interests
  - Scientific Steering Committee, Software Standards Committee, Verification and Validation Committee, and User Advisory Committee
  - High-level Program Advisory Committee (PAC)
    - Reporting to the top management of the lead institution, composed of scientists external to the project

Management and Structure Requirements

- **Accountability**
  - Make clear who is ultimately responsible for project deliverables as a whole as well as for the individual parts of the project
- **Utility**
  - Mechanisms to evaluate the usefulness of the project, in whole and in parts
- **Delivery**
  - Ensure that release schedules and required capability are achieved
- **Expertise, advice, and evaluation**
  - Identify mechanisms, such as advisory committees and/or panels, by which required expertise is brought into the project
- **Communication**
  - Disseminate project requirements, schedules, progress and issues to the multi-institutional, geographically distributed workforce
- **Best practices and interdisciplinary integration**
  - Project structure should ensure that tasks are executed by teams that have embraced the expertise needed from all appropriate fields
- **Motivation and evaluation**
  - Establish mechanisms to ensure accomplishments are appropriately rewarded

Management and Structure Requirements

- **Technical decision making**
  - Project structure should allow for technical decisions to be made in a manner in which all participants are confident that they are heard
- **Conflict resolution**
  - Management structure must be able to identify the person and/or mechanism by which conflicts will be resolved
- **Delivery and Quality**
  - Identify the mechanisms by to insure deliverables are provided on time and that all quality standards are enforced
- **Staffing and resource management**
  - Dynamically assign resources and staff and establish a mechanism for reassignment of tasks, in partnership with the Department of Energy
- **Risk assessment and mitigation**
  - Quantify risk for each part of the software project and have appropriate backup solutions and/or have recovery methods in place
- **Mentoring and education**
  - Ensure that mechanisms exist for bringing into the project scientifically capable personal and establish liaisons with educational institutions

Conclusions

- The FSP committee and workshop report will:
  - Identify key scientific issues that can be addressed by integrated modeling that takes advantage of the physics, computer science, and applied mathematics knowledge base
  - Identify the critical technical challenges for which predictive integrated simulation has a unique potential for providing answers in a timely fashion
    - In a way that traditional theory or experiment by themselves cannot
  - Establish a clear plan to improve the fidelity of the physics modules required for predictive tokamak whole device modeling
    - Well supported theory and experimental fusion programs are essential
  - Identify the critical areas of computational science and infrastructure in which investments would likely produce the tools required for the FSP to achieve its goals
  - Address issues associated with project structure and management of the proposed FSP
- Essential to produce, in a timely way, advanced whole plasma simulation capability using high performance computers to:
  - Provide key scientific deliverables
  - Make accurate predictions for burning plasma experiments