FUSION SIMULATION PROGRAM (FSP) BRIEFING

DOE OFFICE OF SCIENCE (DOE-SC)

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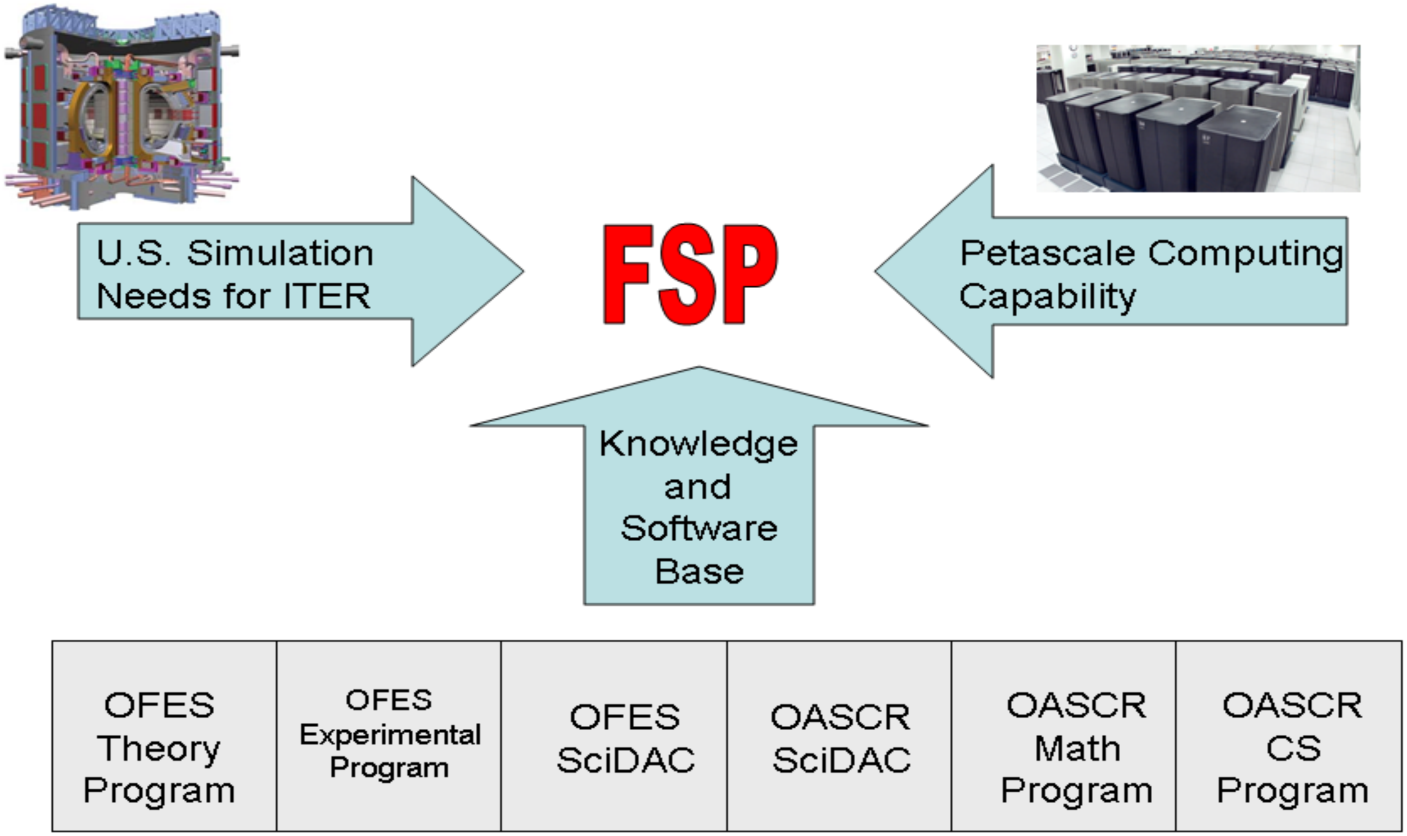
FUSION SIMULATION PROGRAM (FSP)

Outline of FSP Briefing:

I. Motivation, Mission, & Vision
II. Situation Analysis
III. Science Challenges & Opportunities for FES
IV. Materials Challenges & FSP
V. Illustrative New FES Results enabled by ASCR
VI. Milestones & Deliverables
VII. Planning Elements
    -- cross-coordination between groups
VIII. Risks
IX. Concluding Comments

FSP: Timely Opportunity to Accelerate Scientific Progress in FES

- Predictive simulation capability needed for harvesting scientific results from experiments worldwide, including *participation in ITER* & reducing risks in plans for future devices
- Powerful (“Leadership Class”) Computational Facilities worldwide moving rapidly beyond the petascale *(10^{15} floating point operations per second)*
- Interdisciplinary *collaborative experience*, knowledge, & software assembled over 8 years under SciDAC plus ongoing FES and ASCR base programs



U.S. Simulation Needs for ITER

FSP

Petascale Computing Capability

Knowledge and Software Base

OFES Theory Program

OFES Experimental Program

OFES SciDAC

OASCR SciDAC

OASCR Math Program

OASCR CS Program

FSP MISSION & VISION

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.

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.

CURRENT FSP SITUATION ANALYSIS

- The FSP team is funded to conduct a detailed two-year “planning study” (beginning July of FY ‘09 & ending July of FY ‘11) -- in coordination with DOE - Office of Science (OFES and OASCR)
  - *Team of 6 national labs, 2 companies, and 9 universities*
- Deliverables include:
  - Mission & vision statements
  - Assessment of current capabilities and gaps analyses
  - Implementation plan with initial roadmap of scientific software deliverables/milestones and time-lines
  - Work breakdown structure (WBS)
- Similar to “Project Definition” phase in leading to *CD-1*
  - FSP is not under DOE Order 413.3 A, but will use similar management structures as appropriate
  - Build on “lessons learned” from other major scientific software development projects such as ASC [e.g. -- FY06 ASC Program Plan]

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

The FSP offers an opportunity for transformational science in support of critical programmatic needs

Though equations are well-known (Boltzmann-Maxwell), the problem is a physics grand challenge

$$\frac{\partial f}{\partial t} + \mathrm{v}\cdot\nabla f + \frac{q}{m}\left[E + \mathrm{v}\times B\right]\cdot\nabla_{\mathrm{v}} f = C(f) + S(f)$$

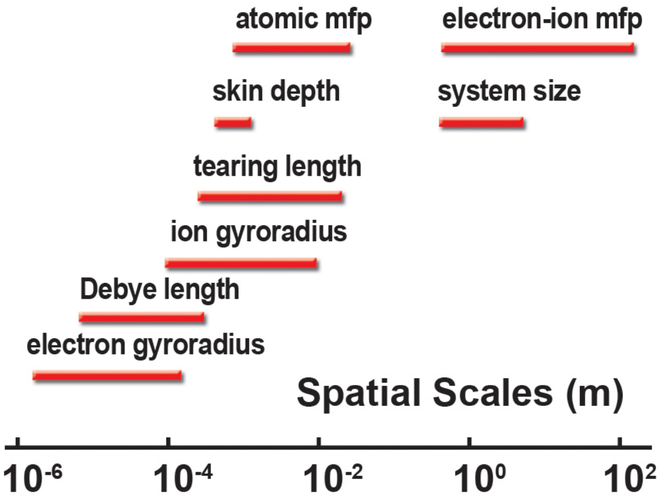
convection in space

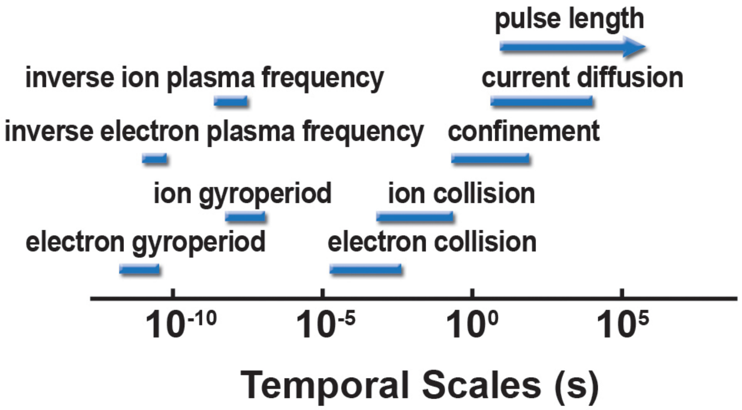
convection in velocity space

collisional relaxation

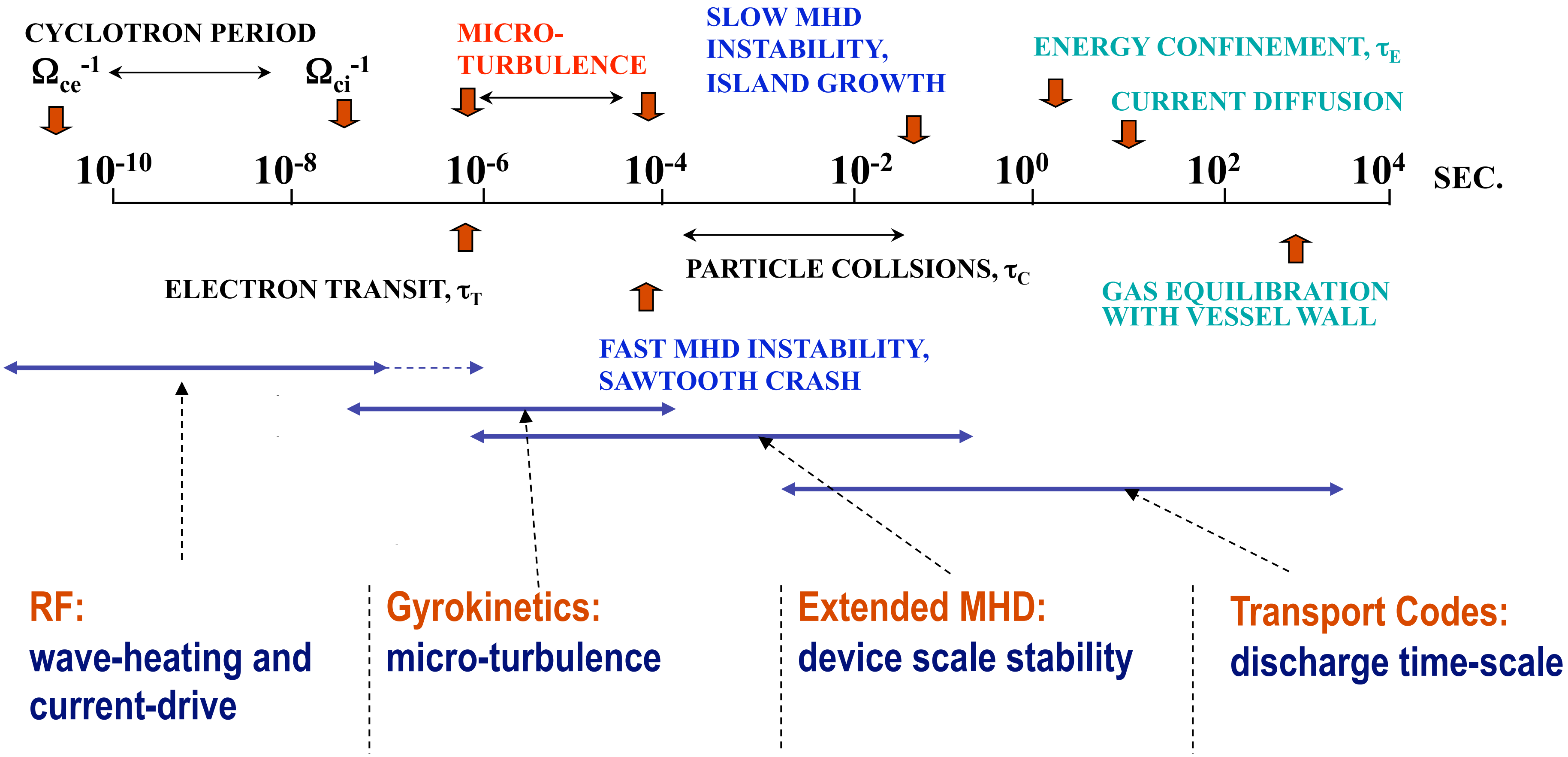
particle sources

- Seven dimensional equation of motion in phase space, f(x, v, t) for each species and 2 coupled vector fields
- Extreme range of time scales – wall equilibration/ electron cyclotron O(10^{14})
- Wide range of spatial scales – machine radius/electron gyroradius O(10^4)
- Extreme anisotropy – mean free path in magnetic field parallel/perpendicular O(10^8)
- Intrinsic nonlinearity (e.g. plasma distributions generate significant E and B fields through Maxwell's equations)
- Sensitivity to geometric details





Progress Achieved Historically Through Separation of Physics Domains



CYCLOTRON PERIOD

Ω_{ce}^{-1} ↔ Ω_{ci}^{-1}

MICRO-TURBULENCE

SLOW MHD INSTABILITY, ISLAND GROWTH

ENERGY CONFINEMENT, τ_E

CURRENT DIFFUSION

10^{-10} 10^{-8} 10^{-6} 10^{-4} 10^{-2} 10^{0} 10^{2} 10^{4} SEC.

ELECTRON TRANSIT, τ_T

PARTICLE COLLSIONS, τ_C

GAS EQUILIBRATION WITH VESSEL WALL

FAST MHD INSTABILITY, SAWTOOTH CRASH

RF: wave-heating and current-drive

Gyrokinetics: micro-turbulence

Extended MHD: device scale stability

Transport Codes: discharge time-scale

- A similar approach divides the problem spatially between Core, Pedestal, Boundary Layer, Plasma Wall Interactions
- However, this approach is fundamentally limited and inadequate!

Accurate Modeling Requires Going Beyond This Historical Paradigm

- Overlap in scales (time and space) often means strong ordering is not possible
- Additional physics enters (Nuclear reactions, atomic physics, neutral transport, radiation transport, plasma-material interactions)
- We've currently identified 5 "Science Drivers" which exemplify and span these two challenges
  - Boundary Layer
  - Nonlinear turbulent transport and macro-stability in the plasma core
  - Wave particle interactions
  - Disruption avoidance, detection and mitigation
  - Whole device modeling
- Science development roadmaps under development for each

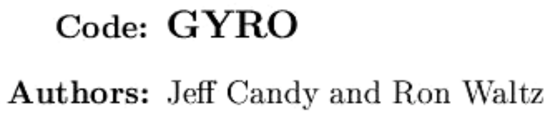
- Integration challenges in physics, applied math, and computer science
- Computing platforms at the petascale and beyond are also needed

Science Driver: Plasma Boundary Layer

- Crucial unresolved issue for fusion reactors, impacts:
  - Heat and particle loads
  - Erosion of first wall
  - Tritium fuel cycle – retention in first wall
- Key Scientific Challenges
  - Requires self-consistent solution of plasma and wall-interaction
  - Couples plasma turbulence, macro-stability, neutral transport, atomic physics, PWI, materials chemistry and morphology
  - Lack of spatial scale separation (gradients, gyro-radius, neutral mfp, photon mfp)
  - Magnetic topology: open and closed field lines
- Payoff
  - Choice of first wall materials
  - Design of plasma facing components and plasma shape
  - Robust plasma exhaust strategy

Science Driver: Nonlinear Turbulent Transport and Stability

- Key Scientific Challenges
  - Self-consistent, global solutions of micro- and macro-nonlinear dynamics
  - Meso-scale phenomena (between gyro-orbit and device size)
  - No strong scale separation – understanding nonlinear physics interaction on these two scales
- Payoff
  - Predictability of plasma profiles, operational limits (plasma pressure) and performance (fusion yield)
  - Ability to extrapolate to future devices

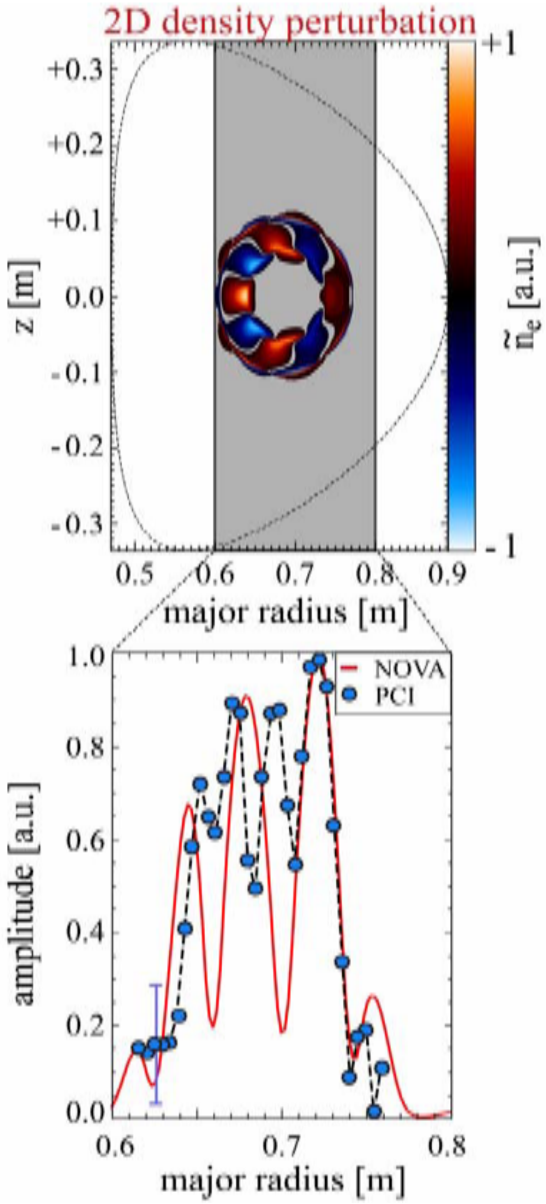


Code: GYRO

Authors: Jeff Candy and Ron Waltz

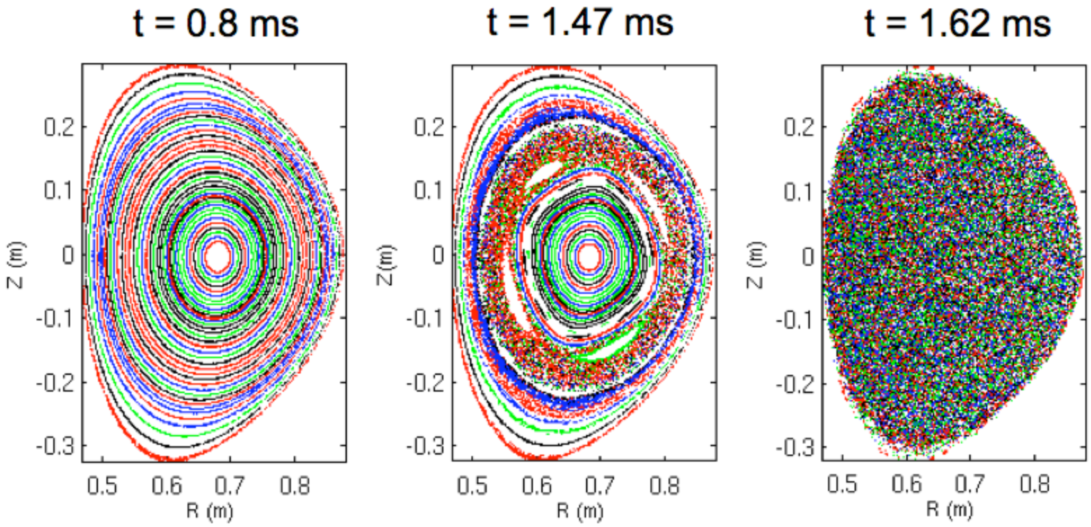
Science Driver: Wave Particle Interactions

- Fusion product, alpha particles born at 3.5 MeV and superthermal particles from RF or Beam heating and current drive
    - Thermalization without loss is essential
    - Represents potent sources of free energy for instabilities
- Key Scientific Challenges
    - Self-consistent description of phase space distribution on energy confinement and/or slowing down times which are many orders of magnitude longer than time scales for underlying wave-particle interactions (Alfvenic)
    - Strong nonlinearities and mutual coupling to transport through pressure, velocity, and current profiles and fluctuation spectra
- Payoff
    - Predictable fusion yield
    - Steady-state operation



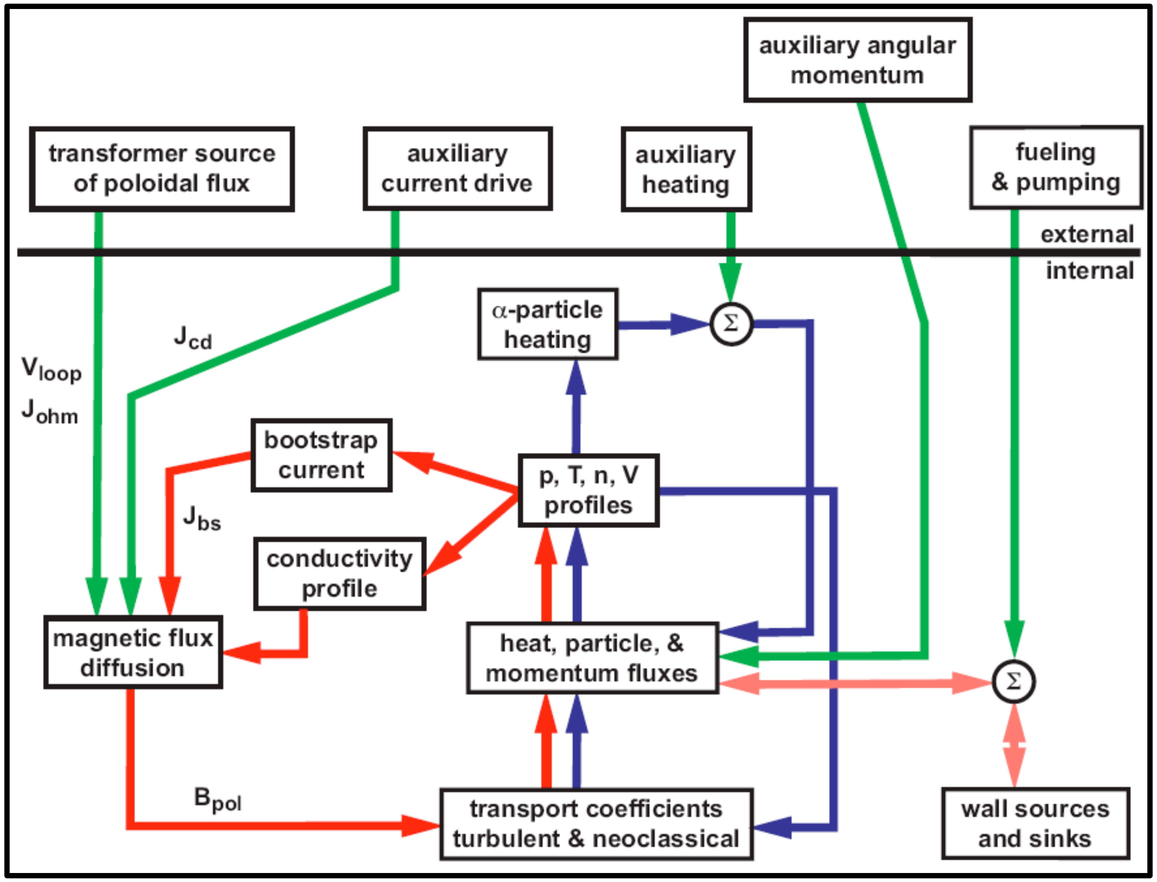
Science Driver: Disruptions

- Needed to predict, avoid and mitigate effects of disruptions
  - Effects include severe heat loads, JxB forces, run-away electron generation
- Key Scientific Challenges
  - Strongly nonlinear MHD, with large Lundquist number ($t_{\text{magnetic diffusion}}/t_{\text{Alfven}}$)
  - Coupled to plasma pressure & current, atomic physics, neutral and impurity transport, radiation transport, relativistic electron transport
  - Coupled to electromagnetic model of machine (complex wall geometry, power supplies, coils, etc)
- Payoff
  - Survivability of first wall components
  - Steady-state operation



Science Driver: Whole Device Modeling

- Key Scientific Challenges
  - Requires integration of all relevant physical models
  - How to couple and integrate advanced physics modules?
  - How to produce accurate and computationally tractable reduced models?
- Payoff
  - Scenario design for existing and planned machines (especially ITER)
  - Reliable design of future devices



Materials Challenges & FSP

The FSP will be a key customer for emerging models of plasma-wall interactions and will address this challenge as a component of its strategic vision.

[From S. Zinkle's Plenary Presentation at FES Grand Challenges Workshop, Spring '09]

- Current assessments indicate wall loads will impose extreme operating conditions on the materials surrounding a burning plasma
- Plasma Facing Components (PFC) issues include high heat fluxes, erosion/re-deposition, gas entrainment (T_2 retention, etc.)

Recommendation: "High performance computational simulations, performed in concert with appropriately designed model experiments, will be essential for accelerating the rate of development of fusion energy."

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

Recent LCF-enabled simulations provide new insights into plasma turbulence

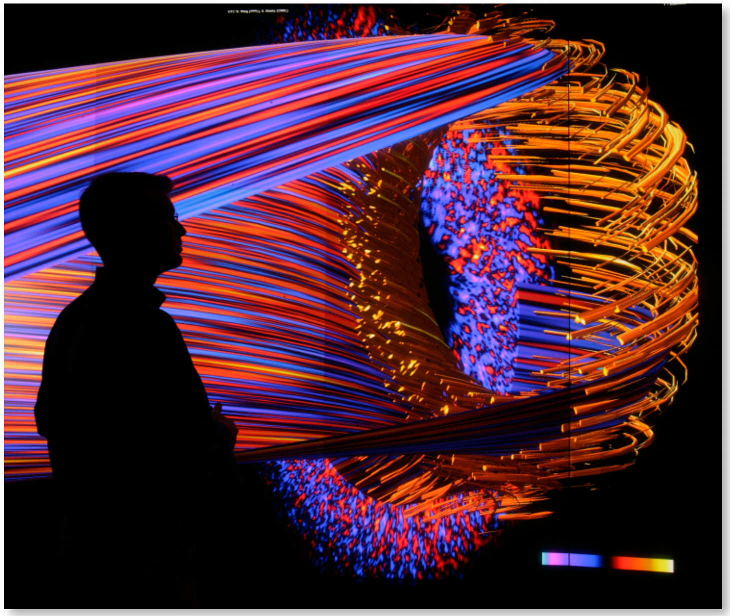
Teraflops-to- petaflops computing power have accelerated progress in understanding heat losses caused by plasma turbulence

Multi-scale simulations accounting for fully global 3D geometric complexity of problem (spanning micro and meso scales) have been carried out on DOE-SC Leadership Computing Facilities

Excellent Scalability of Global PIC Codes (e.g., XGC-1) *enabled by strong ASCR-FES collaboration* in SciDAC proto-FSP CPES project (NYU, ORNL, LBNL, …..)

Exascale-level production runs are needed to enable running codes with even higher physics fidelity and more comprehensive & realistic integrated dynamics

e.g. -- Current petascale-level production runs on ORNL's Jaguar LCF require 24M CPU hours (100,000 cores × 240 hours)



Mission Importance:

Fusion reactor size and cost are determined by balance between loss processes and self-heating rates

FSP Program Definition Milestones

- Identify science drivers for FSP with associated *"gaps analysis"*
  - *Establish criteria for choosing science drivers and assessing both science gaps and software gaps -- identified, e.g., in recent major community workshops: (1) FES ReNeW; (2) DOE-SC Workshop on "Grand Challenges in FES; and (3) 2007 FSP Workshop Report.*
- Develop *program and management plans to address the gaps*, and produce a *living-scientific-road-map that identifies deliverables*
  - *Cognizance of strategic importance of delivering some nearer-term software capabilities to the user community as well as connection to longer-term development of those capturing the needed science.*
- Develop plan for *coupling to requisite expertise from FES & ASCR communities needed to address prioritized FSP goals*
  - FSP information briefings/site visits beginning in October '09 to discuss proposed plan with larger community [e.g., at ANL (7/09), PPPL (9/09) & planned at GA, MIT, ORNL, LANL, IFS, U. Wisconsin, …….)]
  - Public meetings of the working groups (e.g., on Science Drivers @ recent APS-DPP Meeting and at future public venues such as TTF, Sherwood, etc.)
  - National web-site (http://www.pppl.gov/fsp/) and working group "wikis" (up and operating now with continuing improvements including FAQ's)

FSP Planning Activity

Deliverables

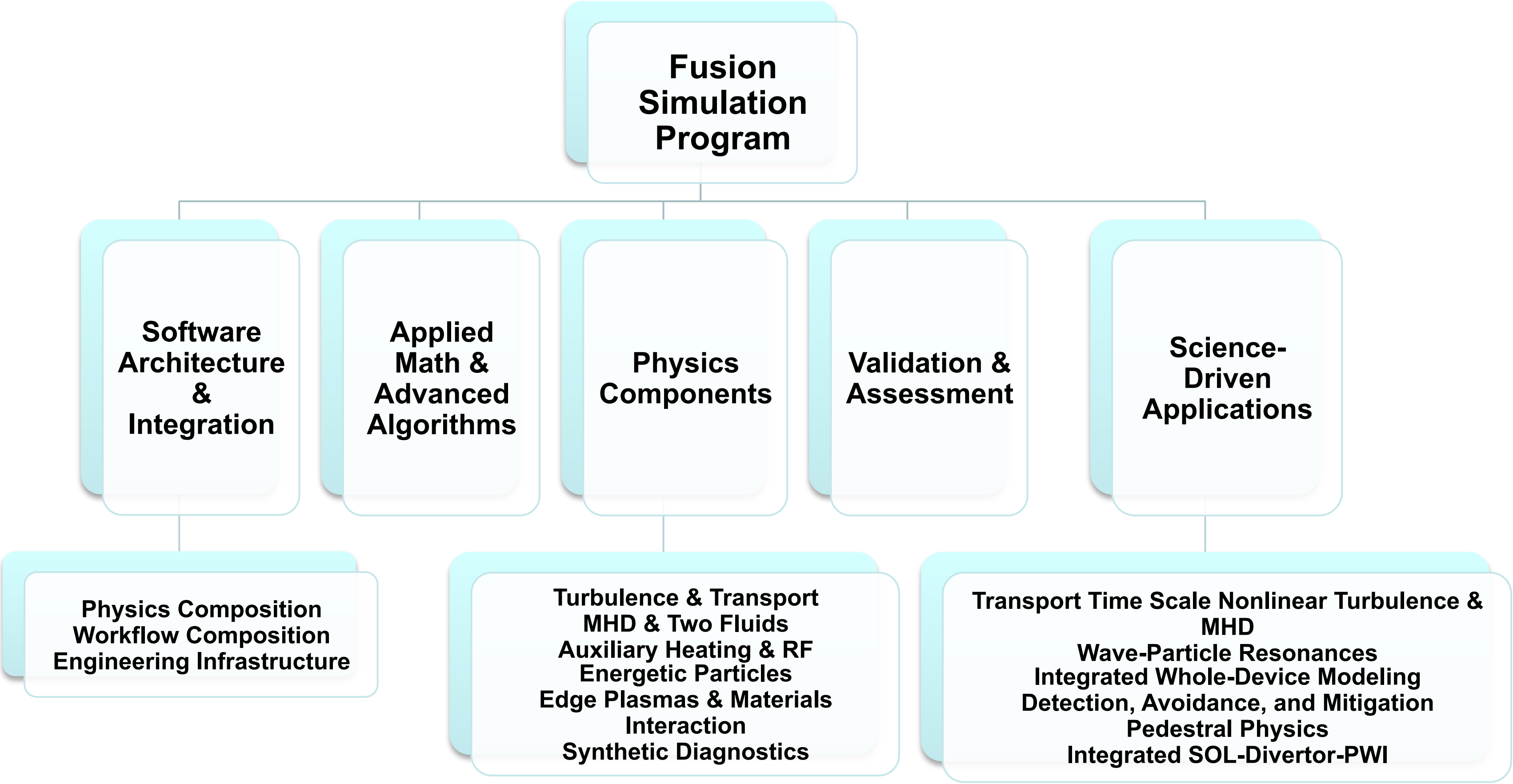
- **Overall Deliverables:**
  - **Frameworks:** *(1) Sections in FSP Integrated Plan & in FSP Requirements Plan; (2) Report on Frameworks Workshop; (3) Report on Community Input for Frameworks*
  - **Validation:** *(1) Predictive Modeling Best Practices Document; (2) Sections in FSP Integrated Plan & in FSP Requirements Plan; (3) Data Management Plan; (4) Experimental Plan*
  - **Components:** *(1) Sections in FSP Integrated Plan & in FSP Requirements Plan; Report on Selection & Prioritization Process for New Components Development – complementarity with SciDAC & base Theory/Modeling Programs*
  - **Science Drivers:** *(1) Sections in FSP Integrated Plan & in FSP Requirements Plan; (2) Report on Community Input for Science Drivers*
  - **Detailed list of documents to be delivered with associated quarterly time-line** ***(summary table on next slide)***

FSP Planning Activity Deliverables

Fiscal Year Quarter	Q409	Q110	Q210	Q310
Deliverables	✓FSP Kickoff meeting held on July, '09 ✓Communication logistics (web-site, wikis) ✓FSP PAC organized and first meeting held (Sept.'09) ✓Mission and vision statements	✓Joint ASCR/FES Collaboration Agreement in place (DOE-SC action) ✓FES Management Plan ✓Strategic Plan ✓Framework stakeholders	✓Integration/Outreach Plan ✓Risk Management Plan	✓Requirements Mgt. Plan ✓Program Tracking Plan ✓Validation Best Practices ✓Data Management and Requirements Plan ✓Community Input on Science Drivers & Applications collected ✓1st Draft – time estimates for initial Frameworks tasks & analysis of 2 science drivers ✓1st Draft – Components gaps analysis & process for selection and prioritization of new components development
Fiscal Year Quarter	**Q410**	**Q111**	**Q211**	**Q311**
Deliverables	✓Change Management Plan ✓Quality Management Plan ✓1st Drafts: (1) Frameworks time estimates for initial tasks & analysis of science drivers; (2) Components gaps analysis & process for selecting/prioritizing new components development; and (3) Validation gaps analysis and remediation	✓ Infrastructure Plan ✓1st Drafts: (1) Overall Implementation Plan; (2) Framework Implementation Plan; (3) Validation Plan; (4) Experimental Coordination Plan; (5) Components Execution Plan; and (6) Prioritizing and sequencing of Science Drivers	✓Implementation Plan ✓1st Draft - Project Execution Plan (PEP) ✓Frameworks Community Input Workshop Report ✓Reports on Validation Metrics for Data Mgt. Prototypes ✓Components Program Plan ✓Report on why FSP is required by each Science Drivers	✓Project Execution Plan ✓Final FSP Planning Package ✓Frameworks Section of FSP Plan ✓Validation Section of FSP Plan ✓Components Section of FSP Plan ✓Science Drivers Section of FSP Plan

FSP Strategic Plan

A Partial Work Breakdown Structure (WBS)



Fusion Simulation Program

Software Architecture & Integration

Applied Math & Advanced Algorithms

Physics Components

Validation & Assessment

Science-Driven Applications

Physics Composition
Workflow Composition
Engineering Infrastructure

Turbulence & Transport
MHD & Two Fluids
Auxiliary Heating & RF
Energetic Particles
Edge Plasmas & Materials Interaction
Synthetic Diagnostics

Transport Time Scale Nonlinear Turbulence & MHD
Wave-Particle Resonances
Integrated Whole-Device Modeling
Detection, Avoidance, and Mitigation
Pedestral Physics
Integrated SOL-Divertor-PWI

The WBS will likely evolve during the FSP definition and planning phase as a result of discussions with clients, customers, and users.

FSP Risks

- **Science Drivers**: (1) underlying physics models not sufficiently complete to adequately resolve scientific issues consistent with experimental reality; and (2) major challenge of reaching agreement on importance of any given science driver due to varying needs in different parts of FES community
- **Frameworks**: (1) chosen framework technologies may prove incompatible with future computational architectures; and (2) existing components found to be insufficiently engineered and/or robust for use in the more demanding framework environment
- **Components**: balancing the needs of delivering advanced physics code software products and the exploratory research needs for producing the physics capabilities required to resolve the FSP science drivers' challenges
- **Validation**: The US has the best plasma diagnostics, but there are practical limitations of experimental measurement – particularly the ability to comprehensively measure all important parameters with the needed spatial coverage and resolution
- **Verification**: dealing with challenges associated with integrated vs. single physics – especially "model uncertainty quantification"
- **General Risks**:
  - Managing a major software R&D project of the scale of FSP is unprecedented in DOE-SC
  - New challenges for FES & ASCR communities in managing such a large, multi-disciplinary, multi-institutional software R&D project with prioritized deliverables tracking a specified time-line

CONCLUDING COMMENTS

- **The FSP represents a unique and important opportunity to make substantial advances in experimentally-validated predictive simulations to enable a shorter path to the achievement of magnetic fusion energy.**

- **The FSP team is currently funded to carry out a detailed 2-year "planning study" (July of FY '09 to July of FY '11) -- in coordination with DOE-SC (FES and ASCR) with deliverables including:**

  FSP vision/mission statements, management plan, and implementation plan with a "living roadmap" of scientific software deliverables/milestones and associated time-lines with work breakdown structure (WBS)

- **A key element of the FSP planning effort will be an active outreach to the FES (theory, modeling, and experimental) and ASCR communities to help define scientific priorities and establish mechanisms for productive collaborations both nationally and internationally.**
  - **A successful FSP will require a strong and active ongoing program in the FES and ASCR core R&D areas**