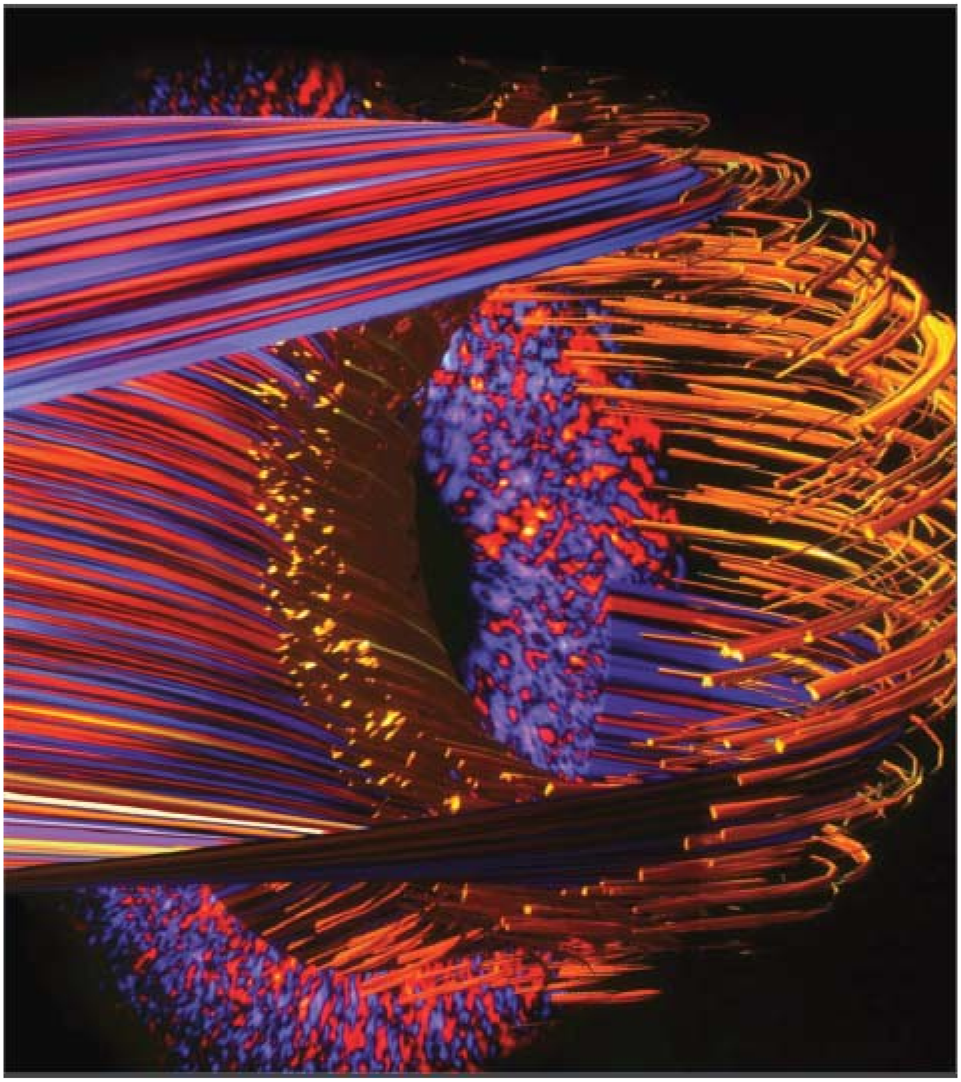
FSP Science Drivers

Detailed Reports From Community Teams



FSP Science Drivers

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Introduction

The reports contained in this document were prepared by small groups of technical experts at the request of the FSP planning team. They represent a bottoms-up attempt to define plans for addressing critical programmatic issues that require integrated simulations. The reports cover the six science drivers identified by the FSP: Boundary/PWI; Pedestal; Core Profiles; Wave-particle interactions; Disruptions and Whole Device Modeling.

Each report is organized along the following lines:

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1. BOUNDARY SCIENCE DRIVER

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1.A. Background and motivation

The boundary region in a fusion device includes a narrow region where plasma parameters change very rapidly and the near surface of adjoining materials know as plasma-facing components. Processes in this region determine the distribution of high levels of plasma exhaust particle and heat fluxes to surrounding materials and the associated response of the material (*e.g.*, heating, erosion, and tritium trapping). Simultaneously, the eroded material becomes part of the ionized plasma and its intrusion into the hot core region must be understood and controlled. Issues associated with plasma exhaust, material erosion, tritium trapping, dust, and impurity intrusion are among the most challenging for the successful development of fusion via magnetic confinement devices focused on here, as well as inertia confinement devices. A predictive simulation model of this region requires coupling of a number of disparate physics models describing plasmas, neutral gas, radiation, solid and possibly liquid materials operating on a wide range of space and time scales.

The strong motivation to have predictive models of boundary region processes is summarized, *e.g.*, by the recent ReNeW activity report [ReNeW 2009] and Fusion/Exascale-Computing Workshop [Exascale 2009]. These critical issues include: 1) lifetime of plasma-facing material components (estimates vary from hours to days to years), 2) unacceptable levels of tritium co-deposition in re-deposited material and tritium trapping in bulk surface material, 3) effect/limitations on the plasma including core plasma contamination by surface emitted material, 4) accumulation of dust that can be easily dispersed during an unintended vent, and 5) impact on additional core issues such as toroidal rotation, edge transport barrier, and tokamak density limits.

A brief characterization of the main physical processes in the boundary regions follows, beginning with the boundary plasma and continuing through to the surface material:

The behavior of the boundary plasma is strongly influenced by changing topology of confining magnetic field, **B**, from being composed of closed fields lines to open fields lines that intersect material surfaces; the poloidal magnetic flux surface where this transition occurs is called the separatrix. The region outside the separatrix is called the scrape-off layer (SOL). Because of the much more rapid parallel plasma transport along B than across it, most of the heat and particle fluxes are concentrated on flux surfaces that map along **B** to the near the separatrix. Consequently, the SOL plasma is thin, yielding large radial gradients, can have substantial poloidal variations, and a range of collisional parallel mean-free paths to scale lengths. These features distinguish the SOL plasma from that in the core, and the gradients are a potential source of strong plasma instabilities, including short wavelength microinstabilities and long wavelength edge localize modes (ELMs), that impact particle and energy dispersal to surfaces.

A substantial neutral particle component typically exists in the SOL owing to plasma-material interactions (PMI) yielding recycled main fuel hydrogenic (deuterium and tritium, DT,) atoms and molecules, and neutral sputtering wall impurities via physical or chemical mechanisms as discussed below. Owing to the lower electron temperatures in the SOL, neutrals can penetrate some distance into the plasma volume before being ionized, providing refueling and contamination mechanisms for the core plasma. Strong recycling can substantially lower the plasma temperature and increase in plasma density and radiation near material surfaces, especially in the divertor region. Neutral penetration across the separatrix may play a role in the H-mode pedestal [Park 2007] formation. Plasma chemistry can also play an important role, especially for carbon-base devices where neutral chemically sputtered particles are usually in the form of hydrocarbons (*e.g.*, HC_4) that are subsequently broken down into their constitutive elements by the plasma.

Excitation, ionization, and recombination processes can produce a substantial energy-loss mechanism via line radiation that broadens the total heat-flux profile. The atomic rates can depend on plasma density, temperature, and local transport that involve detailed atomic physics models. The impurity density is generally low enough that the plasma is optically thin to impurity radiation, but the hydrogen atom densities may be high enough that emitted photons, especially Lyman-α, can be reabsorbed before escaping the divertor [Post 1995]. The resulting photon trapping not only affects the distribution and spectrum of emitted radiation, it alters the ionization balance for the atoms [Reiter 2007]. The light emitted by neutral atoms, regardless of their origin, is the basis for a wide variety of important diagnostic techniques.

The boundary between the gaseous SOL and the solid material or radio frequency (RF) antenna is the plasma sheath. The sheath controls the energy and angle of incidence of impinging ions from the plasma, including re-deposited surface material ions. Most of the impinging ion energy is acquired in the sheath. For the tokamak divertor type, with highly oblique strong magnetic field incidence to the surface (order of 1-2°), the sheath consists of a Debye sheath, of order 10 μm, and a magnetic sheath, of order of 3 times the D-T ion gyroradius, or ~1 mm. Average angles of incidence for D-T ions are about 50° from the surface normal, such angles generally involving a major enhancement of sputter yields over normal incidence. Plasma currents and surface roughness can play important roles in the sheath characteristics as well [Ryutov 2008].

Understanding and managing plasma/material interactions are probably the most critical issues for fusion technology [Federici 2001]. Basic processes can be separated into those that occur in the near-surface region, say the first tens of microns, and those that occur throughout the bulk. The near-surface region is the focus here where the impinging plasma and neutrals contribute, while the bulk properties are impacted by deeply penetrating neutrons and thermal excursions. The fundamental processes of backscattering and sputtering are understood theoretically for well-characterized materials (*e.g.*, binary collision models for backscattering and physical sputtering [Eckstein 1991], and molecular dynamics for chemical sputtering [Nordlund 2006]) and are able to reproduce data from laboratory experiments. Likewise, there are basic models for migration and trapping of hydrogenic species within materials [Hillis 2001?, Pigarov 2009?]. However, surface materials in fusion are reprocessed in that substantial gross erosion and re-deposition occurs, resulting in irregular surfaces with complex structure. In devices with mixed materials (*e.g.*, ITER with Be walls and C or W divertor plates), the surface composition itself is uncertain. Development of adequate models to understand and predict the behavior of such material surfaces is in its infancy. It is important to move beyond qualitative models that require empirical coefficients to more physics-based simulations, which will require a substantial increase in funding.

Practical considerations, based on tritium retention, fuel inventory and erosion management, lead to a design preference for the use of tungsten as the divertor material, and possibly also the entirety of the plasma facing components, in future fusion reactors. In fact, the 'all metal' ITER design option involves replacing the current graphite design with tungsten strike points that would operate at temperatures above 1000 K. In such environments, tungsten will experience high heat loads and exposure to various hydrogen and helium isotopes and impurity species, possibly including beryllium, carbon and argon (which is added to enhance radiative plasma losses). To date, only limited experience exists with solid tungsten in magnetic fusion confinement devices, while recent laboratory based plasma exposure experiments involving hydrogen and helium implantation on tungsten have demonstrated a very rich, and as yet poorly understood surface response behavior.

Finally, the response of the SOL and especially wall materials to transient events such as edge localized modes (ELMs) and disruptions (including vertical displacements) must be understood. In addition, the interaction the boundary plasma and material with radio frequency (RF) antennas, and associated electromagnetic fields, requires much better integration into boundary models. For controllable ELMs, the main issue is what defines acceptable ELM characteristics in terms of size, duration, and frequency to avoid excessive material erosion. For disruptions, the location and damage to materials from high heat flux including runaway electrons needs quantification. RF sources inject power into the SOL plasma and drives potentially large RF sheaths, and in turn, the plasma gives rise to antenna sputtering. All of these transient and RF processes produce supra-thermal particles and thus ultimately require kinetic descriptions in 3D.

1.B. Goals

The survivability of fusion plasma facing materials places constraints on the impinging plasma fluxes. A boundary plasma model capable of predicting those fluxes will allow future devices to be designed and operated in a manner consistent with those constraints. Such a model should, first, be able to reproduce the parametric scaling of the following quantities in existing experiments, and, second, incorporate a fundamental understanding of the underlying physical processes, allowing the model to be extrapolated to future devices with confidence.

- Heat loads to material surfaces both during steady state operation (in L-mode and H-mode between ELMs) and in transients (ELMs, disruptions)
- Fluxes of particles to material surfaces, including those of deuterium, tritium, helium, and all impurities.
- Fluxes of particles back into the boundary plasma due to plasma-material interactions, including:
  - Impurity generation by physical and chemical sputtering,
  - Recycling of deuterium and tritium,
  - Removal of deuterium, tritium, helium and other particles from the system by pumping mechanisms.
- Transport of those particles through the boundary plasma and the resulting sources of particles, momentum, and energy in the pedestal and core plasma.
- Tritium recycling, transport, and retention in materials; implicit in the above, but listed separately because of its importance.

- Particle, momentum, and energy sources in the boundary and core plasma due to external fueling, including gas puffing, pellets, and other techniques.
- Modification of plasma facing materials due to plasma fluxes and externally applied treatments (*e.g.* boronization), including erosion, re-deposition with mixed materials, dust generation (and transport).

1.C. Components:

1.C.1. Requirements for physics codes (components) that need to be integrated in order to achieve the goals associated with the science driver.

The basic physics equations used in the models for plasma, neutrals, and photons, either fluid or kinetic, are usually differential equations of either the Eulerian or Lagrangian form. The plasma Eulerian or continuum models are multi-dimensional partial differential equations with convection and diffusion operators plus source terms – akin to Navier-Stokes equations in fluid dynamics. The Lagrangian or particle formulation describes the trajectories of a large ensemble of particles or fluid elements in response to various forces. Each type of model for charged particles also includes an Eulerian field equation for the electrostatic potential (Poisson's equation or a current continuity equation) and sometimes the magnetic field using typically reduced Maxwell equations. [some references] Kinetic models required a model for collisions processes, which in the case of the plasma, is the 2nd order differential operator (convection and diffusion in velocity space) Fokker-Planck equation. Sometimes models reduce the size of the problem by averaging over one or more of the dimensions, a procedure that can result in integro-differential equations to describe nonlocal processes.

Table 1. Requirements for Boundary SOL plasma models

Model	Capability	Space/time scales	Input/output
Magnetic equilibrium, mesh, and wall position/ composition	Provides magnetic flux surfaces for mesh construction and B-field components	Usually 2D axisymmetric; may include 3D perturbation;	<u>In:</u> Coil and plasma current/pressure. Also wall geometry <u>Out:</u> flux-surfaces in (R,Z) leading to mesh conforming to divertor/wall

Transport - fluid	Yields plasma profiles & flows via fluid eqns for e, D, T, multi-charge-state impurities; couple to neutrals; electrostatic potential	2D with toroidal symmetry, or 3D; from pedestal to wall and divertor at arbitrary angle to magnetic flux surfaces; Time~10^{-8} s (elec. || conduc.); ~0.1 ms (ELM crash); 1 ms (blobs); 10's ms (btwn ELM cycle); to steady state	In: Magnetic field, mesh, anomalous fluxes, atomic rates, power from core, wall conditions Out; 2D plasma profiles of density, momentum, and energy
Transport - kinetic	Adds kinetic effects to fluid transport along and across B-field; computes distribution function; e, D initially, then impurities, T, and couple to neutrals; electrostatic	2D axisymmetric configuration, 2D velocity spaces; from pedestal to wall/divertor; Time ~10^{-9}-10^{-7} s (e-i grid transit) ~10^{-7}–10^{-5} s (e-i bounce times); + fluid scales	In: Magnetic field, mesh, anomalous fluxes, atomic rates, power from core, wall conditions Out; 2D plasma profiles of density, momentum, and energy, adds 2D velocity space particle distribution functions
Turbulence - fluid	Evolves drift-type instabilities to find nonlinear steady-state turbulence & associated anomalous transport; e, D initially, then impurities, T, and couple to neutrals; electrostatic, magnetic fluctuations	3D; from pedestal to wall/divertor; Time - sub drift-wave and maybe Alfven wave (~10^{-7} s); saturation ~0.3 ms	In: Magnetic field, mesh, initial plasma profiles, core, wall boundary conditions Out; 3D plasma fluctuation levels and turbulent fluxes; often average toroidally for interpretation & coupling to transport
Turbulence - kinetic	Adds kinetic effects to fluid turbulence for e, D initially, then impurities, T, and couple to neutrals; electrostatic, magnetic fluctuations	3D configuration, 2D velocity spaces; from pedestal to wall/divertor; Time, similar to kinetic transport	In: Magnetic field, mesh, initial plasma profiles, core, wall boundary conditions Out; 3D plasma fluctuation levels and turbulent fluxes; velocity-space distribution

Sheath model	Computes thin electrostatic sheath separating plasma and materials	2D, 3D configuration and 3D ion, 2D electron velocity space; inclined B-field; later rough surfaces; Time - plasma frequency, ion cyclotron frequency	In: Magnetic field, mesh, plasma profiles, wall material Out; 1D or 2D magnetic and Debye sheath structure
Concludes plasma models			

For neutrals, ballistic particle trajectories between collisions are much simpler than for the plasma owing the absence of electromagnetic forces. The nature of collisions is more varied and often very dominant. Chief among collision processes are prompt charge-exchange with ions and ionization/recombination/excitation producing nonlocal transport in velocity space. Neutral-neutral collisions require another (nonlinear) model. As for the plasma, both fluid and kinetic descriptions can be used with the kinetic model most rigorous, but also costly. The most common kinetic approach is Monte Carlo. At a numerical model level, photon transport is very analogous to that of neutrals. Both neutral and photon transport depend on atomic cross-sections that are usually included as a table lookup function with interpolation between values as a function of particle energy and density. For dense plasmas, excited states become an important complication.

Table 2. Requirements for Boundary SOL neutral, photon, dust, and atomic physics models

Model	Capability	Space/time scales	Input/output
Fluid transport	Determines neutral species profiles in the plasma; (in order) D density & flow , impurity atoms, D temperature, D_2 density, T (generalize to all isotopes)	2D axisymmetric, extend mesh to walls to allow accurate PMI, 3D (if needed); Time, $>10^{-7} - 10^{-6}$ s (CR validity, grid transit)	In: Plasma profiles, wall geometry and albedo, recycling coeff. Out; 2D or 3D profiles of neutrals in the SOL, core

Kinetic transport	Adds kinetic effects to fluid model – long mean-free path; Initially: H (all isotopes), H_2, H_2+, impurity atoms; then: nonlinear H & H_2, H_2(v) (and associated species), impurity molecules, (on faster time scales, or if required by radiation trapping) H(n), H_2(n,v)	2D axisymmetric, 3D; Time, >10^{-7} – 10^{-6} s (CR validity, grid transit)	In: Plasma profiles, wall and pump geometry, recycling, backscatter rates, material composition Out; 2D or 3D profiles of neutrals in the SOL, core; CX-fluxes to walls
Photon transport	Determine how released photons escape the plasma/neutrals; Ly-α (escape probability), Ly-α (Doppler & Stark broadened, Zeeman splitting), Ly-α (add anisotropic line shape, fine structure), Ly-α, add lines for T, and other lines as needed.	2D axisymmetric, 3D	In: Neutral and plasma profiles, wall geometry, Out; Re-adsorption and emission of photons; 2D or 3D profiles of photon flux to walls
Dust transport	Traces trajectories and ablation of dust particles in SOL; macroscopie particles of wall material, *e.g.,* C, W, Be; 10 nm to 100 µm in size; negative charge; ablation requires plasma model & radiation loss	3D trajectory throughout SOL; Time, 10's of msec	In: Dust source, B-field, plasma and potential profiles, wall geometry, Out; 3D distribution of dust particles in SOL including flux across separatrix

Atomic rates	Provides, relevant to the above, cross sections (differential where needed) and kinetic data for reaction products, collisional radiative models for transport time scale simulations, especially for hydrogen atoms & molecules; tractable models for high-Z atoms and hydrocarbon breakup.	(Determined by time scales resolved in collisional radiative models)	In: Electron temperature and density Out; atomic rates averaged over Maxwellian for fluid models or differential cross-sections for kinetic codes
Concludes neutral, photon, and atomic physics models			

For the material surfaces, the basic physics equations used are of the general type described above, though here particle methods are more common. The most fundamental model of the material is Molecular Dynamics where individual projectiles are followed in the electrostatic potential of the lattice structure of the material, breaking bonds between lattice elements and reforming a new arrangement, which can result in the ejection of a lattice atom into the vacuum (sputtering)… (more?)

Table 3. Requirements for Boundary material models

Model	Capability	Space/time scales	Input/output
Basic backscattering/ sputtering rates	Determines PMI rates for various process; Energy and angular resolved backscattering & physical sputter yields; backscattered & sputtered velocity distributions for H, Be, C, Mo, selected C chemical sputter yields	~0-10 nm; Time, 1 ps	In: Incident ion energy, mass, and angle to surface Out; backscatter and sputtering rates

Hydrogen transport	Computes hydrogen transport, trapping, and release from materials; T co-deposition rates as a function of surface temperature, other T trapping	~0-10 nm	In: Material, temperture, possible defects/traps, transport coefficients, initial H concentration, incident H flux Out; Profile of H into the material, number releasable
Re-deposition	Provides location and rate of re-deposition of previously sputtered material for all candidate surface materials	~0-1 cm; Time, ~0-10 μs	In: Plasma fluxes and profiles, sputtering rates, surface material & temperature, B-field Out; location and rate of impurity flux back to surface
Material evolution/ dust production	Describes how surface materials evolve from strong plasma fluxes; Mixed materials (e.g. Be/W, C/W) formation/plasma interaction properties; He/W micro-structural evolution and response; dust composed of loosely bound macroparticles	Microscopic processes:~0-10 nm; Macroscopic processes, *e.g.*, dust production up to 100 μm; Time, ~1 ns – 1000 s	In: Location and rate of impurity fluxes to surface, temperature Out; Evolution of surface including composition
Concludes material models			

1.C.2. Plans for adapting older components and as well as plans for developing new components.

1) Plasma transport

Several codes exist capable of calculating plasma transport in the pedestal and SOL in the fluid approximation for long, transport time scales (excluding calculation of the turbulent transport itself). The most common of the 2-D codes, which were developed for tokamak applications and thus assume axisymmetry, are UEDGE [Rognlien 94] and SOLPS [Schneider 06] although other codes have been developed for application to specific tokamaks (*e.g.*, EDGE2D [Simonini 94] and KTRAN [Kim 05]). For an fluid transport FSP component, all of these codes have the basic features desired, but do differ in a number of deals, including solution algorithms. UEDGE is developed in the U.S. and is a component in FACETS, but has focused (not limited to) on coupling to fluid neutrals and only occasionally Monte Carlo neutrals. SOLPS is being developed in the EU has a larger development team (often postdocs/students), and has focused on coupling to Monte Carlo neutrals. SOLPS is in use in the U.S., but there is limited experience with code details.

Kinetic transport codes for the boundary region have and are being developed that solve for the 2-D velocity space particle distribution functions under the assumption that the third gyrophase velocity coordinate can be averaged over. Models assuming only 1-D spatial variation along **B** have been developed and performed a number of test problems [Batishchev 1997; Matte 1988]; here careful attention was given to the Fokker-Planck collision operator. More recent codes have added a second spatial dimension assuming toroidal symmetry and either use a particle-in-cell method [Chang 2004] or a continuum method where the distribution function is represented on a 4-D grid [Xu 2007]. While these latter codes include neoclassical drift-orbit effects, the collision operators have not been stressed for collisional SOL plasmas and this highlights an important area that needs further development, i.e., a 4-D kinetic transport code with an accurate and efficient collision module. The FSP should be able to leverage the kinetic transport work started in CPES (XGC0 [Chang 2004]]) and ESL (TEMPEST [Xu 2007], COGENT [Dorr 2010]). A key need here is Fokker-Planck collision model capable of truly spanning the long-to-short mean free path regimes found in the SOL.

2) Plasma turbulence

Plasma turbulence in the SOL is a difficult problem owing to the large amplitude and thus highly nonlinear physics involved. Most progress has been made with two-fluid (ion and electron) models. There are 2-D models in simplified geometry that show some of the basic characteristics of the SOL microturbulence [Garcia 2003; Russell 2009]. Here the detail magnetic geometry and thus strong magnetic shear is not included, and the third spatial coordinate is represented by an eikonal approximation for the wave variation. The most general fluid model that includes the full tokamak toroidal geometry with magnetic shear and the divertor plates is the 3-D BOUT code [Xu 2009]. An advanced, flexible version based on the BOUT code (called BOUT++) has recently been developed using on the C++ programming language [Dudson 2009]. BOUT++ has also been used recently to model ELMs [Xu 2010]. While some kinetic 5-D turbulence simulations have been performed using XGC1, that modeling has focused on the region inside the separatrix.

For fluid turbulence, BOUT++ is well suited for the SOL and is the only known code to include some region inside the separatrix, with the exception of a developing effort in France. BOUT++ is relatively mature having being a major rewrite in C++, but using many of the same algorithmic pieces from the original BOUT. Further, BOUT++ is an open-source code being developed both in the U.S. and the U.K. For kinetic turbulence, we again look to the CPES and ESL projects, though such 5D simulations are in their early stages at best.

3) Neutral transport

The implementation of detailed atomic and PMI physics models is most straightforward in a kinetic, Monte Carlo neutral transport code. Two widely used codes of this type are EIRENE and DEGAS 2. The Monte Carlo algorithm also allows the experimental geometry to be replicated in as much detail as is desired. The principal drawbacks to the Monte Carlo approach are the statistical noise in the results and the computational resources required to simulate short mean free path regimes. Because the Monte Carlo algorithm parallelizes naturally, the severity of both of these is mitigated by the continued increase in the number of CPUs available for production calculations.

The particular code which should be developed into the kinetic neutral transport component is not clear. EIRENE contains more physics than DEGAS 2 and is more widely used. On the other hand, no development support for it is available within the US fusion community. With sufficient manpower, the physics capabilities of DEGAS 2 can be brought up to the same level as those in EIRENE. However, the computational tasks undertaken by these codes can be neatly broken down into flexible, easily extended "objects". Consequently, a third option of developing a new code becomes viable if a programming language and development environment or framework can be identified that allows this representation to be straightforwardly implemented.

Fluid neutral transport models suffer from neither of the shortcomings of kinetic Monte Carlo, but are more restricted in the level of physics detail that can be incorporated into the calculations. Because fluid neutral models provide a precise, albeit approximate, neutral density profile for a given plasma, they are typically the default treatment of neutrals in fluid plasma transport codes, such as SOLPS/B2 and UEDGE. The absence of statistical noise in the neutral solution also permits an implicit approach to solving the coupled plasma – neutral equations, allowing the tight coupling associated with the charge exchange process to be handled efficiently.

A hybrid fluid-kinetic neutral transport model would treat short mean free path regions efficiently while retaining fully detailed kinetic behavior elsewhere. Although algorithms for such a hybrid model have been contemplated [Karney 1998], viable implementations do not yet exist. Likewise, methods for substantially reducing statistical noise in Monte Carlo calculations (correlated sampling, quasi-Monte Carlo, backward Monte Carlo) have been developed for other applications, but have not been incorporated into fusion neutral transport codes.

4) Radiation transport

The inclusion of radiation transport increases the complexity of a divertor transport simulation since plasma, neutrals, and radiation are tightly coupled and must be computed consistently. Moreover, all processes impacting the photon line shapes (Doppler and Stark broadening, Zeeman splitting) should be included [Reiter 2007]. The similarity between the neutral and radiation transport equations facilitated the incorporation of the latter into the EIRENE Monte Carlo transport code with straightforward extensions [Reiter 2007, Kotov 2006]. An alternative, approximate approach utilizes effective collisional radiative rates for hydrogen ionization and recombination having an additional dependence on an optical depth parameter characterizing the distance to the material boundary weighted by the neutral density along that path [Scott 2004]. These rates were obtained by incorporating a simplified, partially ionized, plasma transport model into the non-linear thermodynamic equilibrium radiation transport code CRETIN [Adams 2004] and can be easily incorporated into existing plasma and neutral transport codes [Scott 2004]. Because of the relatively high opacity of detached plasmas, an approximate treatment of this sort may suffice [Kotov 2006].

5) Dust

Dust production and transport has been recognized as a safety concern for fusion devices owing to its potential role in tritium retention, impurity transport and ease of mobilization during a vent. All present tokamaks produce some level of dust, but the amount is projected to increase very substantially with long-running devices such as ITER and beyond. Most theory/modeling progress has been made in understanding the mobilization and ablation of dust during a plasma discharge via the use of the macroscopic particle model DUSTT [Pigarov 2005] using a stationary UEDGE plasma background. More recently, DUSTT has been dynamically coupled to UEDGE [Smirnov 2010]. The DUSTT is the most advanced transport model known and should provide a good starting point for further work within the FSP. On the other hand, the production of dust is much less understood and here models need to be developed.

6) Sheath

There are existing codes, *e.g.* BPHI-3D [Brooks *et al.* xxx] for computation of sheath parameters and ion transport for a 3-D, tokamak geometry (near-tangential B-field), time-independent sheath. One need is for inclusion of RF induced sheath models/codes for plasma facing surface response.

7) Sputtering and transient response in materials, including D-T transport/accumulation

This topic area includes a number of strongly interacting effects, and thus the models used are discussed under this one subsection.

Plasma/material response has been the subject of 20+ years of analysis and model and code development (inasmuch as plasma facing component performance/lifetime is probably the single most technology feasiblility issue for fusion power). There are existing code packages for the steady state response, *in particular the* REDEP/WBC sputtering erosion/re-deposition code package [Brooks 2002, 2009], and the transient response HEIGHTS code package [Hassanein 2002, 2003, 2009]. These two packages include numerous sub codes for sputter yield, bulk material response, tritium trapping, and related areas *e.g.* as summarized in [Exascale 2009]. Briefly, the REDEP/WBC package computes the (3D,3v) kinetic, sub-gyro-orbit transport of sputtered (and thermally etc. emitted) impurities within a few gyro-radii of the surface (atoms and ions), while farther into the plasma, it uses a guiding-central (2v) ion model. The resulting surface response is simulated, including mixed-material evolution and tritium co-deposition. HEIGHTS computes the material response to transient events like ELMs, disruptions, Vertical Displacement Events, and associated runaway electrons. HEIGHTS can treat the 3D cases, including vapor formation, radiation transport, and surface thermal evolution. Both REDEP/WBC and HEIGHTS have been extensively developed, including some parallelization, and could be used in their existing state. REDEP/WBC has been coupled with a UEDGE SOL simulation, but to date only via a manual iteration cycle [Brooks] The REDEP/WBC and HEIGHTS sub-codes/packages could also supply important components to be combined with others in the FSP.

Comparatively recently, another code called WallPSI [Pigarov 2009] has been developed to consider the dynamics and meso-scale transport of hydrogenic species in carbon and beryllium. This code computes the recycling and sputtering of material in response to plasma/neutral fluxes, and solves for the dynamic temperature hydrogenic content of the material. WallPSI presently provides the wall model for the FACETS project [Cary 2009].

At a more fundamental, and therefore shorter timescale, other codes are exploring the material behavior at the atomistic level and pioneering ways to couple such results to more

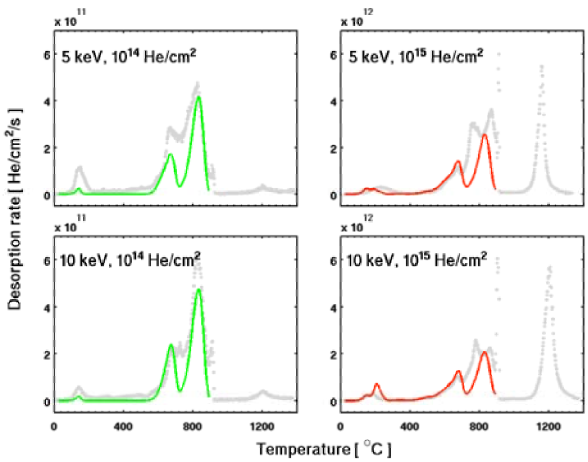

Fig. 1. Cluster dynamics simulation of Hydrogen desorption for different temperatures (needs explanation).

macroscopic, long timescale models. For example, the application of the codes based on Molecular Dynamics (AMD, LAMPPS, MDCASK, etc. by A. Voter, LANL, P. Krstic, ORNL, J. Marian, LLNL, *etc.*) as well as Kinetic Monte Carlo, and Cluster dynamics (TRIM, PARASPACE, PLEXIES by J. P Allain, Purdue, B. Wirth, UTenn) approaches were able to explain important experimental data on the sputtering of mixed materials; chemical erosion and hydrogen desorption from carbon, and helium dynamics in tungsten (*e.g.* see Fig. 1). Simulation of pores in tungsten caused by He irradiation and formation of bubbles [Sharafat 2009] shows a good agreement with experimental observations. A basic visco-elastic model of the "fuzz" growth for tungsten material in plasma containing helium reproduces major experimental finding [Krasheninnikov 2010].

1.D. Framework requirements

1.D.1. Analysis of the requirements for composition of the physics components (including data exchanges and algorithms)

Because the boundary region includes a number of strongly interacting species and processes, coupling of different elements is essential to obtain a predictive model. While some existing codes combine different elements in a type of direct coupling, *e.g.*, fluid plasma and neutral components may be solved simultaneously on the same mesh, here we consider coupling between the most basic physics elements.

Table 4. Requirements for coupling components

Coupling	**Particle species/fields**	**Type, size, frequency of coupled data;** **mesh structure**	**Algorithmic needs**

Plasma transport/ turbulence	Turbulent fluxes or transport coeff; axisymmetric profiles	Volumetric coupling; implicit; for fluid, 2D fluxes/profiles for 4 or more moment variables – 4x50x25 minimum; if kinetic, divide by number of fluid moments/multiple by velocity space (~50x50); with fast turbulence, may only need a coupling frequency of 1/(eddy turn-over time) or transport time scale; flux-surface mesh, nonorthogonal for wall structures	Implicit desirable; preconditioning/solving large linear system
Fluid plasma/ fluid neutral	Plasma source/sink due to neutrals; neutral sources (plasma fluxes to surfaces); plasma parameters; plasma/neutral collisional forces	Volumetric; implicit; sizes same as for plasma turbulence/ transport except may have 3rd spatial dimension; frequency depends on ionization/cx or either i/n transport times; plasma needs flux-surface mesh, neutrals unrestricted	Option of implicit coupling
Fluid plasma / kinetic neutral	Plasma source/sink due to neutrals; neutral sources (plasma fluxes to surfaces); plasma parameters;	Volumetric; sizes same as for plasma turb/transport except may have 3rd spatial dimension; frequency as for neutral fluid; plasma needs flux-surface mesh, neutrals unrestricted	Reduce / eliminate Monte Carlo noise in neutral data; develop capability for implicit coupling. Verify. Approaches to simulating neutral response to large amplitude, intermittent turbulent plasma.

Kinetic plasma / kinetic neutral	Kinetic specification of neutral sources (kinetic characterization of plasma fluxes to surfaces); plasma & neutral fluid parameters; later: plasma & neutral distribution functions	With exchange of fluid parameters, same as above. With exchange of velocity distribution functions (VDF), scale by number of parameters required to specify VDF in each cell; frequency as for neutral fluid; plasma needs flux-surface mesh, neutrals unrestricted	Ensure conservation of mass, momentum, and energy in plasma-neutral exchanges (not guaranteed with moments exchange). These techniques can be used for nonlinear neutral transport also. Approaches to simulating neutral response to large amplitude, intermittent turbulent plasma. Implicit desirable
Photon transport / neutrals & plasma (Adams / Scott approach)	Optical depth; modified effective rates for ionization & recombination	Volumetric times an order of unity factor; frequency on transport time scale; unrestricted mesh	(More thorough verification required.)
Photon transport / neutrals & plasma (coupled line transport)	Neutral & plasma parameters; rates for line absorption and radiation stimulated ionization	Volumetric times an order of unity factor; frequency on transport time scale; unrestricted mesh	(Any approximations require adequate verification)
Eroded & re-deposited particles / plasma & sheath	Sputtered impurity neutrals/ions; dust; fluid or kinetic plasma; sheath model	Surfacial: plasma flux to surface/wall release model and impurity flux to SOL plasma model several ion radii from surface. Volumetric: hydrogenic plasma/neutrals density, momentum, energy, and potential as background to evolve eroded particles/dust. flux-surface plasma mesh or interpolation to other mesh	Noise reduction to improve noise from using particle data in continuum plasma models

Hydrogenic & impurity fluxes / material evolution	Incident particles; surface/near surface stoichiometry and structure	Surfacial with net particle flux to surfaces; couples to material code to describe diffusion/trapping of plasma species in the material & resulting material structure	
Plasma/neutrals to the pedestal/core	Fluxes of particles, momentum, and energy; potential; consistent physics models, e.g., transport coefficients on each side	Surfacial, typically fluxes; change in dimensionality (2D edge, 1D core) introduces need for averaging edge before coupling; frequency on transport (or tubulence if coupled) time scale; consistent B-field at coupling point; overlap region useful	implicit desirable
Concludes coupling requirements			

There is also a question of where time-implicit coupling is important. The answer to this question depends on the shortest timescale in each component. In general, if an time-implicit component is explicitly coupled to a second component that has a fast timescale (whether that second component is implicit or explicit), the timestep required for the first component will likely degrade to that required for the explicit timescale of the second.

A few examples of present-day experiment in coupling boundary components follows in the next two paragraphs. The various processes in the SOL just described are generally tightly coupled, and some of the existing models include this coupling at some level. Foremost in this regard are the SOL/edge transport codes that include plasma, neutrals, and PMI models. The coupling between plasma and neutrals is treated either by using fluid neutrals that fit efficiently into the time-dependent algorithm for the plasma equations, or by using kinetic Monte Carlo neutral particles, which are more accurate but where efficient time-dependent coupling is an issue. Atomic-physics rate coefficients are used by both plasma and neutral models, and should be consistent. Transport of photons in the optically thick regime, especially Lyman-α, can be done directly via a nonlinear Monte Carlo technique, as exemplified by the treatment in EIRENE [Reiter 2007]. In this case, the solution is obtained in an iterative manner; this approach, along with some associated approximations, should be verified. A simpler alternative approach is to incorporate radiation trapping effects directly into the effective hydrogen ionization and recombination rates via an additional optical depth parameter [Scott 2005], eliminating the need for explicit coupling to a radiation transport calculation. This technique was verified with a 1-D plasma-neutral transport tightly coupled to the radiation transport code, CRETIN [Adams 2005].

The coupling between transport and PMI codes is typically rudimentary in that only a single iteration is done and/or assumes a static wall [Brooks 2006]. A dynamic wall model has been coupled to a simple 1D plasma model [Pigarov 2008], and the FACETS SciDAC project is working toward coupling SOL/edge transport and dynamic wall codes as well as a core model [Cary 2009]. The coupling between transport codes and turbulence codes has been performed for isolated cases [Rognlien 2005], but important averaging issues and dynamic coupling are largely untouched. Furthermore, turbulence codes themselves do not include dynamic neutrals or impurities. Finally, plasma chemistry related to hydrocarbons in carbon walls has only been studied in isolated near-wall plasma/neutral models.

1.D.2. Analysis of the requirements for the full workflow (task composition)

The Boundary Science Driver shares with other science drivers the need to plan and execute simulations with a variety of components that can have very different computational requirements; *e.g.*, in the coupling of turbulence and transport, the turbulence simulation will take much more CPU time and memory requirements than transport (unless the turbulence code performs both tasks). While all drivers will share the need for build systems, batch submission interfaces, and the like, we first mention some general capabilities of interest to the Boundary group. The framework should have the capability of efficiently testing individual components as well as various combinations of components. For the testing of individual components, a default static model of essential missing components should be available. For example, a plasma model should have access to a static neutral component and vice versa. It will also be important that the framework allow some level of user-controlled steering for exploratory simulations. With respect to legacy codes, there is an issue if it is worthwhile for their elemental subcomponents to be exposed to the framework such that substitute subcomponents can be explored. This step requires a judgment of the value of the subcomponent, which is difficult to generalize. Finally, all science drivers will need ready access to high-quality visualization tools of simulation results and to experimental data accessible through the framework.

Framework task composition needs for the Boundary Science Driver that are at least quantitatively different from most of the other science drivers are as follows: As stressed earlier, the Boundary has a number of strongly interacting components within it own region that require strong coupling. Thus, while use of file-based coupling has some utility for special interactions, tight coupling will be much more important (see Table 4). If one or more of these components is omitted from a composed task, the substituted representation (say, for neutrals or wall recycling/sputtering) should be of sufficient quality that the approximated behavior is captured. For example, an edge transport simulation without any neutrals will far from experimental reality. Second, several processes are typically represented by data tables that use interpolation, such as ionization, recombination, sputtering, *etc.* Access to documented standardized tables as well as common variations is important. Third, the configurational dimensionality of boundary is at least 2D and more generally 3D. Consequently, data visualization for simulation results and experimental results will be more demanding that for other regions.

1.E. Validation requirements

1.E.1. Measurement requirements

A crucial task of all FSP Science Drivers is the validation of both individual components and integrated models against measurements from experiments. In the Boundary Science area, special measurement challenges arise. The boundary plasma and surrounding surfaces are inherently 2-D or 3-D and typically feature steep spatial gradients, and the plasma is subject to highly intermittent and often strong turbulence, which dictates that PMI itself will be intermittent. The validation of integrated models will require advanced and in some cases new diagnostics. In particular, diagnostic techniques must extend beyond the realm plasma diagnosis to measurement of surrounding material surfaces. These surface diagnostics are very different from the largely spectroscopy techniques used for the plasma. In the table below we list the physics areas and measurements needed for validation, as well as important measurements that are not currently provided by the commonly available diagnostics.

Table 5. Critical physics and required measures for Boundary model validation

Issue	Critical Physics	Measurements Needed	Important Gaps
Cross field transport	- Collisional and turbulent transport of heat, particles and momentum - Effects of meso-scale short wavelength MHD-like modes - Blobs (transport via coherent structures) - Role of magnetic topology, magnetic shear, x-point and wall/divertor contact geometry	- Time-averaged profiles of ne, Te, Ti, perp. and parallel flows - Spatiotemporal resolved fluctuation fields in near and far SOL for ne, Te, ϕ, B and flow velocities including amplitude, relative phase, cross-coherence - Plasma turbulence mapped along field lines to wall	- Ti profiles - Te, B fluctuations and their correlation with ne, ϕ - 2D coverage for profiles and fluctuations - Synthetic diagnostics (e.g. probe theory, turbulence imaging) - Simultaneous fluctuation measurements along a field line

Heat and particle loads	- Integration of perp. and parallel transport, flows, atomic and neutral physics - Momentum transport – plasma-neutral interactions - Fueling, recycling and retention - Sheath heat transmission physics - Radiation transfer - Transport in and through private flux region - SOL currents	- Surface temperature evolution - Local plasma profiles, plasma potential and fluctuation near material surfaces - Neutral densities, transport - In situ measurement of fuel retention vs material, depth, temperature - Spectral measurements to determine radiation opacity - Tile currents - Poloidal field	- Local measurement of recycling coefficients - Atomic physics - 2D coverage for plasma profiles, potential - 3D coverage - Transient measurements - Synthetic diagnostics - Kinetic data in plasma volume and at surfaces
Impurity generation and transport	- Impurity sources - Collisional and turbulent transport including flows - Impurity sinks – condensation, chemical bonding, implantation, co-deposition	- Characterization of impurity sources - Impurity profiles and transport (fluxes) - SOL flows	- 2D coverage for sources - 3D coverage for impurity profiles - Transient measurements - Hot walls

Evolution of material surfaces	- Plasma heat and particle sources - Plasma material interactions and evolution of surface and sub-surface structures - Surface chemistry - Effects of applied surface coatings and cleaning - Dust generation	- Net erosion/deposition rates - Offline measurements of surface chemistry and morphology (at all scales) - In situ measurement of surface stoichiometry, morphology and dust	- In situ measurements - Steady state plasmas - Hot walls
Interactions with RF fields	- Creation of RF sheaths - Impurity generation - Ionization and heating of SOL plasma - Effects on launching structures	- RF sheath potentials - Ion distribution functions - Impurity generation - Local Te, ne and ionization rates in SOL - Characterization of launching structure surfaces	- 2D, 3D coverage - Plasma measurement in presence of strong RF fields
Concludes critical physics/measurements for validation			

1.E.2. Plans for validation of critical physics associated with the science driver

The level of measurements available in confinement devices necessarily impacts validation plans. It should be noted that highly resolved plasma and surface diagnostics are often readily available in linear plasma devices, and that to the extent possible, boundary science validation should exploit these devices to the fullest (*e.g.* PISCES, DIONISOS), With respect to the boundary area of confinement devices, the measurement challenges can be set into three broad categories which are described here:

1. <u>Deployment of mature diagnostics with sufficient spatial extent and coverage</u>. This topic is particularly important because it identifies a near-term (and relatively low risk) route by which boundary science validation is greatly improved. This includes
   - scanning and fixed Langmuir probes with large poloidal coverage of SOL. This meets many of the requirements for 2-D static and fluctuating plasma fields and associated transport (density, temperature, flows); gas-puff imaging also provides

important fluctuation measurements, though the impact of neutral profiles requires synthetic diagnostics that model neutral profiles

- Thomson scattering measurements of electron density and temperature usually extend into the SOL and profile key profile information, though multiple diagnostic signals typically need to be averaged owing to the intermittent nature of large fluctuations and the short duration of the Thomson data window
- scanning of fixed potential probes. These may be Langmuir probes or other special designs (emissive probe, ion sensitive probe)
- infrared thermography and thermocouples to provide high resolution energy /power balance to materials, especially the divertor plate regions
- optical spectroscopy for impurity (gross) influx from surfaces, spatial profiles and impurity temperatures; validation of the long-range transport will require profiles of the impurity content, as well as plasma flow.

2. Allocation of experiments dedicated to boundary/PMI diagnosis. This category highlights the requirements for controlled, long-term exposure of plasma-facing surfaces in confinement devices, if ex-situ analysis of materials is required. Such experiments provide controlled and diagnosed exposure of surfaces in an integrated manner, however they require the dedicated, long-term use (multiple days typically due to short pulse lengths) of the confinement device. Examples include:
   - exposure of material samples on retractable probes
   - removal and analysis of plasma-facing components during vent access
   - operationally "perturbing" experimental device operation: *e.g.* hot walls, oxygen baking
3. Development of new in-situ diagnostics. This approach includes either developing completely new diagnostic methods and/or the adaptation of existing ex-situ diagnostics to the confinement devices. Important diagnostic developments here are:
   - main ion temperature in the SOL and divertor. The role of ions in heat exhaust is essentially completely unknown at this point; such measurements would be key in validating heat transport models in the SOL/divertor
   - fast optical techniques to resolve geometric features of turbulence and plasma flows in high-temperature H-mode
   - plasma-facing surface diagnosis: erosion, stoichiometry, hydrogen isotopes
   - velocity distributions of electrons and ions to examine kinetic effects

All of the options just mentioned can be considered with respect of a strategic plan. However, option 2) has been the status quo for much of PMI studies, and it is generally acknowledged that leads to very incomplete and ill-controlled measurement picture. In addition it is unlikely that confinement devices will switch large portions of their run time to boundary/PMI studies. Therefore it is likely that the optimal strategy will be

1. Short term program of increased deployment of standard diagnostics (2-3 years)
2. Proof of principle development of new diagnostics in 3-5 years. These can be performed either in off-line facilities or at small scale in confinement devices. Highest priority should be given to

- o Ion temperature
- o In-situ surface diagnosis
- o Velocity distribution and flows

3. Deployment of new diagnostics in confinement devices (4-10 years)

1.F. Connections to other work

1.F.1. Relation to other work within the FSP

Development of an integrated plasma boundary model will depend on tools and codes produced by other groups within the FSP. In turn, other science application areas will require a boundary model, at some degree of complexity and fidelity, as an element in their own codes. The most direct connection is with the pedestal, which covers an overlapping spatial domain and a great deal of common physics. The physics of turbulence, cross-field transport and neutral transport are continuous across the separatrix with pedestal structures extending some small distance into the open field line region. Thus certain advanced components, for example for implementing gyrokinetic turbulence, Fokker-Planck collision operators, and kinetic neutral transport could be shared. We note, for example, experimental observations of an E_r shear layer in the SOL of L-mode plasmas [LaBombard 2005] and the connection between SOL flows, equilibrium topology and the L-H threshold [Ritz 1990]. Initially, codes for each region will require simplified models to serve as boundary conditions for profiles and a calculation from the pedestal group of transient heat and particle loads from ELMs. The coupling likely requires consideration of fluctuation propagation, flows and other phenomena suggesting that ultimately, a common model for the boundary and pedestal plasmas will be required. As more sophisticated plasma-material models are developed, calculation of transient loading from disruptions will be needed as these can cause discontinuous change in the morphology and chemistry of the first wall. Wave-particle codes will need a plasma boundary model to account for the physics of parasitic losses and RF sheath generation. The two groups will need to work together for calculations of the resultant impurity production and local heat deposition. The boundary group will need to produce reduced models, perhaps at various levels of fidelity, for whole device modeling especially for impurity sources and fueling. Finally, production of the boundary model will also require the set of common FSP components, for example for 2D and 3D MHD equilibria and inclusion of the slow evolution of the equilibria, along with tools and infrastructure for software development support, user support, data management, software testing and release.

Table 6. Connections to other FSP activities

Application Area	Capabilities Needed From Boundary	Capabilities Provided to Boundary	Capabilities Shared with Boundary

Pedestal	Heat, particle, momentum fluxes Neutral and impurity fluxes	Heat, particle, momentum fluxes	Gyrokinetics Fokker-Planck Collisions Kinetic neutral transport
Wave-Particles	Plasma profiles Fluctuation levels	Local heat deposition from fast particles and RF	Parasitic RF losses and impurity sources
Disruptions		Transient local heat and particle loads	Atomic and neutral physics, radiation transport
Whole Device	Reduced models for boundary, especially fueling, fuel retention impurity sources	Heat, particle, momentum fluxes	

1.F.2. Relation to work outside the FSP

In its early stages, the plasma boundary model will depend on adaptation of existing physics components. Further development of foundational theory will be required for the boundary model in several important areas…

- Foundational theory
    - Kinetic theory applicable in boundary (perturbation size, scale separation, momentum equations, collision operators? …)
    - Sheath (and probe) theory including RF and surface roughness
    - Models appropriate for multi-scale (space/time) materials modeling
- Development or adaptation of existing components including those for
    - Fluid and kinetic turbulent transport
    - 3D neutral transport
    - Atomic physics packages
    - Radiation transport models
    - Materials and PWI models

1.G. Schedule and resources

The boundary region has a number of components of varying complexity that need to be coupled to provide a realistic model of this region. Consequently, there are a number of tasks that need to be carried out simultaneously, with lower-level models (*e.g.*, fluid versus kinetic) providing the first coupled results that give way to more sophisticated models over time. The current coupled model can provide an evolving boundary module to be used for whole-device simulations at any time. An overview of the projected schedule of the work to be carried over a 15 year time period is provided by the following figure where the abscissa denotes years.

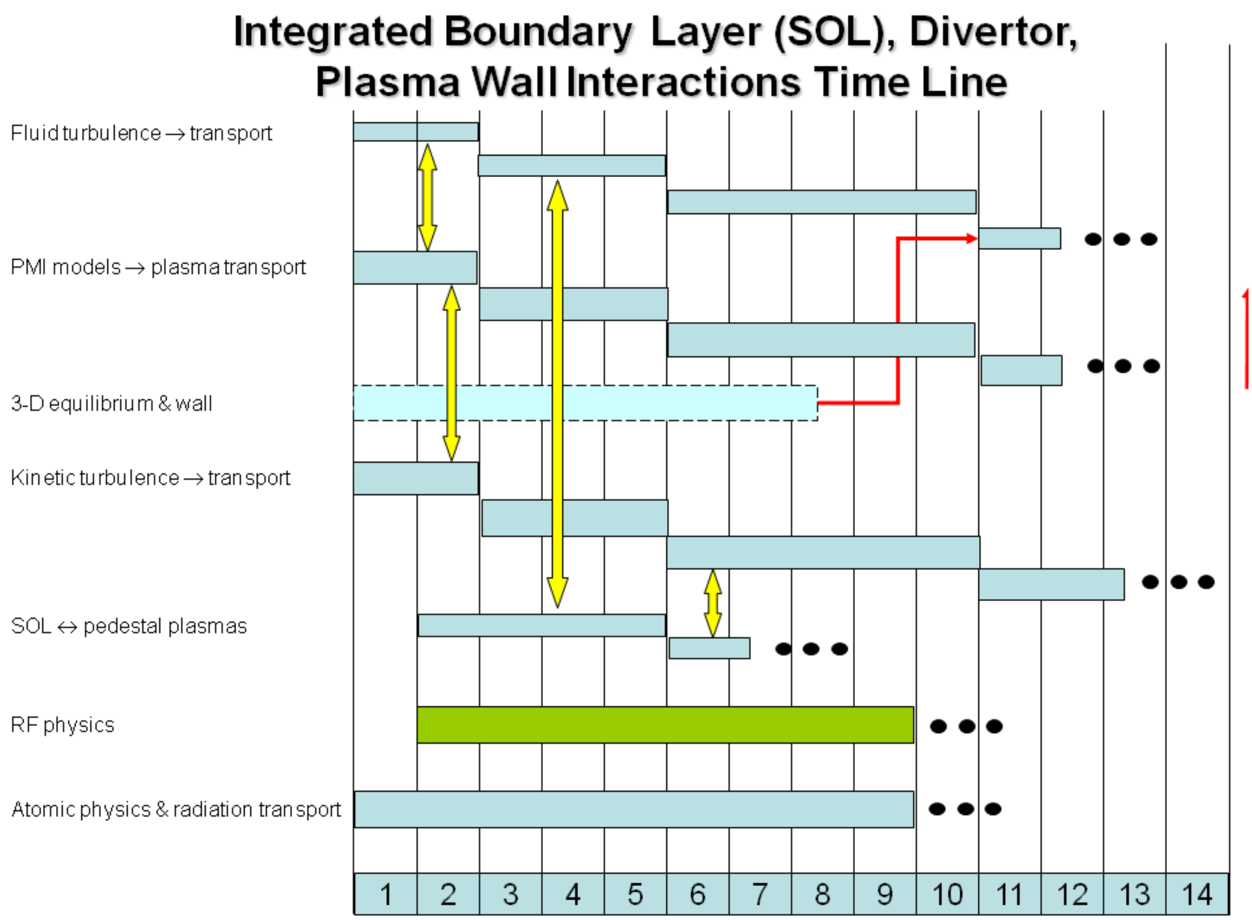

Fig. 1.2 Projected time line for development of coupled Boundary Science Driver components Each line in the chart corresponds to a separate Science Driver task; the height of the bars is intended to qualitatively reflect the relative manpower requirements associated with each task. The horizontal axis corresponds to calendar years. The dashed border of the "3-D equilibrium and wall" task indicates that this work is being undertaken by the base program outside of the FSP. The different color of the "RF physics" task indicates that it is part of a separate Science Driver. The yellow arrows indicate multiple exchanges of information & capabilities; similar exchanges for RF and atomic physics are not shown for clarity. Red arrows denote one time or infrequent exchange of information between tasks.

The elements of the boundary module are divided into tasks corresponding approximately to the rows in Fig. 1, though owing to staged development, some subtasks do not appear sequentially in the table. The schedule and resources for each is given below (PFTE=physicist FTE and CFTE=computational/math FTE):

Task 1: Coupling fluid plasma turbulence, transport, and neutrals in the SOL

- Years 1-2 [continuation of some of the development begun in FACETS]
  - Couple SOL fluid plasma transport/turbulence; suitable micro-turbulence and/or transport codes exist; either iterative coupling between codes or long-time turbulence simulation with continuously evolving profiles: 1 PFTE/yr, 1 CFTE/yr
  - Couple neutral model, initially fluid; likely embedded in plasma fluid codes for coupling efficiency; verify with Monte Carlo: 0.25 PFTE/yr, 0.25 CFTE/yr.
- .
- Years 3-5
  - Couple impurities and radiation transport models; impact of turbulence on impurity transport: 1.0 PFTE/yr, 1.0 CFTE/yr for 1.5 years.
  - Extension of fluid turbulence to foot of pedestal region, begin to include long toroidal wavelength ELM modes: 0.5 PFTE/yr, 0.5 CFTE/yr.
  - Couple dynamic kinetic neutral model; likely Monte Carlo: 0.5 PFTE/yr, 0.5 CFTE/yr for 1 year
  - Couple evolving MHD equilibrium to account for shifting separatrix: 0.5 PFTE/yr, 0.5 CFTE/yr for 1 year.
  - Extend fluid neutral model to include additional species and equation for neutral temperature: 0.5 PFTE/yr, 0.5 CFTE/yr for 1 year.
  - Improve coupling to kinetic Monte Carlo neutral model to reduce or eliminate statistical noise: 0.5 PFTE/yr, 1.0 CFTE/yr for 1 year
- Years 6-10
  - 3D plasma transport; peaking factors of heat flux, PMI
  - 3D magnetic fields
  - 3D kinetic radiation transport
- Years 11-15
  - ?

Task 2: Coupling plasma-material interaction models with plasma transport

- Years 1-2
  - Couple dynamic wall model for hydrogen wall uptake/recycling with dynamic 2D SOL plasma model 0.25 PFTE, 0.5 CFTE/yr
  - Initiate full coupling between near-surface, particle-based sputter erosion/re-deposition code for 2D impurities and SOL 2D fluid plasma model. Resolve possible particle-noise issues. 1.5 PETE+CFTE/yr
  - Provide the interface and a reduced material model that uses as input ELM and disruption characteristics, *i.e.,* frequency, duration, and power, and can output the material response corresponding to *non-melting* (acceptable) or *melting* (non-acceptable) condition. 1.0 PETE+CFTE/yr

    - Improve data transfer between MD simulations and PMI models; 0.25 PFTE, 0.25 CFTE/yr
- Years 3-5
    - Couple initial surface evolution model and near-surface plasma model; 1 PFTE/yr, 1 CFTE/yr
    - Couple kinetic SOL to dynamic SOL models: 0.5 PFTE/y, 0.5 CFTE/yr
    - Improve near-surface model coupling to MD model; 0.5 PFTE/y, 0.5 CFTE/yr
- Years 6-10
    - Couple 3D SOL code to 3D near-surface and PMI codes: 1.0 PFTE/yr, 1.0 CFTE/yr
    - 3D impurity transport, surface evolution, improved plasma/material interaction models
    -
- Years 11-15
    -

Task 3: Couple kinetic plasma turbulence and transport in SOL

- Years 1-2
    - Couple (2D, 2v) kinetic SOL plasma with nonlinear Fokker-Planck collision model capable of full short-to-long mean-free path (leverage CPES and ESL): 1-2 PFTE/yr, 1 CFTE/yr
    - Initial coupling (perhaps non-conservative) of kinetic plasma code to kinetic neutral model; demonstrate strong recycling and near steady-state 0.5 PFTE/yr, 0.5 CFTE/yr.
    - Develop and extend kinetic Monte Carlo neutral transport component: 1 PFTE/yr, 0.5 CFTE/yr.
- Years 3-5
    - Couple kinetic (first electrostatic, then EM) turbulence to kinetic transport from foot of pedestal to wall: 2 PFTE/yr, 1 CFTE/yr.
    - Improved (conservative, more efficient) coupling of kinetic plasma code to kinetic neutral model: 1 PFTE/yr, 1 CFTE/yr.
    - Apply similar technique to nonlinear neutral transport problems in kinetic Monte Carlo code: 0.5 PFTE/yr, 0.5 CFTE/yr.
- Years 6-10
    - Couple kinetic impurities to main ion transport; 1 PFTE/yr, 1 CFTE/yr
    - Extend kinetic domain well into pedestal; either couple to pedestal model or extend domain of single kinetic model
    - Couple Kinetic ELM simulations; ejection, heat footprint

- Develop hybrid fluid-kinetic neutral transport component: 1 PFTE/yr, 1 CFTE/yr.

- Years 11-15
  -

Task 4: Couple SOL and Pedestal plasmas

- Years 2-5
  - Begin extending fluid and kinetic transport well across separatrix (see Tasks 1 and 3)
- Years 6-10
- Years 11-15

Task 5: Couple RF antennas/physics with SOL and PMI models

- Years 2-5
- Years 5-10
- Years 10-15

Task 6: Atomic physics models

- Years 1-5
  - Develop tractable characterization of high-Z atoms (already underway): 1 PFTE/yr.
  - Calculate kinetic details for hydrogen molecular physics and incorporate into kinetic neutral transport model: 1 PFTE/yr.
  - Identify and obtain data for molecular species pertinent to mixed material environment of ITER: 2 PFTE/yr, 0.5 CFTE/yr.
  - Assemble improved data and simplified models for breakup of hydrocarbon molecules: 2 PFTE/yr, 0.5 CFTE/yr.
- Years 6-10
- Years 11-15

Table 7. Summary of Schedule and Resources

(P/yr = PFTE/year and C/yr = CFTE/year)

	Year 1-2	**Year 3-5**	**Year 6-10**	**Year 11-15**
Task 1 fluid plasma/neutrals transp/turb	2.5 P/yr; 2.5 C/yr	1.7 P/yr; 1.8 C/yr		
	Coupled SOL fluid transport/turbulence; coupled wall	Couple impurities, kinetic neutrals, extend turb.		

Task 2 PMI models				
Task 3 kinetic plasma/neutrals transp/turb.				
Task 4 couple to pedestal				
Task 5 couple to RF				
Task 6 couple to disruption				
Task 7 atomic/ molecular physics				
Concludes summary of schedule and resources				

1.H. Milestones

High-level goals and milestones are as follows:

Milestone	**Year from inception**
Self-consistent SOL fluid plasma turbulence and transport (heat-flux width)	2
Dynamic coupling between PMI model and SOL plasma (integrated particle inventory)	2
Electrostatic kinetic turbulence and transport in SOL	5
Surface evolution model	5
Extension of kinetic transport and turbulence into pedestal or coupling with pedestal model	10
Tritium transport and retention	10
Electromagnetic kinetic turbulence and transport	
3D kinetic transport – peaking factors	15

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2. PEDESTAL INTEGRATED PLANNING TEAM REPORT

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This report from the Pedestal Integrated Planning Team lays out a set of scientific goals and challenges, and proposes a roadmap for addressing these issues. Background and motivation for the work is provided in Sec A, and goals, including a proposed roadmap, are given in Sec B. A set of required components (Sec C), frameworks (Sec D), and plans for validation (Sec E) and coupling to other efforts (Sec F), are provided. A proposed schedule and estimates of resource requirements (Sec G) and milestones (Sec H) are also provided.

2.A. Background and Motivation

High performance ("H Mode") operation in tokamaks is achieved via the spontaneous formation of a transport barrier (or "pedestal") in the outer few percent of the confined plasma. This edge transport barrier strongly improves global energy confinement, and also generally improves global stability, resulting in dramatically enhanced fusion performance and the potential for more cost effective fusion reactors. However, the free energy in the large pressure gradient and the resulting bootstrap current in the pedestal can drive instabilities called Edge Localized Modes (ELMs), which deposit heat and particles on plasma facing surfaces, and may constrain component lifetimes in reactor scale devices. A predictive understanding of pedestal formation and structure, as well as the physics of ELMs, is essential for prediction and optimization of the fusion performance of ITER and future reactors.

The plasma pressure typically increases by 1-2 orders of magnitude from the bottom of the pedestal to the top, and increases by less than an order of magnitude from the pedestal top to the magnetic axis. Hence, while the pedestal occupies a relatively narrow radial region, it contains far more pressure scale lengths than the core plasma. The pedestal accounts directly for a significant fraction of global confinement, and its impact on global confinement is further amplified via coupling to the core plasma. In the core, transport is typically dominated by turbulence driven by microinstabilities. This transport is fairly stiff, meaning that the core profiles are closely correlated to the microinstability critical gradient scale lengths. As a result, the core pressure increases roughly linearly with the pedestal pressure (or "pedestal height"), and the fusion power output scales roughly as the square of the pedestal height. Furthermore, the pedestal height is quite sensitive, for example to small changes in the plasma shape, or changes in collisionality or safety factor, and hence provides a powerful lever for performance optimization of fusion systems.

While the performance benefits of H-mode operation are dramatic, there is a potential drawback. The large pressure gradients in the edge barrier lead to large localized currents, via the bootstrap effect, and the substantial free energy present in both the pressure and current gradients can drive the repetitive instabilities known as ELMs. While ELMs are largely benign in existing devices, and can aid in density and impurity control, ELMs deposit a highly impulsive heat and particle load on plasma facing surfaces. Empirical scaling of ELM heat loads to ITER- or reactor-scale devices suggests that unmitigated ELMs could substantially reduce the lifetimes of plasma facing components. Hence it is important to understand heat and particle loads produced by ELMs, as well as to consider methods for mitigating or eliminating ELMs. A number of ELM control methods have been explored, including active control of ELMs via 3D resonant magnetic perturbations (RMP), or triggering of rapid, small ELMs via pellet injection, magnetic perturbations, or rapid displacements of the plasma. Pellet pacing and RMP ELM control are both presently under consideration for ITER. Operation in steady state without ELMs or with very small ELMs has also been achieved in a number of regimes. One regime of interest is Quiescent H-Mode (QH), in which a saturated mode called the Edge Harmonic Oscillation (EHO) drives transport and allows steady state ELM-free operation in the low collisionality regime of interest for ITER and reactors.

The goal for ITER and future fusion reactors is thus to achieve a high, essentially steady-state pedestal to optimize fusion performance, while also eliminating or strongly mitigating ELMs. To achieve this goal, the transition to H-mode (or "L-H transition"), and the transition to high-performance H-mode will have to be achieved, with as low auxiliary power input as feasible.

2.A.1. Challenges

The pedestal presents a daunting set of challenges to traditional theoretical and computational methods. Because the pressure varies by 1-2 orders of magnitude across the pedestal, and the density, temperature, flow velocity, radial electric field and current also vary substantially, a very wide range of key dimensionless parameters is encompassed in this region. For example, the pedestal often transitions from highly collisionless near the top, to strongly collisional at the bottom, requiring methods appropriate for both regimes.

More fundamentally, the broad range and overlap of spatiotemporal scales across the pedestal deeply challenges the assumed separation of equilibrium ("macro") and turbulence ("micro") scales upon which most existing theory and computation relies, and thus extensions of basic theory and massive computational resources are expected to be needed. For example, across a single pedestal, the timescales associated with electron drift waves span a wide range (due to the wide variation of equilibrium quantities) which overlaps with the wide range of temporal scales associated with Alfven waves, which in turn overlaps ion drift wave and ion transit temporal scales, which in turn can overlap the fast timescales on which the equilibrium itself is observed to evolve, for example during an ELM. The range of overlapping temporal scales often exceeds six orders of magnitude. A similar overlap is found in physically relevant spatial scales, where the gyroradius and ion drift wave scales can overlap the short gradient scale lengths. In principle, a fully self-consistent simulation must then treat the full range of scales, challenging even the most powerful supercomputers envisioned to be available in the near future.

Furthermore, perturbations can be large compared to the background equilibrium, for example during ELMs or so-called "blob" transport, presenting a challenge to perturbative methods. Flows and sources, including impurity radiation and atomic physics, are expected to be important, bifurcations and operation near marginality must be considered, and geometry is complex, particularly in problems for which coupling to the boundary region outside the separatrix is strong. In addition, in plasmas with ELMs, the pedestal region does not generally reach a steady state, but rather continues to evolve throughout the ELM cycle. The ELM itself is a highly complex event, involving both MHD and transport physics, and extending from the pedestal region, where it is primarily driven, out into the open field line region, and finally onto material surfaces, with coupling back to the deeper core via the evolving pedestal profiles.

2.A.2. Progress

Despite these challenges, there has been substantial recent progress in understanding key pedestal physics issues, and in developing computational tools suitable for pedestal studies.

The onset of ("Type I") ELMs, and a crucial constraint on the pedestal height, has been found to be due to the onset of intermediate wavelength MHD modes, known as "peeling-ballooning modes" because they are driven by a combination of the pressure gradient (ballooning) and edge current (peeling or kink) drive. Efficient linear codes have been developed for calculating the peeling-ballooning mode onset condition, and in numerous studies on several devices, this calculated onset condition has been found to agree with the observed ELM onset condition and to a constraint on the pedestal height as a function of the edge barrier width (or "pedestal width"). Model equilibrium studies have been used to apply the peeling-ballooning constraint predictively, and to explore its parametric dependencies. Nonlinear simulations using Braginskii, extended MHD, and gyrofluid codes have explored ELM dynamics with increasing physical realism. For example, recent improvements in numerical methods and available computing power have allowed extended MHD ELM simulations with realistic values of resisitivity and viscosity, yielding agreement with linear onset dynamics, and beginning to explore nonlinear dynamics at realistic collisionality, in some cases including the effect of flow.

Static models of the pedestal height and width have been developed by combining the peeling-ballooning constraint with another linear constraint, such as that for stiff onset of kinetic ballooning modes. These models, without any fit parameters, have proved to be reasonably accurate in predicting the pedestal height in the high performance H-mode regime on a number of devices, though a number of extensions can be considered.

A number of computational tools have been developed to begin the study of dynamic evolution of the pedestal. Neoclassical transport codes, including fast steady-state solvers, and large scale initial value simulations have been developed to treat the pedestal region, and tested, identifying significant ion thermal transport and potential effects due to ion orbit losses. Closed field line gyrokinetic solvers initially developed for the core have been extended to include fully electromagnetic perturbations and more realistic collision operators, potentially enabling their use in pedestal studies, both linear and nonlinear. Gyrokinetic codes incorporating both the closed field line (pedestal) region, and the open field line boundary region are under development by a pair of US projects (CPES and ESL).

There has also been substantial progress in experimental measurement of profiles and turbulence in the pedestal region, as well as measurements of ELM dynamics and heat loads on material surfaces. A number of tokamaks have developed and are continually improving systems for measuring profiles with the high spatial resolution required to determine the pedestal width and, more challenging, gradient scale lengths within the edge barrier. A number of analysis challenges remain, however. Measurements of pedestal turbulence on ion and in some cases electron scales have been conducted on several devices, and ELM dynamics have been observed with a number of fast diagnostics. A large database of pedestal measurements is available, and opportunities for model validation are abundant, at several levels of comparison.

2.B. Goals for the Pedestal Science Driver

The practical goal for pedestal research is to achieve operation with a high pressure pedestal with a profile relaxation mechanism which does not present the material interface with unacceptable transient heat loads – that is to operate with small or no ELMs. For modeling, the goal is to develop the capabilities to understand and predict:

(A) the onset of edge barriers (or "L-H transition") as well as the transition from low to high performance H-mode,

(B) the structure of the barrier in all profiles (with particular initial emphasis on the pressure at the top of the pedestal), and

(C) the nature of the pedestal relaxation, particularly ELMs, and to identify and optimize methods for reducing transient heat deposition on material surfaces (including ELM-free and small ELM regimes, as well as suppressing or mitigating ELMs via external control techniques, including magnetic perturbations or pellets).

Since the pedestal height strongly influences overall plasma performance, accurate pedestal modeling is essential for an overall predictive capability for fusion plasmas. Development of a validated predictive capability for the pedestal structure will allow coupled pedestal-core optimization of global fusion performance, which is essential both for attaining high performance in existing devices and for designing future reactors.

Related to the above goals, there are several notable gaps in present understanding. There are fundamental experimental observations that cannot yet be modeled with sufficient accuracy, representing important areas where substantial scientific progress is needed to achieve goals described above. These include:

- L-H transition, particularly in terms of input power
- Prediction of large scale radial electric field (Er) and plasma rotation
- The wide variety of ELM types and ELM-free H-modes
- Heat and particle loads from large Type I ELMs
- Plasma fueling across the pedestal region

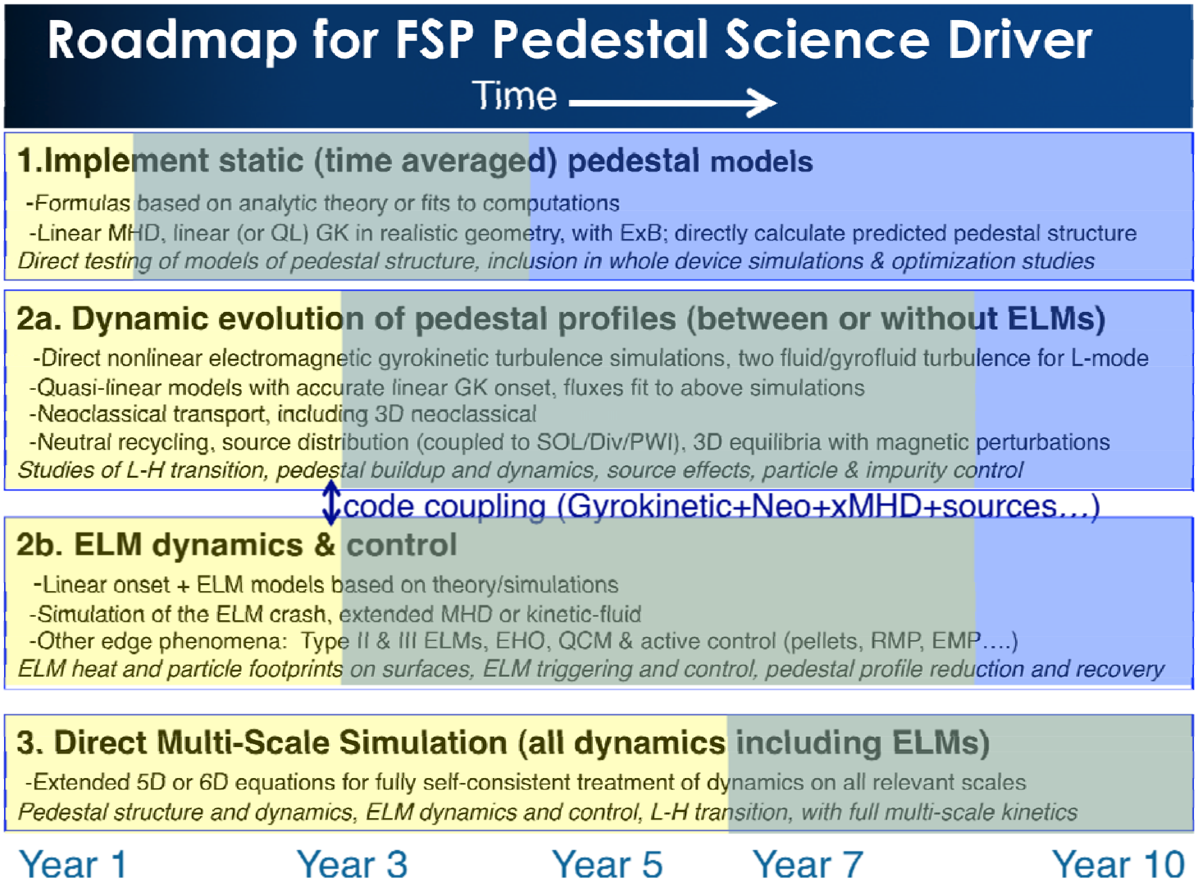


Figure 1: The three level roadmap for the pedestal science driver, indicating sets of major tasks (1, 2a&b, 3) that are planned. All levels are to be initiated at the onset of the project in Year 1. Each level of the roadmap (1,2 &3) will begin with a development, implementaion and verification stage (shaded yellow), followed by a validation and ongoing development stage (shaded green), and finally a stage of routine application, with minor ongoing development (shaded blue).

2.C. B.1) Roadmap for the Development of Pedestal Simulation

The goals, challenges and progress described above lend themselves to a three level plan for the FSP pedestal effort. This plan, illustrated in Fig 1, addresses both the need to deliver world-leading capability on a relatively short timescale, and the need to address the deeper fundamental challenges associated with pedestal dynamics, taking advantage of peta- and exa- scale computing capability as it becomes available.

As described above, there are a number of computational approaches which can be applied with increasing physics fidelity but also with increasing challenge to theory and computation. At the first level, the physics of the static (ie time-averaged) pedestal can be addressed via linear physics models, based on existing models and their extensions. Simple models such as EPED are based on linear calculations of instability thresholds and strong onset of transport or ELMs above those thresholds. At the 2nd level, dynamics of the pedestal are considered, but a separation is maintained between the physics models for the ELM event itself, and the dynamics between, or in the absence of, ELMs. A wide variety of available and developing tools can be used to treat neoclassical and turbulent transport between ELMs, including electromagnetic gyrokinetic simulation codes (and in some limits gyrofluid and Braginskii turbulence codes). Full f codes can potentially be used to treat larger perturbations, but will require further development. At this level, the ELM event itself will be treated separately, via calculations of its onset and dynamics with extended MHD or gyrofluid codes. Finally, at Level 3, dynamics across all relevant scales, including ELMs, will be treated self-consistently with a single simulation code. Additional advancements in theoretical gyrokinetic algorithms, and possibly formulations, to allow fully electromagnetic simulations of arbitrary scale electromagnetic modes in pedestal geometry may be required. The most complete models would be 6D full kinetic simulations using the full collision operator. The computational challenge that this would present suggests that its use, at least initially, would be for assessment of the less complete models, though in the longer term, with sufficient computational power becomes available, more extensive use could become practical. This general outline leads to a corresponding development roadmap with three levels and four major elements, illustrated with a timeline in Figure 1:

Level 1. Linear models for pedestal structure

This step would begin with componentization of existing models that solve for static (time averaged) pedestal structure via linear stability analysis, for example, that of peeling-ballooning and kinetic ballooning modes. Improvements can come through use of linear or quasi-linear gyrokinetic calculations, more realistic geometry and inclusion of ExB stabilization. Extended models could include shorter wavelength driftwave modes (eg electron temperature gradient modes) and neoclassical effects. This analysis typically requires hundreds or thousands of independent MHD and/or gyrokinetic stability calculations with trial equilibria. Key issues are robustness, error checking, automation, and, particularly in the case of gyrokinetic calculations, efficiency. Extensive comparison with experimental data sets will be carried out. It is expected that this capability can be made available relatively quickly, allowing a world-leading capability for coupled pedestal-core optimization of fusion systems.

Level 2. Dynamic evolution of the pedestal via separate inter-ELM and ELM components

2a. Dynamic evolution of pedestal profiles between ELMs

The fundamental tool for calculating pedestal transport between ELMs is expected to be electromagnetic gyrokinetic simulations of turbulent transport, coupled to separate calculations of neoclassical transport and sources. In some limits, gyrofluid or Braginskii simulations may also be employed. It is envisioned that nonlinear simulations will be employed both for development of simplified transport models, as well as for direct calculations of particle, momentum and heat transport. Neoclassical calculations will eventually include 3D equilibrium effects, such as neoclassical toroidal viscosity. Source models should include neutral transport and pellet fuelling – and eventually to a more complete model of the boundary plasma, recycling, impurity sources, etc. All of these models would need to be appropriately verified, including extensive verification of reduced dynamic models against direct nonlinear simulations, and validated against experimental measurements.

2b. ELM dynamics & control with fluid or kinetic-fluid hybrid models

The models described above would be extended by simulation of phenomena which limit or control the pedestal pressure gradients. These would include spontaneous plasma behavior [ELMs of various types, Edge Harmonic Oscillation (EHO), Quasi-Coherent Mode (QCM), etc.] and active control through pellets, resonant magnetic perturbations (RMP), electromagnetic perturbations, etc. The work could begin with linear onset from peeling-ballooning calculations, coupled to simple ELM crash models. The next step would be direct simulation of ELM dynamics using extended MHD or two-fluid and/or kinetic-fluid codes. These codes would need to include realistic calculations of parallel transport and through coupling to boundary models, compute transient heat and particle loads onto material surfaces. Validation experiments could compare ELM (or other mode) structure, dynamic modification of pedestal profiles, heat and particle footprints and ELM control mechanisms.

Level 3: Direct Multi-Scale Simulation

The prior computational stages use gyrokinetic calculations for modeling the micro-scale and extended MHD for the macro-scale. However, as noted above, these overlap strongly in the edge barrier. Some systematic study will be required to test the assumption of spatiotemporal scale separation, to determine when and how it breaks down and to assess the consequences. Numerical and theoretical progress will be required to develop and implement verified formulations and codes which can simulate multi-scale electromagnetic modes and turbulence in separatrix geometry. Several approaches are possible including gyrokinetic treatments without the high-n approximation, kinetic-fluid methods and 6D Vlasov treatments including the full collision operator. The last of these, in particular, will require substantial progress in numerics to be practical. These models would support the most fundamental studies of pedestal physics including threshold, coupling of turbulence and equilibrium scales, ELMs and ELM control.

2.D. Components

b. Requirements for physics codes (components) that need to be integrated in order to achieve the goals associated with the science driver.

As indicated in the roadmap in Figure 1, we have identified three levels of pedestal modeling development. We organize the anticipated physics components by the level in which they first are required; Tables 1, 2, and 3 present the components for levels 1, 2, and 3, respectively. For each component, we provide a description of the capability to be provided by the component as well as the important inputs and outputs for the component.

Physics Component	Capability	Inputs	Outputs
Geometry and Mesh Conversion	Provides equilibrium magnetic field coordinates from core to walls; convert between various coordinate systems (e.g. (R,Z,ζ) to (ψ,θ,ζ)) and mesh	Equilibrium profiles and magnetic field expressed in input coordinates and mesh	Equilibrium magnetic field expressed in output coordinates and mesh
Linear MHD Profile Stability Analysis	Determines the static (time-averaged) linear stability of peeling-ballooning modes and MHD ballooning modes to predict ELM onset and critical pedestal profiles in realistic geometries.	Equilibrium magnetic flux surfaces; main ion, impurity ion and electron density and temperature profiles; pressure and current density as functions of magnetic flux	Linear ELM threshold and pedestal profile at criticality
Linear Electromagnetic Gyrokinetic Profile Stability Analysis	Determines the linear stability of kinetic ballooning modes, ETG, ITG, TEM (or other micro-instabilities) to predict critical pedestal profiles and microinstability growth rates and	Equilibrium magnetic flux surfaces; main ion, impurity ion and electron density and temperature profiles; pressure and current density as functions of magnetic flux	Pedestal profile at criticality; growth rates and stiffness of microinstabilities

	spectra in realistic geometries.		

Table 1. Level 1 Components: Required to implement static (time-averaged) pedestal models

Physics Component	Capability	Inputs	Outputs
Closed-flux-surface Gyrokinetic Turbulence	Evolves a nonlinear, electromagnetic gyrokinetic turbulence model on closed field lines. Is capable of computing accurately both electron and ion scales and includes a realistic collision model.	Equilibrium magnetic flux surfaces; initial profiles; boundary conditions	Turbulent particle, momentum, and energy fluxes across pedestal and to core and SOL. Fluctuation levels and spectra
Cross-separatrix Gyrokinetic Turbulence	Evolves a nonlinear, electromagnetic gyokinetic turbulence model on both open and closed field lines. Is capable of computing accurately both electron and ion scales and includes realistic collisions and realistic boundary conditions at material surfaces.	Equilibrium magnetic flux surfaces; initial profiles; boundary conditions	Turbulent particle, momentum, and energy fluxes across pedestal and to core and material surfaces. Fluctuation levels and spectra
Neoclassical Transport	Evaluates neoclassical transport fluxes, radial electric field and/or rotation in magnetic separatrix geometry in the presence of neutral particles and wall.	Plasma profiles; magnetic and wall geometry; sources	Neoclassical transport fluxes; radial electric field and/or rotation, bootstrap current
Pedestal Profile Evolution Reduced	Reduced models of transport and MHD	1D transport model; 1D MHD activity	Plasma profile across

Models	activities as part of the reduced model whole device modeling, derived from direct nonlinear simulations.	model	pedestal
Kinetic Neutral Transport Model	Provides interaction of neutral particles with fluid plasmas.	Plasma distribution (fluid or kinetic); geometry, reaction cross sections	Particle and heat source, 6D neutral distribution function
Radio-Frequency Heating Edge Model	Provides RF wave interaction with the pedestal plasma, including during ELMs.	RF amplitude, direction and spectrum; kinetic edge plasma profile	Heat and momentum sources
Pellet Fueling Model	Models ablation of fuel pellets as source of plasma.	Pellet size and speed; geometry; plasma profile	Local particle source
ELM Control and Mitigation Model	Releases the free energy from the steep pedestal before the onset of ELM crash.	Plasma profile and geometry; kinetic information	Relaxed pedestal pressure profile
Nonlinear Extended MHD	Evolves fully nonlinear, non-ideal, fluid plasma model on open and closed field lines from electromagnetic instability through relaxation	Plasma parameters and geometry	Edge localized mode crash, relaxation and recovery; Pedestal profile evolution (turbulent particle, momentum, and energy fluxes) to core and SOL, Fluctuation levels and spectra
Fokker-Planck Collision Operator	Provides fully nonlinear, conserving approximation of Coulomb collisions	5D plasma distribution	Collisionally relaxed 5D plasma distribution functions

Table 2. Level 2 Components: Required for separate dynamic models of inter-ELM and ELM dynamics.

Physics Component	Capability	Inputs	Outputs
Multi-scale gyrokinetics or 6D kinetics	Evolves nonlinear, electromagnetic kinetic turbulence model in realistic beta, with a model that includes include tearing-parity, finite toroidal mode number n (all n's from 0 and 1 up to electron gyroradius scales) and that allows for overlap of turbulence and equilibrium scales.	Plasma profiles and geometry	Electromagnetic turbulence and transport including finite-n tearing modes, ELMs of all types, Quasi-Harmonic Oscillations, Quasi-Coherent Modes

Table 3. Level 3 Components: Required for multi-scale dynamics including micro-, meso-, and macro-scales, ELMs and inter-ELM dynamics, all in a single, self-consistent framework with kinetic effects.

c. *Plans for adapting older components and as well as plans for developing new components.*

For each component, we identify existing technologies that could either be used directly or as starting points for the required components. In several cases, identified components will require new development efforts.

1) *Geometry and Mesh Conversion*

This component is fundamental to most device simulation codes, and a variety of coordinate systems are in use for toroidal systems including Cartesian, cylindrical, toroidal, axisymmetric magnetic flux coordinates, and Hamada-Boozer magnetic flux coordinates. Thus, many codes already either include some internal mesh and geometry package or rely on external packages. Examples of such external packages include the EFIT equilibrium-fitting code [??] and the Corsica code [??]. It is expected that the geometry/mesh component will leverage much existing code, however improvements will need to be made. In particular, capabilities to automate the conversion between different meshes and coordinates, as well as the interpolation of the physics information between meshes, are desired.

2) *Linear MHD Stability Analysis*

Many codes have been developed that can provide the desired ideal MHD stability analysis in various limits. For low-n modes, this include the axisymmetric eigenvalue codes GATO and PEST, and the stability threshold code DCON. The ELITE code is eigenvalue code optimized for the study of intermediate-to-high-n modes. Several high-n balloon codes also exist including HINST, CAS3D, balloo and BAL-MSC. Other codes that coould provide extensions from current approaches include linear studies with extended and two-fluid MHD initial value codes such as BOUT++, M3D-C1, M3D and NIMROD. The EPED model combines peeling-ballooning and KBM linear thresholds in a structure that could be directly componentized. Clearly, there are many existing technologies that will serve as the basis of one or more linear MHD stability analysis components can be built. Desired extensions include the effects of ExB stabilization, two-fluid models, toroidal and poloidal rotation and the generalization to regions with open field lines.

3) *Linear Electromagnetic Gyrokinetic Profile Stability Analysis*

   There are also several linear electromagnetic gyrokinetic candidate codes for linear gyrokinetic profile stability analysis. These include the eigenvalue code FULL [??], the initial-value code GS2/GKS [??], and the eigenvalue/initial-value code GYRO [??]. In addition, the linear gyrofluid transport code TGLF [??] could be used for rapid calculation of approximate linear growth rates. The linear electromagnetic gyrokinetic profile stability analysis component will be based off of one or more of these existing codes. These will include ExB stabilization, shorter-wavelength drift (ETG) modes, and will be extended to include a full collision operator.

4) *Closed-Flux-Surface Gyrokinetic Turbulence*

   Work on core turbulence has led to the development of several closed-flux-surface, electromagnetic, gyrokinetic codes including the continuum code GYRO [??]; the PIC, delta-f code GEM [??]; and the continuum, flux-tube codes GS2 [??] and GENE [??]. The component(s) for this functionality will be based on one or more of these existing codes. Desired capabilities include full electromagnetic turbulence with realistic pedestal geometry and boundary conditions; multiple species; efficient treatment of electron-ion scales (implicit-explicit or fully implicit treatment); and realistic collision operators. Note that some of these capabilities already are implemented in existing codes. Extensions to incorporate alternate pedestal-specific gyrokinetics orderings would be or great interest.

5) *Cross-Separtrix Gyrokinetic Turbulence*

   Several gyrokinetic turbulence codes applicable to both open and closed flux surface geometries have been and are under active development. XGC1 [??] is a 5D PIC, full-f electrostatic, delta-f electromagnetic code operating on separatrix geometries. COGENT [??] is a 4D continuum, full-f electrostatic code that is currently based on Miller equilibrium geometries, although it will soon incorporate separatrix geometries. XGC1 is already a key component in the CPES proto-FSP [??] and is a candidate for a general gyrokinetic turbulence component in the FSP. More so than the closed-flux-surface gyrokinetic codes, the cross-separatrix gyrokinetic codes still require advancements in the areas of fully electromagnetic turbulence in realistic edge geometry and boundary conditions; multiple species; efficient treatment of electron-ion scales (implicit-explicit or fully implicit treatment); and realistic collision operators.

6) *Neoclassical Transport*

   Many codes can compute neoclassical transport, including the continuum codes NEO [??] (steady state closed flux surface) and COGENT (cross-separatrix initial value) and the PIC codes GTC-NEO [??] (closed flux surfaces) and XGC0 [??] (magnetic separatrix and wall), the latter of which also handles three-dimensional magnetic field perturbations). Existing codes will again serve as the basis of the neoclassical component(s). Desired extensions to existing codes include three-dimensional geometric and electrostatic potential effects.

7) *Pedestal Profile Evolution Reduced Models*

There are several existing reduced models that support core transport, for example, MMM [??] and TGLF [??]. While these may serve as a starting point, higher-fidelity edge transport and MHD models will be deduced from first-principles codes and made into suitable components.

8) *Kinetic Neutral Transport Model*

Many existing kinetic neutral transport models are based on Monte Carlo techniques, such as DEGAS2 [??], EIRENE [??], or the 2D Monte Carlo neutral atoms in XGC0 [??]. Alternatively, codes such as GTNEUT [??] use a continuum approach (in this case the Transmission and Escape Probabilities method). Any of these technologies can be used to develop a neutral transport component. The ultimate capability for such a component would be to simulate directly kinetic-kinetic, neutral-plasma interactions, i.e. a fully kinetic neutral model tightly coupled through realistic collisions with the plasma species.

9) *RF Heating Edge Model*

Initial components implementing an RF heating model specific to the edge will be reduced models of some kind. NEED MORE INFORMATION HERE. DOES ANYTHING CURRENTLY EXIST? The ultimate goal will be to develop a direct-simulation capability that couples the fully kinetic plasma interaction with the RF wave.

10) *Pellet Fueling Model*

Initial components implementing a pellet fueling model will invariably be reduced models of some kind. NEED MORE INFORMATION HERE. DOES ANYTHING CURRENTLY EXIST? An alternative first-principles approach, FronTier-MHD [??] is a 3D compressible, free-surface MHD code developed by the ITAPS SciDAC Center to model pellet fueling. A full kinetic model will require substantial new theoretical and algorithmic development (IS THIS IN OUR SCOPE?).

11) *ELM Control and Mitigation Model*

(I'M NOT SURE WHAT TO DO WITH THIS COMPONENT. ARE THESE ALL REDUCED MODELS OF SOME TYPE?) *RMP, magnetic jittering, and pellet, snowflake divertor. Self-consistent penetration of RMP and magnetic jittering with pedestal transport response.* Pellet effects on the pedestal profile will require a more tightly-coupled computation of the pellet ablation and motion and its effects on the plasma flow.

12) *Nonlinear Extended MHD*

Many nonlinear, extended MHD codes exist, most notably M3D [??], M3D-C1 [??], NIMROD [??], and BOUT++ [??]. Of course one or more of these will serve as the starting point for an extended MHD component, and many science application areas will require such a component. Extensions that will be necessary for the pedestal application include realistic plasma resistivity toward ITER; improved HPC capability to reduce runtime; two-fluid physics; models of parallel kinetic effects; 3D equilibrium; and coupling to pellet models.

13) *Fokker-Planck Collisions*

While methods have been developed to address the full collision operator, for example Greengard's FFT method [??] and Hinton's Langevin method [??], and previous codes base on pitch-angle scattering have been implemented (what about CQL?), there is still substantial work to be done to develop an efficient, nonlinear Fokker-Planck collision package. This will be a task that must be ultimately addressed for the pedestal science application area and will also be needed for other science areas. One of the challenges will be the development of an accurate, fast implicit time-advancement algorithm for this component.

14) *Multi-Scale Gyrokinetics or 6D Kinetics*

Since this component represents a more fundamental, first-principles model that incorporates micro- through macro-scopic scales, such a component will require substantial computational algorithmic development to reduce computational cost. It will require either a new set of 5D gyrokinetic equations with generalized ordering and a full collision operator or the development of efficient numerical schemes for solving 6D equations without introducing sub-cyclotron time scales. This component represents the most speculative component research and development that should be undertaken for the pedestal application.

2.E. Framework requirements

d. Analysis of the requirements for composition of the physics components (including data exchanges and algorithms)

Shown in Figures 1, 2, and 3 are representative coupling schemes for each of the three levels of development that have been identified. While these are not an exhaustive set of all possible component combinations for pedestal applications, they do represent the key characteristics of the data exchanges and couplings required. We briefly describe the configurations and then discuss physics composition needs in more detail.

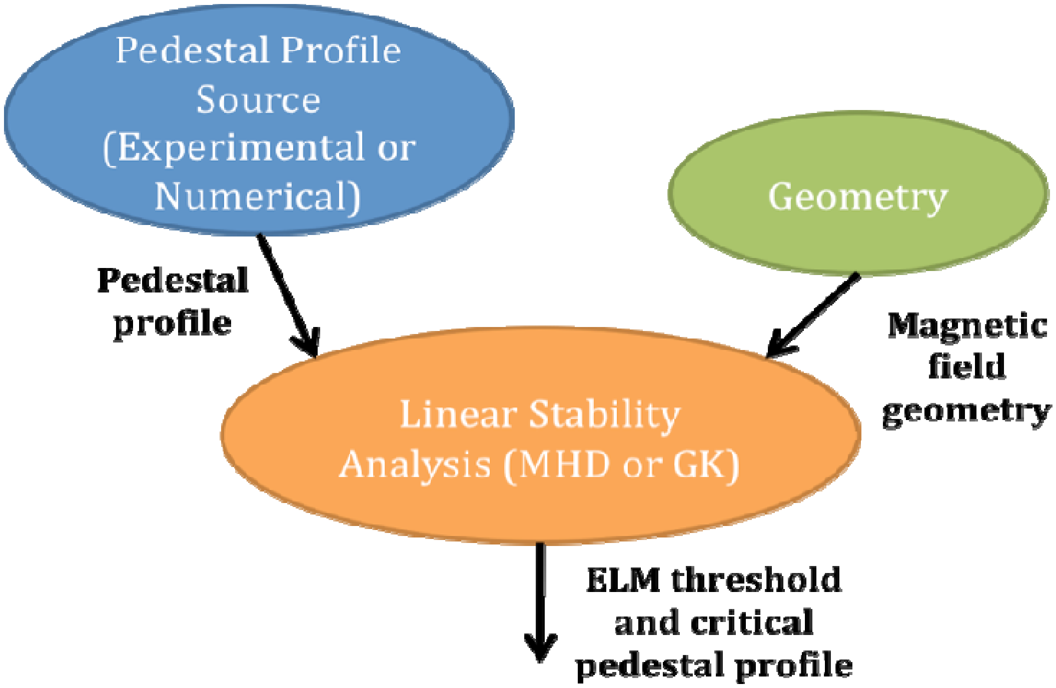


Figure 1. Representative static (Level 1) pedestal component configuration.

Figure 1 represents the static pedestal component, which implements a pedestal profile stability analysis based on some plasma profile input. The pedestal component just takes in one-dimensional profile data and computes instability thresholds and critical profiles using a linear MHD and/or linear gyrokinetic model. The coupling is weak; this analysis is not tightly coupled to plasma evolution equations, but serves as a periodic check on the pedestal profile, allowing coupled core-pedestal optimization via weakly coupled pedestal and core models. Only a small amount of data is exchanged, and this could be done either through files or in memory.

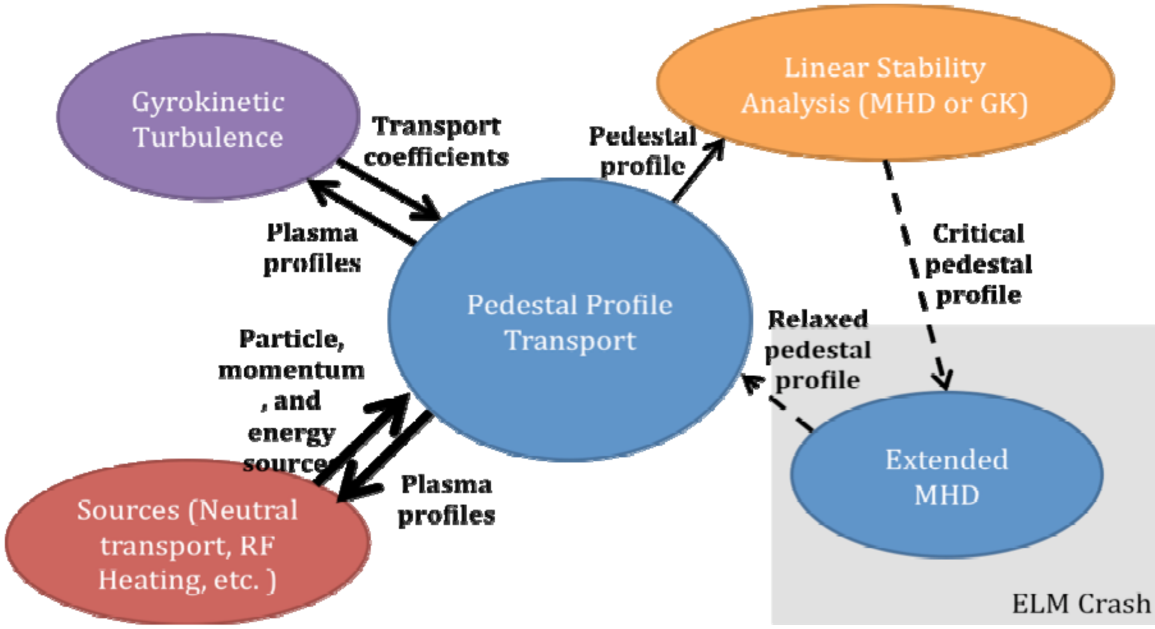


Figure 2. Representative dynamic (Level 2) pedestal component configuration.

Figure 2 represents a very general configuration for a dynamic pedestal component that relies on a variety of subcomponents to accomplish different portions of ELM evolution. At the core is a linear or quasi-linear profile transport component (envisioned to include neoclassical transport calculations), which might be a reduced model, a transport model of advection-diffusion-reaction type, etc. The profile transport code provides the pedestal profile for linear stability analysis as before, but also interacts in a bi-directional way with a kinetic turbulence component. In this interaction, the turbulence component provides transport coefficients, while the transport code provides the current plasma state as initial (profiles) and/or boundary conditions (fluxes) for the turbulence component. This type of coupling is stronger than for the stability computation, but the relative cost and time-scale disparity of the two components means that in general, the exchange will not occur every time step in a tightly-coupled manner. The strongest coupling involves the volumetric coupling between the transport component and the source components; effects such as pellet injection, neutral transport, RF heating require local plasma conditions from the transport component and return sources (the "reaction" terms) to the transport process. Such tight coupling will need to occur frequently (i.e., every time step) and most likely will require some form of implicitness to ensure self-consistency.

Also shown in Figure 2 is a relationship that can be used to model ELM evolution though an ELM crash. In some cases, a nonlinear transport component may be able to directly simulate the pedestal instability, ELM crash, and recovery. The configuration shown is a more componentized model where the transport component handles profile evolution until the linear stability analysis component determines that instability occurs. The linear stability analysis component provides the critical plasma profile to a nonlinear, extended MHD component that handles the ELM crash and ultimately provides the relaxed profiles (and evolution responsibilities) back to the transport component.

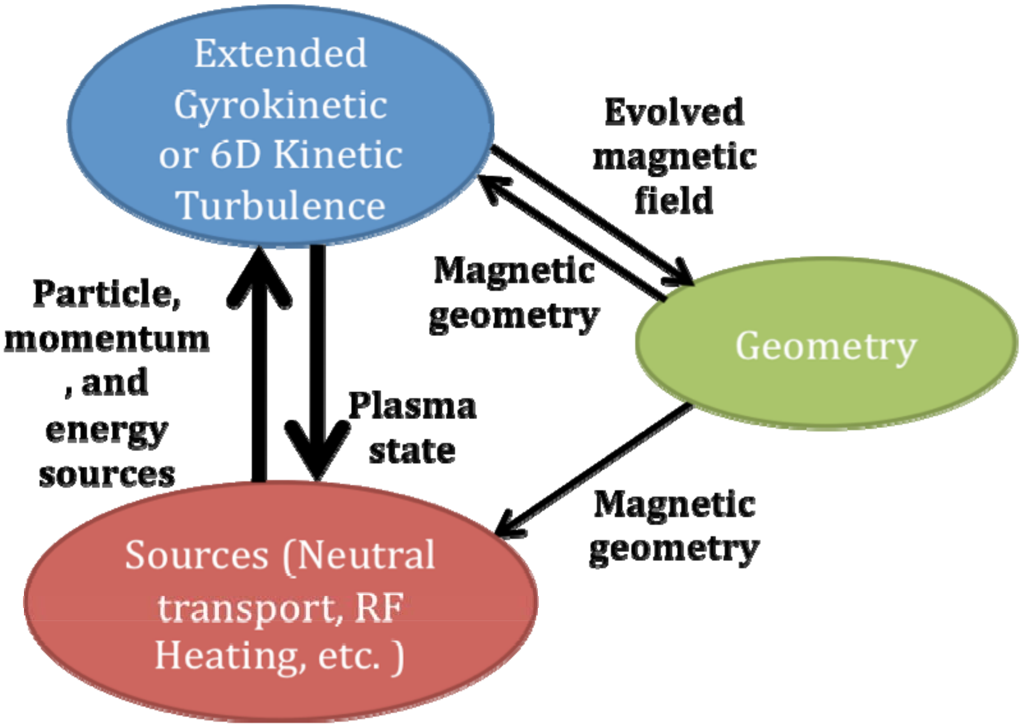


Figure 3. Representative, tightly-coupled, dynamic (Level 3) pedestal component configuration.

Finally, Figure 3 shows the third proposed Level of pedestal simulation, where the pedestal evolution, instability, ELM crash and recovery are directly simulated using a kinetic code coupled volumetrically to a variety of source models. Here, as before, the coupling is very tight and implicitness will be required. Note that certain sources, such as neutral kinetic transport, may require boundary (flux) coupling to components external to the pedestal area, for example a plasma-surface interaction component. The magnetic geometry will be evolving in time, and so the kinetic Maxwell-plasma model will need to provide updated magnetic fields to the geometry component and will need to be able to regrid onto the magnetic geometry produced by the geometry component.

Types of coupling

The basic description of physics composition identifies that the pedestal will require capability that supports both weak and strong coupling. The coupling can be achieved in some cases (e.g., static stability) through high-latency coupling through files. Tighter coupling, particularly of boundary and volumetric data, will require in-memory coupling. Framework support for tight coupling (implicit and implicit-explicit time advancement) will be required, particularly for the inclusion of sources like neutral transport.

Interpolation and data representation

Existing technologies on which components will be based rely on many different data representations: particle, finite-volume, finite-element, finite-difference, and spectral/pseudospectral. In addition, different technologies use different grids and coordinate systems. Framework capabilities that define self-describing data representations and that can automate the conversion between different representations would facilitate physics composition. Such capabilities would need to allow for constrained conversions (e.g., conservation-preserving interpolation or limited interpolation to prevent the introduction of artificial extrema).

Inline data reduction

As seen in the representative use cases, data exchanges (and out put diagnostics) frequently involve data derived from the primary data of the component, for example, transport coffeicients, averaged profiles, boundary fluxes, etc. Coupling between particle and continuum codes will require some form of filtering for noise reduction. Because these exchanges will often be done in time-advancement loops, they will need to be efficient. Many data reduction algorithms will result from similar operations, and so it would be advantageous for the framework to provide capabilities for efficient data reduction.

Algorithmic needs

The algorithmic needs of the pedestal application are not particularly unique to the area. Diffusion operators (transport, Fokker-Planck collisions), finite-element, and implicit time discretizations will require efficient, scalable linear and nonlinear solvers and robust preconditioners. Common interface to these solvers will need to be provided by the framework. Because of the ranges of time scales, we expect that explicit multi-rate, implicit-explicit, and fully implicit time integration algorithms will be required, and the framework will need to provide a capability to combine different components under these different time advancement techniques.

Restart capability

It is expected that each component will at minimum have the ability to store its state to file and to restore its state from file. The framework must provide the capability to initiate and coordinate the check-pointing and restart for all components combined in a physics simulation. Ideally, the framework would provide a common set of check-point and restart tools that components could leverage.

Parallel configuration of components

Different components will require different types of parallelism. For some components, such as a linear MHD eigensolver, it makes little sense to parallelize the problem. Kinetic components, however, will benefit substantially from both data and task parallelization. The framework must provide a capability to specify the parallel decomposition of different components in different ways and must support distributed and threaded parallelism. Ideal, from an allocation of processors, the framework will allow the user to specify that some components are to be run on a subset of dedicated processors, while other components may share or overlap on the same processor and memory space. This will further require framework support for data exchanges both directly in memory, through messages, and through interaction with a parallel file system.

Support for stochastic algorithms

A candidate technologies for kinetic components is a stochastic approach (Monte Carlo, PIC) that relies on pseudo-random number generation on potentially massively parallel machines. The framework will need to provide capability to support these stochastic algorithms, both with respect to providing reproducibility (for a given random seed, the ability to produce the same results) for testing and verification and also with respect to providing access to a robust, parallel pseudo-random number generator.

b. *Analysis of the requirements for the full workflow (task composition)*

With respect to task composition, we have not identified any requirements that are unique to the pedestal science application. We nevertheless briefly address the needs as identified at the Boulder Workshop.

Workflow software

The framework must provide capability to assemble components into an integrated simulation. This can be done either through graphical-based approaches, such as Kepler [??], or through some scripted or file-based (programming) interface. Such a capability must make it clear for the user how to connect the interfaces of two or more components and provide some consistency checking prior to batch execution. The workflow software must also allow for the composition of conditional component configurations, for example, to accommodate the separate ELM build-up and crash configurations described above.

Provenance

The metadata required to uniquely identify reproduce any simulation (date, platform, component versions, source file identifications, physics composition, parallel decomposition, etc.) must be acquired and preserved. The framework should provide tools to automate the acquisition and storage of provenance information.

Input file preparation

Most components will rely on input files to specify the problem configuration for the component. In addition, various forms of input data files will be used, for example, numerically and experimentally generated field data. The framework will need to provide tools to at minimum check the constancy of input files. Ideally, the framework would provide tools, perhaps graphical in nature, that would allow for easier configuration and that would automatically generate valid input files for each of the components. In addition, the FSP should maintain a repository of input data files, and the framework should provide a capability to easily obtain data from this repository.

Batch and interactive data analysis and graphics

As identified above, there will be needs for data analysis (e.g., synthetic diagnostics) and visualization of 1D, 2D, and 3D scalar and vector data. As a postprocessing activity, these make require both interactive and batch processing, both of which should be enabled from withint the framework.

Steering/Monitoring

The framework should provide mechanisms to monitor submitted simulations and their completion, as well as progress, as they execute. We do not currently anticipate the need to steer simulations; steering is a questionable practice in that the user intervention raises doubts about rigorous verification and validation of the results.

Regression testing and UQ studies

For good software quality practices and to facilitate verification and uncertainty quantification studies, the framework should provide capability akin to a testing harness that allows for automated execution of pre-defined test problem, semi-automated convergence studies for code verification, and the incorporation of sensitivity analysis infrastructure. The framework should ease the incorporation of code verification problems into the automated regression testing suite. Some UQ frameworks already exist [??] that incorporate sampling strategies, sensitivity study definition and execution, and post-processing statistical analysis tools.

2.F. Validation

The plan outlined here envisions phased development of increasingly sophisticated physics models. As noted, work on these models will be carried out in parallel, with the simpler models coming on line earlier. Validation activities will begin on each model as it reaches some minimum level of maturity. (While it is important that the codes and calculations are verified, they need not be "complete" before validation begins. Validation should be an ongoing process that helps guide development by assessing the adequacy of the physical model and identifying the most important needed improvements.)

The table below attempts to summarize the overall requirements for validation of pedestal models. (Future versions will lay out a schedule of requirements that is consistent with the plan for model development.) For each of four areas, it lists the critical physics that must be validated, the corresponding measurement set required and highlights important gaps – diagnostic needs that will require significant innovation and investment. The emphasis is on measurements which we believe will be the main challenge for pedestal model validation. The worldwide set of existing and planned experiments, including ITER, should be adequate given sufficient run time.

Table 1. Validation Requirements For Pedestal Science Application

	Critical Physics	Measurements Needed	Important Gaps
Transition Physics	- L-mode turbulence and transport - Turbulence suppression mechanisms - Feedback loops	- Edge profiles for ne, Te, Ti, Er, J(r) - Edge fluctuations for ne, Te, ϕ, B including amplitude, phase, cross-coherence - Near SOL profiles of ne, Te, Ti, perp. and parallel flows - Near SOL fluctuations for ne, Te, phi, B including amplitude, phase, cross-coherence	- J(r), magnetic shear - Resolution - 2D coverage - Non-Maxwellian ion temperatures - , Edge fluctuations for quantities other than n_e - Wave-number range and resolution - Synthetic diagnostics
Pedestal Evolution and Structure	- Micro/meso stability - Quasi-linear and neoclassical transport - Nonlinear turbulent transport - Particle and energy sources	- Pedestal profiles as above - Pedestal fluctuations as above	- Fully resolved transient measurements - Other gaps as above - Synthetic diagnostics
Steady-State Transport within Barrier	- Quasi-linear and neoclassical transport - Nonlinear turbulence and transport - Sources and sinks - Neutral and atomic	- Pedestal profiles as above - Pedestal fluctuations as above - Neutral profiles - Impurity profiles	- J(r), magnetic shear - Resolution - 2D coverage - Pedestal fluctuations for quantities other

	physics		than n_e - Synthetic diagnostics
Relaxation Mechanisms	- Nonlinear extended MHD and gyrokinetic models for ELM onset, nonlinear evolution and effects on plasma - Coherent mode stability, nonlinear evolution and effects on plasma - 3D equilibrium effects including non-axisymmetric B fields	- Fast evolution of profiles - Pedestal fluctuations for ne, Te, ϕ, B over wide range of frequencies and wave-numbers	- Fully time resolved transient measurements - 2D and 3D coverage - Synthetic diagnostics

2.G. Connections to Other Work

2.G.1. Coupling Requirements and Collaboration Opportunities within FSP

The edge pedestal module in the FSP will need to be coupled with the core, scrape-off, and wall interaction modules, to respond to and to influence the plasma behaviors in those regions. The coupling includes heat and particle fluxes, plasma equilibrium and transport properties, neutral particles, and instabilities. The fundamentally nonlocal properties, such as RF and large scale instabilities/turbulence, may require different types of couplings across the radial layers considered here. The edge pedestal module needs to build up the pedestal with Er/rotation and simulate both small and large scale instabilities, if present, and their effect on the pedestal plasma profile consistently with the heat and particle fluxes, the height and slopes of the plasma density and temperatures, and the radial electric field and rotation from the adjacent regions. Considering the multiscale nature of the plasma in the edge, such a surfacial coupling is a challenging problem. Some progression from relatively simple couplings in Level 1 (see Fig 1) to more sophisticated couplings (Level 2a & b), through to direct connection, at least to the SOL region, and possibly also the core, is planned.

Several of the required components are expected to overlap significantly with the needs of other groups. Notably, a closed flux gyrokinetic solver is expected to overlap with the needs of the Core Profiles group, though there are several pedestal-specific requirements, and the cross-separatrix gyrokinetic solver is expected to overlap strongly with the needs of the Boundary group. The extended MHD components are expected to overlap with needs of the Disruptions group, though there are many pedestal-specific needs.

2.G.2. Requirements for work outside FSP

The advances required for each component are given in Section C. The development of several of these components is expected to be aided by theoretical progress outside FSP. In particular, Level 3 of the plan represents a substantial advance over existing simulation capabilities. While theoretical progress has been made in developing extended 5D gyrokinetic orderings, these have not yet been demonstrated computationally, and it is likely that substantial progress both in theory and in computation will be required for the successful attainment of the Level 3 goals.

2.H. Schedule and Resources

The three level plan for the pedestal science driver is illustrated in Fig 1, and described in Sec B.1. Fundamentally, the plan is designed to provide a substantial level of functionality early on (Level 1), offering unique opportunities for global prediction and optimization of magnetic fusion energy systems, while then taking advantage of and advancing leading gyrokinetic and extended MHD simulation capability in Level 2, before finally moving to fully self-consistent multi-scale simulations which will address the most fundamental challenges of the coupled multi-scale pedestal region, while strongly pushing the limits of the computational capabilities that should be available across the next 15 years (Level 3).

As illustrated in Fig 1, all three levels of tasks will be undertaken from the beginning, with a staggered schedule progressing from a development, implementation and verification stage (shaded yellow in Fig 1), to a validation and ongoing development stage (green in Fig 1), and finally to a full production stage with routine application, user support and minor ongoing development (blue in Fig 1).

The resource requirements below reflect the plan in Fig 1. Here we ignore the potential overlap of some of these efforts, particularly with the Boundary Plasma and Core Profiles efforts, and provide resource estimates as if we could not leverage work in other science areas. We do assume the existence of external groups developing framework, testing, and other development support that is funded separately. We provide rough estimates based on the type and importance of tasks. We also try to make realistic estimates for manpower needs, ignoring the inevitable budgetary constraints.

Level 1: Static (Linear) Models for Pedestal Structure

Assumptions: Much of the existing technology already exists (at least for a first pass), so this primarily constitutes componentization of the existing technologies, documenting the components to the requirements of the FSP, and verification and validation of the components.

Tasks:

1) Documentation of components, verification test problems: **0.25 PhD FTE/yr**
2) Componentization of existing codes (definition and implementation of interfaces, incorporation of common framework tools, bringing under common version control, attaching to regression system, unifying build systems, etc.) : **0.5 PhD FTE/yr; 1 FTE BS/MS FTE/yr**
3) Validation, incorporating UQ sensitivity analysis; publishing results: **1 PhD FTE/yr**
4) Development of extensions (new modes, neoclassical effects, other improvements): **1 PhD FTE/yr years 1-2; 0.5 PhD FTE/yr years 3-4**
5) Continued support and maintenance (years 5+): **0.1 PhD FTE/yr; 0.1 FTE BS/MS FTE/yr**

	PhD FTE	**BS/MS FTE**
Year 1	2.75	1
Year 2	2.75	1
Year 3	2.25	1
Year 4	2.25	1
Year 5	1.75	1
Years 6+	0.1	0.1

Level 2: Dynamic Evolution of Pedestal Profiles

Assumptions: Existing substantial efforts in edge and core gyrokinetics and extended MHD provide a good starting point. Thus, initial efforts will involve adapting existing components to requirements for the FSP. This is a large, broad task and substantial resources will be required. Bulk of effort will initially be towards development, with emphasis switching to new science and V&V in out years.

Tasks:

1) Documentation of components, verification test problems: **0.5 PhD FTE/yr**
2) Componentization of existing and new codes (definition and implementation of interfaces, incorporation of common framework tools, bringing under common version control, attaching to regression system, unifying build systems, etc.) : **0.5 PhD FTE/yr; 1.5 FTE BS/MS FTE/yr years 1-5; 1 BS/MS FTE years 6-15**
3) Validation, incorporating UQ sensitivity analysis, calculation verification: **0.5 PhD FTE/yr years 1-3; 1.5 PhD FTE/yr years 4-15**
4) Design and development of new/extending existing capabilities (e.g., free boundary equilibrium solver accurate to SOL; ion-electron GK with magnetic perturbations, etc.): **2 PhD FTE/yr years 1-8; 1 PhD/yr years 9-12; 0.5 PhD/yr years 13-15**
5) New science investigations: **1 PhD FTE/yr starting year 3 -10**

	PhD FTE	BS/MS FTE
Year 1	3.5	1.5
Year 2	3.5	1.5
Year 3	4.5	1.5
Year 4	5.5	1.5
Year 5	5.5	1.5
Year 6	5.5	1.5
Year 7	5.5	1.5
Year 8	5.5	1.5
Year 9	4.5	1.5
Year 10	4.5	1.5
Year 11	3.5	1
Year 12	3.5	1
Year 13	3	1
Year 14	3	1
Year 15	3	1

Level 3: Direct Multiscale Simulation

Assumptions: We will target something like 6D direct simulation, or 5D with a substantially extended ordering. This is high-risk work that will require significant advances in algorithms and hardware. Resource requirements might decrease as the field evolves outside of the FSP. Also, we assume sufficient tools exist that direct BS/MS support need not be identified by this point; new technologies will be developed using existing tools and framework.

Tasks:

1) Design and development of new capabilities (e.g., 6D direct simulation, theoretical extension of gyrokinetic models, etc.; also includes componentization as part of development): **1 PhD FTE/yr years 1-6; 1.5 PhD FTE/yr years 7-9; 2 PhD FTE/yr years 10-15**
2) Documentation of components, verification test problems: **0.5 PhD FTE/yr starting year 7**
3) Validation, incorporating UQ sensitivity analysis, calculation verification: **0.5 PhD FTE/yr years 10-12; 1 PhD FTE/yr years 13-15**
4) New science investigations: **0.5 PhD FTE/yr starting year 6 , up to 1 FTE starting in year 10**

	PhD FTE	**BS/MS FTE**
Year 1	1	0
Year 2	1	0
Year 3	1	0
Year 4	1	0
Year 5	1	0
Year 6	1.5	0
Year 7	2.5	0
Year 8	2.5	0
Year 9	2.5	0
Year 10	3.5	0
Year 11	3.5	0
Year 12	3.5	0
Year 13	4	0
Year 14	4	0
Year 15	4	0

Total Estimates

	PhD FTE	BS/MS FTE
Year 1	7.25	2.5
Year 2	7.25	2.5
Year 3	7.75	2.5
Year 4	8.75	2.5
Year 5	8.25	2.5
Year 6	7.1	1.6
Year 7	8.1	1.6
Year 8	8.1	1.6
Year 9	7.1	1.6
Year 10	7.6	1.6
Year 11	7.6	1.1
Year 12	7.6	1.1
Year 13	7.6	1.1
Year 14	7.6	1.1
Year 15	7.6	1.1

2.I. Milestones

Suggested high level goals and milestones:

Year 2:

-Componentization of Level 1 models

-Initial validation of Level 1 models against pedestal height and width observations

-Initial coupled pedestal-core optimization of ITER base case with Level 1 models

Year 5:

-Componentization of Level 2 models

-Pedestal turbulence simulations on closed field lines

-Initial development of reduced dynamic models from nonlinear simulations

-Coupled simulation of between-ELM transport with reduced models, and ELM events

Year 7-10:

-Pedestal turbulence simulation on closed and open field lines

-Validation of calculated ELM heat flux on material surfaces

-Validation of pedestal turbulence simulations

Year 15:

-Componentization of Level 3 models

-Verification of Level 2 components using Level 3 component

-Direct multi-scale simulations of transport and ELMs

-Simulation of the L-H mode transition

3. CORE PROFILES

W. Nevins, S. Kaye, P. Diamond, J. Candy, C. Holland, S. Parker, S. Klasky, W. Wang, X. Tang, V. Chan

3.A. Background and Motivation

Modern magnetic confinement devices employ a magnetic geometry in which the magnetic field lines cover a set of nested toroidal surfaces (the magnetic surfaces). Particles, momentum, and energy are transported rapidly within each magnetic surface, and more slowly across magnetic surfaces. This allows us to reduce the problem of computing core profiles of density, plasma flow, and temperature from a problem in three spatial dimensions to a one-dimensional problem (in the flux-surface label, which we take to be *r* in this discussion). In general, one must also solve a subsidiary equation for the equilibrium magnetic geometry with given the plasma profiles.

The dominant mechanisms for cross-field transport are drift-wave instabilities (giving rise to turbulent transport) and Coulomb collisions (giving rise to neoclassical transport). In most tokamak discharges, turbulence is the dominant mechanism for the transport of particles, momentum, and energy. As such, it is the major issue to be addressed in predicting core profiles. Plasma turbulence results from the non-linear development of instabilities driven by gradients in the plasma temperature and density. This turbulence is rigorously described by the coupled gyrokinetic and Maxwell equations. Neoclassical transport results from a combination of the deviations of individual particle orbits from their magnetic surfaces and binary collisions. There is a well-developed theory of neoclassical transport, which provides an adequate description of the residual transport present in the absence of plasma microturbulence. Most previous efforts to simulate the transport-time-scale evolution of core plasma profiles are based on the solution of the 1-D transport equations using approximate transport coefficients obtained through some combination of analytic theory, simulations, and experimental results. This remains a useful approach, which will be carried out within the FSP by the Whole Device Modeling group.

The advent of tera-scale computing opens the possibility of directly computing the turbulent fluxes for input into the transport equations. This more computationally-intensive approach is the main focus of this section. This capability has been successfully demonstrated by both TGYRO (Candy 2009) and TRINITY (Barnes 2010), and is being used for both validation against steady-state discharges in DIII-D and JET as well as for preliminary ITER performance projections. While these past demonstrations have mainly focused on the local transport model (described below), we see no barrier to applying it in situations when meso-scale phenomena are important.

3.B. Scientific Scope for Core Profile Modeling

The ultimate scientific goal is a validated transport model which reliably predicts, for each plasma species, profiles of density, temperature as well as plasma rotation and current and their evolution on transport time-scales. That is, it would encompass all the phenomena that set the core profiles including turbulence (in all relevant fields and at all relevant scales) and nonlinear MHD (i.e. soft limits as opposed to collapses or disruptions). It would to need to solve for turbulence in 3D perturbed equilibria and include the physics that controls transport barriers. Ultimately, understanding plasma transport is central to the design of an engineering test reactor and commercial power plants based on magnetic fusion. In the process, this topic addresses scientific grand challenges including nonlinear coupling of dynamics across a broad range of spatial and temporal scales.

This goal will be addressed via three parallel paths:

1. A local transport model based on coupling many gyrokinetic simulations distributed across the radial profile
2. A transport model based on global simulations which is capable of addressing meso-scale phenonema on transport time-scales
3. Developing a plan for incorporating boundary interactions between the core and pedestal including fluctuations and flows.

A key component of this development plan is the continual validation of these physics models against experimental data throughout its entire duration.

3.C. Model Hierarchy and Associated Components

A core transport model evolves radial profiles, $\mathcal{P}$, of density and temperature for each plasma species together with the electrostatic potential. Symbolically,

$$\mathcal{P} = [n_a(r), T_a(r), \Phi(r)]$$

Some transport model formulations may alternatively evolve one or more of the plasma velocities, but in the present discussion we focus on the rigorous formulation due to Sugama (Sugama 1998) for which the electric field is the primitive quantity. Evolving these profiles requires knowledge of the equilibrium magnetic geometry.

$$\mathcal{G} = [R(r), Z(r), \psi(r), B, q, \ldots]$$

The fluxes of particles, momentum, and energy together with energy exchange (computed at present only by GYRO and GS2) terms:

$$\mathcal{Q} = \left[\Gamma_a, \Pi_a, Q_a, S_a^{\mathrm{exch}}\right]$$

We find it convenient to express Q as the sum of the neoclassical and turbulent fluxes,

$$\mathcal{Q} = \mathcal{Q}^{\mathrm{neo}} + \mathcal{Q}^{\mathrm{turb}}$$

And, finally, the sources of particles, momentum, and energy:

$$\mathcal{S} = [S_{\Gamma,a}, S_{\Pi,a}, S_{\Phi}, n_{\mathrm{fast}}]$$

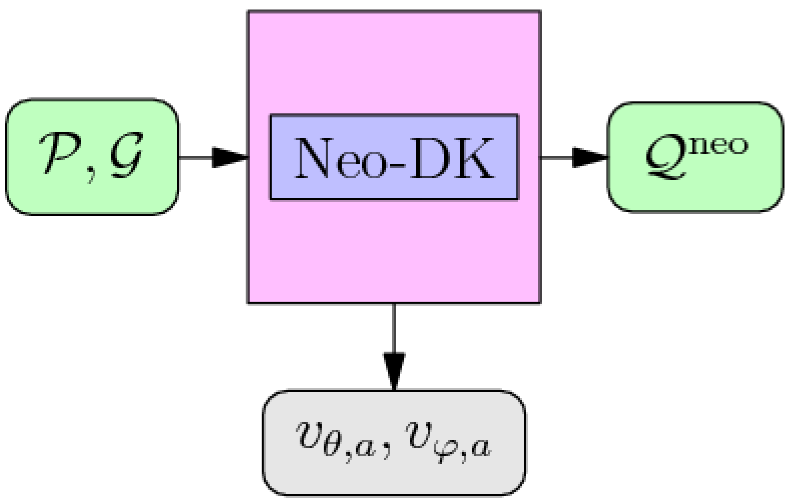
3.D. Local Transport Model

Here, the gyrokinetic/Maxwell equations are integrated on a representative set of flux surfaces for an interval sufficient to allow the plasma microturbulence to reach a statistical steady-state on the gyrokinetic time scale and yielding particle, momentum, and energy fluxes, to be employed to advance density, rotation, and temperature on the transport time-scale. This scheme has been implemented (at least) twice: in the TGYRO (Candy 2009) and TRINITY (Barnes 2010) codes, with some validation of results against experiments on DIII-D and JET.

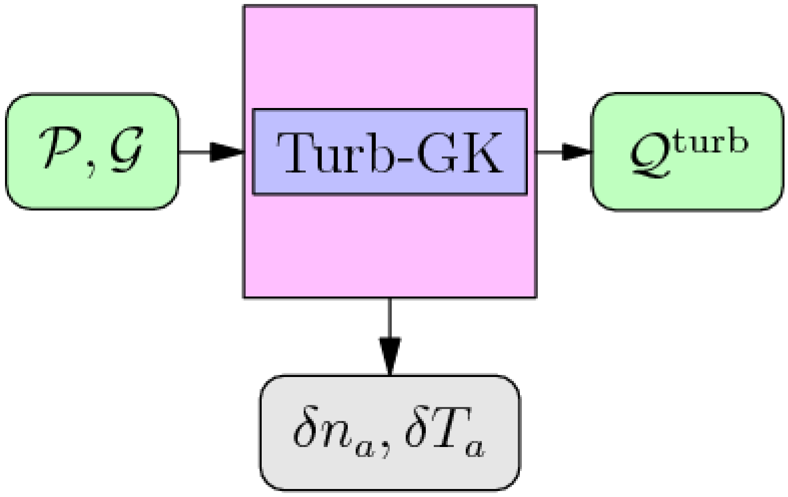
3.D.1. Component Interaction Schema

The components required for a local transport model include:

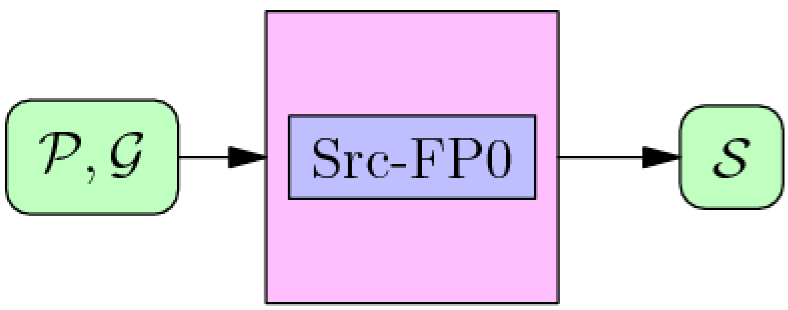
- A *neoclassical* component, which takes $\mathcal{P}$ and $\mathcal{G}$ as input and solves the drift kinetic equation for the neoclassical fluxes, $\mathcal{Q}^{\mathrm{neo}}$ and the poloidal and toroidal rotation velocities of each plasma species (or the neoclassical radial electric field).



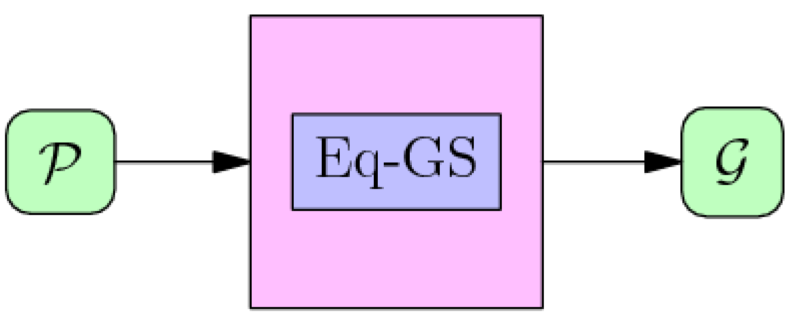
- A *turbulent* component, which takes $\mathcal{P}$ and $\mathcal{G}$ as input and solves the gyrokinetic kinetic equation for the turbulent fluxes, $\mathcal{Q}^{\mathrm{turb}}$.



- A *core source* component, which takes $\mathcal{P}$and $\mathcal{G}$as input (together with some description of the RF heating systems, neutral beams and any alpha heating) and returns $\mathcal{S}$.



- A *magnetic geometry* component, which takes $\mathcal{P}$as input and solves for the magnetic geometry, $\mathcal{G}$.



3.D.2. Transport Equations

3.D.3. Density Transport

$$\frac{\partial \langle n_a \rangle}{\partial t} + \frac{1}{V'} \frac{\partial}{\partial r} \left(V' \Gamma_a \right) = S_{n,a}$$

where

$$S_{n,a} = S_{n,a}^{\mathrm{beam}} + S_{n,a}^{\mathrm{wall}}$$

and

$$\Gamma_a = \Gamma_a^{\mathrm{GV}} + \Gamma_a^{\mathrm{neo}} + \Gamma_a^{\mathrm{tur}}.$$

Variable	**Definition**
Γ_a^{GV}	Gyroviscous particle flux density
Γ_a^{neo}	Neoclassical particle flux density
Γ_a^{tur}	Turbulent particle flux density
$S_{n,a}^{\mathrm{beam}}$	Beam density source rate
$S_{n,a}^{\mathrm{wall}}$	Wall density source rate

3.D.4. Energy Transport

$$\frac{\partial \langle W_a \rangle}{\partial t} + \frac{1}{V'} \frac{\partial}{\partial r} \left(V' Q_a \right) + \Pi_a \frac{\partial \omega_0}{\partial \psi} = S_{W,a}$$

where

$$S_{W,a} = S_{W,a}^{\mathrm{aux}} + S_{W,a}^{\mathrm{rad}} + S_{W,a}^{\alpha} + S_{W,a}^{\mathrm{tur}} + S_{W,a}^{\mathrm{col}}$$

and

$$Q_a = Q_a^{\mathrm{GV}} + Q_a^{\mathrm{neo}} + Q_a^{\mathrm{tur}}.$$

Variable	Definition
Q_a^{GV}	Gyroviscous energy flux density
Q_a^{neo}	Neoclassical energy flux density
Q_a^{tur}	Turbulent energy flux density
$S_{W,a}^{\mathrm{aux}}$	Auxiliary heating power density
$S_{W,a}^{\mathrm{rad}}$	Radiation heating power density
$S_{W,a}^{\alpha}$	Alpha heating power density
$S_{W,a}^{\mathrm{tur}}$	Turbulent exchange power density
$S_{W,a}^{\mathrm{col}}$	Collisional exchange power density

3.D.5. Momentum Transport

$$\frac{\partial}{\partial t}\left(\omega_0 \langle R^2 \rangle \sum_a m_a n_a\right) + \frac{1}{V'}\frac{\partial}{\partial r}\left(V' \sum_a \Pi_a\right) = \sum_a S_{\omega,a}$$

and

$$\Pi_a = \Pi_a^{\mathrm{GV}} + \Pi_a^{\mathrm{neo}} + \Pi_a^{\mathrm{tur}}.$$

Variable	Definition
Π_a^{GV}	Gyroviscous angular momentum flux density
Π_a^{neo}	Neoclassical angular momentum flux density

Π_a^{tur}	Turbulent angular momentum flux density
$S_{\omega,a}$	Angular momentum density source rate

3.D.6. Additional Information

Additional information, including usage scenarios, are given in the March Meeting presentation by J. Candy.

- *Existing components* which might be adapted to fill these roles are described on the "Components" Wiki. They include Neoclassical transport, Turbulent transport, Core sources and sinks, and Magnetic geometry components.

- *Projected schedule* of the work to be carried over a 15 year time period and a realistic estimate of resources required. The development of this local transport model can be accomplished by integrating existing components into the FSP framework, workflow, and data management system. As such, the optimal development path is probably to use this local transport model (and previous implementations like TRINITY and TGYRO) as exemplars of the required workflow in developing the corresponding FSP framework, workflow, and data management systems. This will speed development of the FSP local transport model, ensuring that it can be accomplished early (certainly within the first 5 years). Although many of the required components have already undergone significant interface development in connection with the FACETS, TGYRO, and TRINITY projects, significant support from the developers, and significant effort by the Framework team, will be required to successfully integrate all components into the FSP framework. Presumably each major component will require up to one FTE, distributed between the developer and a computer scientist, to integrate the component into the FSP and provide ongoing code maintenance.

- *Suggested high-level goals and milestones,* at roughly the 2, 5, 10 and 15 year marks. There should be a 2-5 year milestone which demonstrates that the package is operable (say modeling reference steady-state DIII-D discharge?). In addition, there should be a 5-10 year milestone addressing validation of the local transport model (Chris, could you comment?).

3.E. Transport model including meso-scale phenomena

Transport in tokamaks can involve interactions between drift wave turbulence and macroscopic MHD modes as discussed in Drift Wave MHD Coupling. In general, the extension of neoclassical and gyrokinetic theory, including the determination of the lowest-order distribution, to treat low-order (equilibrium) magnetic islands is an unsolved problem. Numerous groups (Cowley, Dorland and others in the US, Wilson and coworkers in the UK) gave this problem significant attention with no clear resolution. Hence, further development of the formalism for coupling plasma micro-turbulence and neo-classical tearing modes is required. However, the substantial progress which has been made in solving for transport in 3D systems, describing the time-evolution of equilibria with magnetic islands, and modeling plasma microturbulence in 3D magnetic geometry separately will enable ad hoc coupling between components to describe the interactions between plasma microturublence and neoclassical tearing modes. Conceptually, the expectation is that general picture presented in the previous section remains largely the same; that is, we seek to evolve $\mathcal{P}$given information about $\mathcal{G}, \mathcal{Q}, \mathcal{S}$. However, various components will require substantial modification, including:

- The transport solver must be modified to take account of the 3D magnetic equilibria [see, for example, H. Grad, Annals of the New York Academy of Sciences (1980); W.A. Houlberg et al, Phys. Plasmas 4 3230 (1997)] and to deal with the presence of magnetic islands [K.C. Shaing et al, Nucl. Fusion <43>, 258 (2003)].

- A component to evolve the 3D magnetic equilibria must be developed. While this component might be largely based on existing components (like PIES or VMEC), attention must be paid to the evolution of the current profile, j_||/B, in the presence of a magnetic island [similar problems have been treated in Strand and Houlberg, Phys. Plasmas <8>, 2782 (2001); and Monticello, White and Rosenbluth, Phys. Fluids ,20>, 800 (1977)].

- The global gyrokinetic code which accepts 3D magnetic equilibria must be developed. While we foresee no over-riding difficulties [a global gyrokinetic code accepting 3D equilibria has been developed in Europe -- see, P. Xanthopoulos et al, Phys. Plasmas <16>, 082303 (2009)], no such code presently exists within the US fusion program.

Likely, the most critical short-term burden imposed on FSP developers by the issue of meso-scale phenomena is to guarantee flexibility of the FSP framework. This flexibility will allow researchers to propose, implement and test independent ad-hoc models. Presumably, the most successful ad-hoc models would be targeted for inclusion into the (released, documented and supported) FSP code base. In parallel, the recognition that rigorous modeling of meso-scale phenomena is not possible due to the lack of a coherent theoretical formulation should drive the worldwide theory program to assign sufficient resources to the development of a tractable formulation of the problem.

3.F. Core-Edge Coupling

Core-edge coupling will require close interaction between the core profile and edge/pedestal groups. Such interaction has yet to occur. Generally, we foresee passing information regarding $\mathcal{P}$, $\mathcal{Q}$, and (possibly) turbulent fluctuation levels at boundary between the core and edge regions between our respective models, and iterating to convergence. We are unaware of any successful demonstration of such a scheme, and anticipate that considerable development will be required.

3.G. Framework Requirements

(Clearly need help here!)

3.H. Validation Strategy

A validation strategy for the core turbulence and transport science driver has been prepared by C. Holland. Based upon the gaps and readiness assessment in that document, the proposed validation strategy is for the core turbulence and transport science driver is to identify a set of increasingly challenging benchmark scenarios, based upon multiple experimental datasets drawn from multiple facilities and spanning a range of operating conditions (e.g. Ohmic, L-mode, and H-mode, along with assorted variations on those confinement modes). For each benchmark case, a set of validation metrics should be developed. Using the experimental datasets to generate common input parameters, relevant combinations of models and formalisms can then be exercised, and their physical fidelity assessed via calculation of the pre-defined validation metrics. By adopting this approach, a quantitative way for assessing relative and absolute fidelity of competing models and formalisms (e.g. local vs. global, δf vs. full-f microturbulence) for real-world applications natural presents itself.

It is envisioned that this strategy would be implemented via multiple iterative multi-code comparison exercises. The results of each comparison study used to identify any needed additional or improved experimental measurements, new validation metrics, and model improvements. The successive atmospheric model intracomparison projects (AMIP 1-3) provide a practical example of how this strategy might be implemented.

The benchmark scenarios are defined as follows. For each scenario, data from Ohmic, L-mode, and H-mode experiments should be obtained as possible. The scenarios are:

- A slowly evolving, MHD-quiescent discharge. This scenario should include some stationary or near-stationary discharges as initial starting points, and cases with both time-stationary and slowly varying sources should be included. The key physics to investigate would be density peaking and intrinsic rotation, as well as possible contributions to electron transport from intermediate and high-k fluctuations.

- The formation of internal transport barrier in a MHD-quiescent plasma. One could also include rapidly modulated sources, and the dynamics of resulting particle/heat/momentum pulses in this scenario, as well as the response of the core profiles to the change in edge parameters at a L-H transition.

- A slowly evolving discharge, including a background of Alfven waves.

- A stationary or slowly evolving plasma which includes a saturated NTM

- Onset of sawteeth and evolution of plasma profiles through multiple sawteeth cycles

This set of scenarios emphasizes testing of microturbulence and neoclassical over MHD physics at the near-term, based on the lack of readiness to integrate MHD and microturbulence. A second set of near-term scenarios focusing on testing MHD-dominated plasmas should be identified which would be pursued in parallel to the above set. These scenarios could include:

- Self-consistent prediction of saturated Alfven eigenmode spectra and fast particle distributions in steady and slowly evolving plasmas

- Simulation of linear growth and saturation of a neoclassical tearing mode, and response to localized RF heating and current drive

- Simulation of sawtooth cycle in presence of a fast ion population

The key experimental gaps for validation are primarily the local of local core velocity and ion temperature fluctuations, which limit our ability to validate ITG mode physics at a fine level. Heavy ion beam probes (HIBP) can be used to measure potential fluctuations and thus perhaps δV_{ExB}, but the diagnostic is generally not cost or space-feasible on larger, high-power machines. Some impurity ion temperature fluctuations have been made by beam emission spectroscopy on TFTR, but this is another highly challenging and cost-intensive measurement. Moreover, this does not provide measurements of the primary deuterium ion temperature fluctuation which would be the most desired quantity for ITG studies. Other notable gaps include high-k Te fluctuations (for assessing the importance of high-k TEM and ETG modes to electron thermal transport) and localized core magnetic fluctuations which would be of particular interest in plasmas with high β.

3.I. Connections to other work

Needs for collaboration with other efforts within the FSP:

- Whole device modeling. Our most important connection is with the "Whole Device Modeling" effort because both groups are offering alternative models of the same physics (transport in the plasma core). It should be possible for "Core Profiles" and "Whole Device Modeling" to employ common Core Source and Magnetic Geometry components; and to employ a common Transport Solver. This transport solver should solve the transport equations in conservative form (as written in Sec. C above) and accept turbulent fluxes (rather than transport coefficients) from the radial array of gyrokinetic flux-tube codes. As it seems likely that there will be significant overlap in verification and validation test cases between the core profiles and WDM groups, the identification and development of such cases should be undertaken in a coordinated fashion.

- Wave Particle Interactions. An important mission of the Wave Particle Interactions group is to provide particle, momentum, and energy source terms associated with auxiliary heating and current drive systems (e.g., RF and neutral beam systems). These source terms need to be incorporated into the shared Transport Solver. In addition, Wave Particle Interactions modeling often involves assumptions and conclusions about the distribution function of various species of ions or electrons. Every effort should be made to ensure as much commonality as practicable between the distribution functions as conceived by the wave particle group and the distribution function described by our gyrokinetic codes.

- Pedestal Modeling. Progress in core edge coupling will require close interactions between the “Core Profiles” and “Pedestal” groups. This interaction has yet to occur.

- Disruption Avoidance. We see the “Disruption Avoidance” group as mainly a customer of “Core Profiles”. What is less obvious is who should have responsibility for modeling the onset of a sawtooth crash (an MHD event similar to disruptions) and the resulting redistribution of density, flow, and temperature profiles within the q=1 surface. The relevant expertise (nonlinear MHD) would seem to lie mainly within the Disruption Avoidance group. The Whole Device Modeling group ought to share our concern with modeling sawtooth crashes, and need to be involved in resolving this issue.

- Data Management. The core gyrokinetic codes used by the core profiles group will produce copious amounts of data. Knowledge of turbulent fluxes over a wide range of operating points (computed in the course of advancing core profiles) will be useful in refining 1.5D core transport models; while analysis of the turbulent fluctuations in the fields (electrostatic and electromagnetic), and sources (densities, current, etc.) will provide insight into the nonlinear development of plasma micro-instabilities and the mechanisms responsible for their saturation. A comprehensive data management system will be required to make proper use of this data.

- Data Analysis. The core fluctuation data described under "Data Management" above will contain a wealth of information about plasma microturublence. Making proper use of this data will require the development and support of data analysis tools which provide realization-indpendent characterization of the plasma microturbulence for comparison with experiment (through support of synthetic diagnostics) and theory (through support of tools to compute spectra, correlations functions, bi-coherence, etc.).

Requirements for work to be accomplished outside the FSP (foundational theory, SciDAC, etc).

- Meso-scale physics. The rigorous formalism describing the coupling between neoclassical tearing modes and plasma microturublence needs to be developed. Unresolved issues include the determination of the equilibrium distribution function in the presence of the neoclassical island and the manner in which the plasma microturbulence reacts back on the development of the neo-classical tearing mode.

3.J. Schedule and resources

This is a substantial effort and requires a fully supported leader (1 FTE). In addition to the over-all leader of the Core Transport science driver, we require a work-force of 8 FTE’s in year 1. We expect that this effort would roughly double by year 5, and continue to increase throughout the FSP project. Details of this estimate are provided below.

3.J.1. Validation

The basis for resource estimate, incorporated into the schedule below, is one FTE/major facility — the experimental analyst. Initial validation effort includes three major facilities (DIII-D, C-

Mod, and NSTX) — so 3 FTE's. This estimate is a bare-minimum for a credible validation effort which assumes both a strong collaboration with existing experimental teams and substantial interest from the major device experimental groups in code validation.

Year 1

Activities: Recruiting personnel, learning code use within FSP environment and helping to insure that the FSP code development effort properly supports Validation (data access/storage, appropriate models, user interface, etc.). Development of appropriate synthetic diagnostics (major device specific). Etc. (Chris, feel free to put your oar in here!)

Resources required: 3 FTEs for activities in support of validation on DIII-D, C-Mod, NSTX.

Year 2

Activities: Local transport model becomes operational. Need to work with developers to insure that it meets needs of Validation effort, integrate tools (like sythetic diagnostics). Plan validation campaigns for year 3.

Resources required: 3 FTEs for activities in support of validation on DIII-D, C-Mod, NSTX.

Year 3

Activities: Meet both year 3 milestones — one relating to transport in MHD quiescent plasmas and another relating to fast particle transport.

Resources required: 3 FTEs for activities in support of validation on DIII-D, C-Mod, NSTX.

Year 4

Activities: Global gyrokinetic models are available. Analysts need to familarize themselves with it, adapt tools (like synthetic diagnostics) to these codes, etc. and plan the year 5 validation campaign. Depending on the success of the validation campaign thru year 3, consider expanding the number of experimental analysis to improve coverage of major US facilities (to cover, in particular, validation of core/edge coupline model) and/or initiate validation campaigns on major international facilities, like JET, JT-60, KSTAR, and EAST. Later course assumes appropriate bi-lateral agreements. Note that it is very much in the interest of the US program that our codes (including particularly the FSP suite of codes) properly describes major tokamaks outside the US.

Resources required: 3-10 FTE's (depending on decision described above).

Year 5

Activities: Complete three validation milestones, (1) comparing local and global models in MHD-quiescent plasmas; (2) in presence of significant Alfven eigenmode activity; and (3) self-consistent islands in the presence of turbulence. Analysts to familiarize themselves with core/edge coupling model, develop appropriate synthetic diagnostics required for validation of this model, etc.

Resources required: 3-10 FTEs (DIII-D, C-Mod, NSTX) plus 3 Additional US experimental analysts plus up to four International experimental analysists (JET, JT-60, KSTAR, EAST).

Year 6

Activities: First iteration of core/edge coupling algorithm is complete. Analysts must develop plans for validation of coupled edge/core model.

Resources required: 3-10 FTEs (DIII-D, C-Mod, NSTX) plus 3 Additional US experimental analysts plus up to four International experimental analysists (JET, JT-60, KSTAR, EAST).

Years 7 - 15

We do not have a detailed schedule for years 7-15, but anticipate that the resource requirements will remain the same to support a continued iteration between validation campaigns and improvements to the underlying models. Depending on the success of the 3-D model we may want to further expand the validation effort to include major international stellerators.

3.J.2. Local Model

The basis of my resource estimate is that we require, at a minimum, one FTE to support each major code. In the context of the "local model" this leads to a minimum of 2 FTE's — one to support the transport solver and couplilng to the underlying gyrokinetic code(s), and (at least) one (or more) to support one (or more) flux-tube gyrokintic code(s). In addition, we assume that 1.5D transport models will be supported by the "whole device modeling" group, and anticipate working with them in improving overall model fidelity.

Year 1

Activities: Recruiting personnel, learning code use within FSP environment and helping to insure that the FSP code development effort properly supports Validation (data access/storage, appropriate models, user interface, etc.).

Resource Requirements: 2 (or more) FTEs to support transport solver and GK code(s) -- depending on number of GK codes supported.

Year 2

Activities: Local model becomes operational to meet milestone "demonstration of local transport model". Incorporate fast particles in anticipation of year-3 milestone.

Resource Requirements: 2 (or more) FTEs to support transport solver and GK code(s) -- depending on number of GK codes supported.

Year 3

Activities: Support validation milestone relating to fast particles. Update codes as required to improve both code fidelity and user interface.

Resource Requirements: 2 (or more) FTEs to support transport solver and GK code(s) -- depending on number of GK codes supported.

Year 4

Activities: Prepare for year-5 validation milestones comparing local and global models. Update codes as required to improve both code fidelity and user interface.

Resource Requirements: 2 (or more) FTEs to support transport solver and GK code(s) -- depending on number of GK codes supported.

Year 5

Activities: Support year-5 validation milestones comparing local and global models. Update codes as required to improve both code fidelity and user interface.

Resource Requirements: 2 (or more) FTEs to support transport solver and GK code(s) -- depending on number of GK codes supported.

Years 6 - 15

We do not have a detailed schedule for years 6-15, but anticipate that the resource requirements will remain the same to support a continued iteration between validation campaigns and improvements to the underlying models.

3.J.3. Global Model

The basis of my resource estimate remains one FET to support each major code. Thus one FTE each for global GK code, 3-D magnetic geometry package, and 3-D transport code. It may be possible to employ a common transport package for both the Local and Global models. However, since we anticipate that the transport solver is shared with “whole device modeling”, this decision needs to be made at a higher level. In estimates below I assume a separate 3-D transport model with one FTE to support it.

Year 1

Activities: Recruiting personnel, learning code use within FSP environment and helping to insure that the FSP code development effort properly supports Validation (data access/storage, appropriate models, user interface, etc.).

Resource Requirements: 3 FTEs to support development of global GK code, 3-D magnetic geometry component, and 3-D transport solver.

Year 2

Activities: Develop required components (3-D GK code, 3-D magnetic geometry component, 3-D transport solver), and begin coupling these components.

Resource Requirements: 3 FTEs to support development of global GK code, 3-D magnetic geometry component, and 3-D transport solver.

Year 3

Activities: Complete coupling of 3-D components to produce functional meso-scale transport model. Support year-3 milestone (initial validation assessment …).

Resource Requirements: 3 FTEs to support development of global GK code, 3-D magnetic geometry component, and 3-D transport solver.

Year 4

Activities: Prepare for year-5 validation milestones comparing local and global models; computing self-consistent turbulence in presence of 3-D islands: validation of free-boundary equilibrium in presence of islands plus turbulence Update codes as required to improve both code fidelity and user interface.

Resource Requirements: 3 FTEs to support development of global GK code, 3-D magnetic geometry component, and 3-D transport solver.

Year 5

Activities: Support year-5 validation milestones comparing local and global models; computing self-consistent turbulence in presence of 3-D islands: validation of free-boundary equilibrium in presence of islands plus turbulence Perform self-consistent calculation sfor narrow islands to determine NTM threshold width. Update codes as required to improve both code fidelity and user interface.

Resource Requirements: 3 FTEs to support development of global GK code, 3-D magnetic geometry component, and 3-D transport solver.

Years 6 - 15

We do not have a detailed schedule for years 6-15, but anticipate that the resource requirements will remain the same to support a continued iteration between validation campaigns and improvements to the underlying models.

3.J.4. Core/Edge Coupling

Year 3

Activities: Finalize plan for core/edge coupling. Recruit personnel, who will learn code use within FSP environment and help to insure that the FSP code development effort properly supports Validation (data access/storage, appropriate models, user interface, etc.).

Resources Requirements: 2 FTEs to support packages which are required for core/edge coupling.

Year 4

Activities: Develop required packages, prepare for Year-5 milestones.

Resource Requirements: 2 FTEs to support packages which are required for core/edge coupling.

Year 5

Activities: Complete code development and demonstrate initial core/edge coupling model.

Resource Requirements: 2 FTEs to support packages which are required for core/edge coupling.

Years 6 - 15

We do not have a detailed schedule for years 6-15, but anticipate that the resource requirements will remain increase to support a continued iteration between validation campaigns and improvements to the core/edge coupling model.

3.K. Milestones

Below we summarize suggested high-level goals and milestones (perhaps at roughly the 2, 5, 10 and 15 year marks).

Here is an initial strawman set:

2 year

- Identify initial verification and validation test cases (including metrics to be used for each case), and integrate all needed experimental data into a generally accessible database.
- Deliver prototype framework for a time-dependant 1.5D transport solver built from legacy components (e.g. "FSP0")

- Complete verification assessment and documentation of existing components and frameworks.
- Demonstration of local transport model operation within the FSP code (by modeling a DIII-D discharge?)

3 year

- Complete initial validation assessment study of relative and absolute local and global gyrokinetic turbulence models for slowly evolving, MHD-quiescent plasmas spanning low-β_N Ohmic discharges to high-β_N H-modes.
- Complete initial validation assessment study of self-consistent fast particle profile and Alfven eigenmode saturation in varying plasma conditions.
- Couple global gyrokinetic codes to a 3D equilibrium code with islands.
- Incorporate kinetic and flow effects in 3D equilibria through gyrokinetic calculation of $\mathbf{j}_\perp$.

5 year

- Complete initial validation assessment study of relative and absolute local and global gyrokinetic turbulence models for quickly evolving, MHD-quiescent plasmas (internal transport barrier formation, core response to edge BC change via L-H transition).
- Complete initial validation assessment of relative and absolute local and global gyrokinetic turbulence models in presence of significant Alfven eigenmode activity, with focus on fast particle transport.
- Complete code development (and demonstrate operation) for 1st cut on core/edge coupling based on local transport model.
- Calculate self-consistent turbulence in the presence of magnetic islands through the coupling of a 3D equilibrium code to a global gyrokinetic code that can properly handle neoclassical effects as well as turbulence.
- Validate self-consistent solutions for free-boundary equilibria with magnetic islands in the presence of turbulence against tokamak data for saturated tearing modes.
- Self-consistent calculations for narrow islands determine the NTM threshold width.

10 year

- Complete 2nd round of validation assessment study of relative and absolute local and global gyrokinetic turbulence models MHD-quiescent plasmas.
- Complete self-consistent calculation of the evolution of 3D equilibria in the presence of turbulence.

15 year

- Milestone relating to validation of core/edge coupling
- Milestone relating to validation of meso-scale transport model

3.L. Applications to ITER.

4. WAVE PARTICLE INTERACTIONS

R. Nazikian, P. Bonoli, H. Berk, E. D'Azevedo, N. Gorelenkov, W. Heidbrink, Z. Lin, C. Phillips, J.R. Wilson, D. Spong, S. Wukitch, J. Cary

4.A. Background and motivation

The realization of fusion energy requires the efficient production of well-confined suprathermal ions (alphas, injected neutral beams, RF heated ions) and the efficient transfer of their energy to the core of the thermonuclear burn. In addition, efficient and reliable methods are needed for initiating and then controlling the fusion burn using radio frequency power in the ion cyclotron, lower hybrid, and electron cyclotron range of frequencies, as well as neutral beam injection

Suprathermal ion heating, particularly neutral beam heating, is generally efficient and reliable in existing experiments, in part due to the low velocity of the injected neutrals compared to the Alfvén velocity. However there are some real challenges facing future reactors where the bulk of the suprathermal ions will have velocities exceeding the Alfvén velocity. Calculations indicate that Alfvén wave instabilities are expected in future reactors and in ITER with consequences that cannot be reliably predicted at present. While extensive data exists on the adverse effects of these instabilities in present experiments, the fusion program lacks the computational capability (algorithms, hardware) needed to simulate existing experiments and extrapolate to the reactor regime.

It is not only the energetic particle driven instabilities that present challenges to the development of a reliable reactor. RF waves are injected into existing experiments for heating, current drive and MHD stability control. Effective RF control of the plasma requires a detailed quantitative understanding of the various mechanisms that can dissipate wave energy as well as the effective control of these mechanisms to efficiently and reliably target the wave energy. Recent advances in RF theory and simulation, coupled with experimental advances enabled by new diagnostics and continuing detailed measurements, have led to an unprecedented understanding of the physics of RF heating and current drive in the plasma core of axisymmetric toroidal magnetic fusion devices. However, the existing models cannot predict the net amount of power that will be coupled into the core of the tokamak plasma instead of dissipated in the launcher or nearby vessel components. Furthermore, questions remain about the detailed resonant interaction of the ICRF and LHRF waves with energetic particles created self-consistently by the RF waves, by NBI, or by fusion reactions.

Waves in the ion cyclotron range of frequencies are used to heat core minority ions or electrons or a combination of the two, while lower hybrid waves and waves in the electron cyclotron range of frequencies are principally used to drive localized plasma current. However, higher order resonant interactions with suprathermal ions and parasitic effects at the plasma edge can lead to additional dissipation channels for ICRF and LH waves that are known to reduce coupling efficiency, operational reliability and potentially compromise reactor safety While coupling of rf power for ECCD is more straightforward, reliable long pulse high power operation of the gyrotrons needed for effective ECCD is still uncertain and models for simulating the stabilization of instabilities, such as neoclassical tearing modes, are still under development. At present the fusion program lacks the modeling and computational tools needed to simulate these processes in realistic geometry and conditions existing in fusion plasmas.

From the above, it may appear that the understanding of RF effects can be decoupled from the understanding of collective instabilities, so that the two topical areas can be treated independently. However this is far from the case. This is because the nonlinear saturation and dynamics of Alfvénic instabilities depends critically on the fluxes of particles in the phase space of the energetic particles. These fluxes are heavily modified in the presence of RF fields as compared to say coulomb collisions and classical slowing down. In addition, the presence of the Alfvénic instabilities will modify the flux further and this will also have an impact on the particle distribution generated by the RF waves. Hence the physics of collective instabilities in the presence of RF waves and suprathermal particles is a strongly coupled problem requiring advanced simulation capability.

Understanding these processes is essential for predicting fusion performance and for protecting the integrity of the fusion facility. Significant progress has been made in understanding the range of wave-particle phenomena relevant to the production and dissipation of suprathermal ions and electrons. However a predictive capability is far from available at present. In the area of collective Alfvénic instabilities, integrated modeling capability is needed to predict the spectrum of unstable modes and to evolve the modes self consistently with the particle distribution. In both the ion cyclotron and lower hybrid range of frequencies, predictive capability is needed for edge dissipation mechanisms and for the self-consistent description of waves in the presence of high-energy ions in the plasma core. Ultimately, these components need to be integrated to develop a self consistent description of the instabilities in the presence of the RF fields and energetic particles.

Practical applications of such an integrated modeling capability will be: the assessment of sawtooth stability in ITER in the presence of Alfvénic instabilities and RF heating; wall loading and fast ion pressure relaxation in advanced tokamak (AT) regimes with RF heating and Alfvénic instabilities. Integration with turbulence simulation codes will help address the role of Alfvénic instability induced zonal flows on the background turbulence and on the role of background turbulence in modifying the distribution of the energetic particles.

4.B. Goals

A critical problem to address in present experiments is the role of Alfvénic modes in modifying the fast ion distribution in the plasma core and enhancing particle losses to the first wall. Experiments in DIII-D indicate that the confined beam ion profile is dramatically flattened under the influence of multiple Alfvénic instabilities in reverse shear plasmas. Similar processes exist in NSTX and other fusion facilities. The level of redistribution of the beam ions in DIII-D is consistent with theoretical calculations given the apriori knowledge of the mode amplitudes, which are measured in the experiment. However there is no modeling capability at present that can predict the self-consistent mode amplitudes and fast ion distribution. A fusion reactor, particularly a steady state reactor, will operate in regimes where multiple Alfvénic instabilities are expected.

A multimode modeling capability with prescribed sources and sinks of fast ions is a near term goal of the FSP and will yield immediate benefits to existing experimental programs. Such a capability can be extended to address additional interactions of the energetic particles with the background plasma (such as turbulent fluctuations and tearing modes) and can be integrated into a transport code to predict whole discharge energetic particle transport and loss and the consequences for the evolution of the discharge.

In RF physics, parasitic loss of applied RF power in the regions beyond the last closed flux surface has been observed in all RF experiments to date and is not well understood. Existing models cannot predict the amount of power that will be available in the good confinement regions of the discharge for profile control aimed at performance optimization. These parasitic power losses in the region between the last closed flux surface and the plasma boundary / RF launcher will become increasingly problematic at the higher powers and pulse lengths required in ITER and future fusion devices.

Experiments on NSTX and on Alcator C-Mod have observed hot spot formation and surface erosion on limiter and divertor surfaces during RF pulses that correlate with a reduction in core RF heating efficiency. The mechanisms involved are not yet understood and could be either related directly to wave propagation and interaction with these surfaces or else to RF-induced acceleration of particles to high energy that then follow field lines and impinge on these surfaces, causing damage. Models could be developed in the near term and compared to experimental studies in order to develop a simplified but validated model for RF wave propagation in the edge plasma regions.

For RF-core plasma interactions, an outstanding issue for ITER is sawtooth stability under the combined influence of RF tail ions, neutral beam ions, alpha particles and localized current drive schemes such as electron cyclotron current drive (ECCD). The self-consistent description of the RF field in the presence of multiple energetic particle species is a critical requirement for predicting the stability of the giant sawtooth. Such a description would also be very valuable to existing experimental studies of sawtooth stability in JET and DIII-D and many other facilities. The physics challenge is to include finite orbit effects on the absorption of RF waves in the plasma core, particularly on energetic ions such as alphas and 1 MeV neutral beam ions. Wave propagation and absorption at high harmonics of the ion cyclotron frequency is problematic to describe successfully in the presence of multiple suprathermal ion species as finite ion orbit width effects can become very important for this interaction.

Ultimately, these distinct modeling activities will be integrated to generate a self-consistent description of RF fields, fast ions, MHD instabilities and turbulent background. Such integration is a long-term goal with many physics challenges because of the complexity of the processes involved. However the physics needs for such a high level of integration is evident in today’s experiments and will motivate the progress towards integration.

One example where a high level of integration is required is the role of MHD instabilities in the regulation of the sawtooth instability. In experiments on TFTR, DIII-D, JT-60U and JET, RF heating leads to extended sawtooth periods and the excitation of Alfvén eigenmodes inside the q=1 surface. The Alfvénic modes clearly influence the fast ion transport across the q=1 surface and the central electron heating, with consequences for the inductive current profile evolution and stabilizing effect of the fast ions on the sawtooth. How the fast ion population evolves in the presence of the RF field and Alfvénic modes is critical to the triggering of the sawtooth crash, yet there is no modeling capability to date that can predict the evolution of the suprathermal ion population under the combined influence of these high and low frequency waves. Another example where integration is required is the self-consistent description of the suprathermal ion population under the combined influence of a turbulent background, tearing modes and the RF field.

4.C. Components:

4.C.1. Energetic Particle Components

A great deal of progress has been made in understanding linear Alfvénic instabilities both in the ideal MHD limit and with kinetic effects of the thermal and fast ions included. However, comparatively less progress has been made in understanding the nonlinear mode dynamics and transport of the energetic particles on the energy confinement or slowing down time scale where the profiles are expected to relax to a steady state.

A present the gyrokinetic, gyrofluid and hybrid-MHD codes are very good for describing the rapid nonlinear evolution of the energetic particle driven instabilities for conditions well above marginality. One near term application of these codes is to assess the extent to which multimode dynamics can force profiles to remain near marginality. Such simulations may not need to be run for a slowing down time but they need to accurately resolve the multitude of unstable modes expected in the system, together with an accurate representation of the classical (or RF/turbulence modified) distribution function of the energetic particles, including multiple ion species (NNBI, alphas, etc). It is also likely that first principles simulation methods will be most effective in the short term in describing rapid transport events such as avalanche phenomena where appropriate initial distributions are given by transport codes. In order to validate these nonlinear code results, robust nonperturbative linear eigenmode solvers need to be developed which are capable of resolving the full spectrum of energetic particle mode (EPM) and gap modes expected in a reactor. Therefore the development of advanced nonlinear gyrokinetic and hybrid-MHD codes together with linear kinetic eigenmode solvers is absolutely essential for making progress on the FSP goals.

A second essential component of the FSP is to develop transport modules that can be integrated into whole discharge simulation codes like TRANSP so as to generate steady state fast ion profiles and mode saturation amplitudes on transport time scales. In the short term (1-3 years) the only tractable approach for whole discharge modeling is the use of reduced models which require much less computation time for for the evolution of the distribution function. One such reduced model approach is to fix the mode structures according to the output of linear eigenmode solvers and to compute the mode amplitudes, phases and flux of energetic particles in phase space by retaining the wave-particle nonlinear interaction physics. These fluxes would then be used to relax the particle distribution function in between the coarser time steps of the transport code and the spectrum of eigenmodes would be recalculated with each time step. By this means, we can attempt to achieve a predictive capability for the fast ion distribution over an entire discharge based on transport coefficients inferred from the detailed phase space dynamics of the wave-particle interactions.

The implementation of a robust quasi-linear model is needed to address this question in the near term. Quasi-linear formulations do exist and provide a basis for addressing realistic systems near marginal stability, where either steady state or bursting behavior can arise. The proposed quasi-linear model extends the conventional quasi-linear formulation in that it treats discrete modes as well as modes that overlap (the regime that conventional quasi-linear theory for which the robust formulation applies). The discrete mode formulation of the model has been validated with theoretical and computational simulations that describe the dynamics of a single resonance. Several issues need to be tested with direct simulation. In particular does the relaxation to a steady plasma turbulent behavior predicted by this quasi-linear theory, correspond to relaxation found in direct simulations, and if not can the difference be understood. If the quasi-linear predictions can be verified, then a tool takes shape that will enhance the turn around time for studying the effect of varying many different parameters in burning plasma experiments.

The output of such a quasi-linear calculation will provide transport coefficients that can be implemented in transport codes to predict the evolution of the discharge between code time steps. Essential to this quasilinear model is the need for a more robust autonomous linear eigenmode solver, (that improves codes such as NOVA in its treatment of the MHD continuum). Once the model is implemented and validated against experiment in a limited range of conditions, then it can be integrated into a transport code such as TRANSP for whole discharge simulation and ITER prediction.

In parallel to the quasilinear effort, a PIC based reduced physics model is needed for evolving the particle distribution between the transport time steps using known particle sources including classical collisions and the effect of the Alfvénic instabilities. In this reduced model, the mode structure of each Alfven mode is again fixed whereas the mode amplitude and phase are evolved due to the energetic particle drive. Because of the assumption of fixed mode structure, the computation of the mode evolution and fast ion transport is much faster than the first principle simulations. Thus this reduced model is expected to be useful for whole device modeling. Such a tool can be benchmarked against analytic theory for single mode nonlinear dynamics and can be validated against experiments for energetic particle transport with multiple unstable modes. One example of such a reduced code, called FMS (Fixed Mode Structure), has been used successfully in the past in modeling the nonlinear evolution of multiple unstable Alfven eigenmodes but with simplified geometry and model assumptions. Such a modeling effort can treat the physics of frequency chirping due to hole-clump dynamics in phase space and can also treat the overlap of multiple resonances in a self-consistent way. The exclusion of the wave-wave nonlinearity and the assumption of fixed mode structure makes the system computationally tractable for incorporation into a transport code.

Examples of a few numerical models that can be used to describe different aspects of the Energetic Particle physics are given in Table Ia.

Table Ia: EP – Wave Particle Components

EP Component Name	Functionality	Integration Aspect
NOVA-K, NOVA-KN	Linear perturbative and nonperturbative, ideal and kinetic stability analysis and eigenmode solver	Provides eigenmodes for quasi-linear and reduced model PIC simulation
CQL3D, ORBIT RF, sMC, NUBEAM	Fokker Planck treatment (continuum or Monte Carlo) of energetic ion species	Provides non-thermal distribution of particles with sources and sinks.
SPIRAL, FMS, ORBIT	PIC guiding center and full orbit codes for calculating particle profiles on slowing down time scale	Outputs relaxed fast ion profiles in presence of multiple instabilities
M3D-K, GTC, GYRO, TAEFL	Nonlinear PIC or two fluid code for full nonlinear evolution	Calculates relaxed particle distributions and losses

4.C.2. RF Component

A self-consistent simulation of ICRF heating and LHRF and ECRF current drive requires a description of three different aspects of the wave-plasma interaction: (1) wave propagation and absorption in the core plasma, (2) the quasilinear response of the plasma to the wave fields, and (3) coupling of high power waves from the RF launching structures to the core plasma. For a rapidly oscillating wave field **E** with frequency ω, Maxwell's equations reduce to the Helmholtz wave equation:

$$-\nabla\times\nabla\times\mathbf{E}+\frac{\omega^2}{c^2}\left(\mathbf{E}+\frac{i}{\omega\varepsilon_0}\mathbf{J}_p\right)=-i\omega\mu_0\mathbf{J}_{ant} \quad (1)$$

The plasma current $\mathbf{J}_p$ is, in general, a non-local, nonlinear, integral operator on the electric field that is given by:

$$\mathbf{J}_p(\mathbf{r},t)=\sum_s\int d\mathbf{r}'\int_{-\infty}^{t}dt'\sigma\left(f_{0,s}(\varepsilon),\mathbf{r},\mathbf{r}',t,t'\right)\cdot\mathbf{E}(\mathbf{r}',t')+\mathbf{J}_{sh}^{rf}(E_{rf})+\mathbf{J}(E_{pump}^{rf}) \quad (2)$$

The long time scale response of the plasma distribution function f_0 can be obtained from a bounce- averaged Fokker-Planck equation of the form:

$$\frac{\partial}{\partial t}(\lambda f_0) = \nabla_{\mathbf{u}_0} \cdot \Gamma_{\mathbf{u}_0} \quad \text{with } \nabla_{\mathbf{u}_0} \cdot \Gamma_{\mathbf{u}_0} = C(f_0) + Q(\mathbf{E}, f_0). \tag{3}$$

In these expressions: $\boldsymbol{u}_0$ is the velocity vector at the outside midplane; $\lambda = \tau_b u_{\parallel 0}$, with bounce time τ_b , $C(f_0)$ is the momentum conserving Balescu-Lenard collision operator, and Q is the RF quasilinear operator. The first term in Eq. (2) is the plasma conductivity kernel, evaluated in terms of an arbitrary particle distribution that can be the non-thermal energetic particle distribution that is generated by the RF power itself or from neutral beam injection or fusion processes. Further nonlinearity is introduced into this coupled system through formation of RF sheaths (J_{sh}^{rf}), and through three-wave coupling processes (J_{pump}^{rf}), such as parametric decay instability (PDI). Equations 1-3 represent a highly nonlinear problem in which the core energetic ions and electrons generated by the waves in conjunction with edge processes can significantly alter the wave propagation and absorption. Examples of a few advanced numerical models that can be used to describe different aspects of the RF wave-particle physics are given in Table Ib.

Table Ib: RF – Wave Particle Components

RF Component Name	Functionality	Integration Aspect
AORSA, TORIC, GENRAY	ICRF, LHRF, and ECRF wave propagation (full-wave & ray tracing)	Provides *Q(f_s)* for Fokker Planck description and RF wave fields for use in NUBEAM
CQL3D, ORBIT RF, sMC	Fokker Planck treatment (continuum or Monte Carlo)	Provides non-thermal f_s for conductivity evaluation in wave propagation calculations and energetic particle component
TOPICA, RANT3D	Linear ICRF and LHRF antenna coupling	Provides boundary conditions for core wave solvers
VORPAL	Nonlinear PIC for ions and fluid electrons	Calculation of edge wave fields in presence of nonlinear effects (RF sheaths & PDI)

Plans for adapting older components and as well as plans for developing new components.

4.C.3. EP:

As stated in the previous section, the continued improvements to the GTC, TAEFL, GYRO, and M3D-K fully nonlinear codes are essential in order to provide detailed fast ion transport assessments on short intervals. These improvements include the addition of realistic (classical) slowing down distributions and other upgrades required to resolve the multimode dynamics and system size expected for ITER. In addition the development of a robust kinetic eigenmode solver is essential for providing input to reduced models and benchmarking fully self-consistent models. The key code here is NOVA-KN. Finally the refinement of the FMS code is needed for realistic geometry and fast ion distributions. A new code is needed for the quasilinear solver. This will require significant analytic work to determine how to upgrade existing models with multiple wave-particle resonances.

4.C.4. RF:

Improvements in algorithms used in the full-wave, Fokker Planck, and antenna solvers will be needed to take full advantage of computing resources on petascale platforms and beyond (as they become available). These enhancements in performance will be needed for improved resolution in the lower hybrid regime, for treating 3D effects, and for including mode conversion in the HHFW, ICRF and sub-cyclotron frequency range. We might even envision the potential application of these codes to the electron cyclotron range of frequencies if scaling of the full-wave solvers maintains itself at the 50,000 – 100,000 processor level. In addition, code changes will be made to take advantage of the graphical processor architecture that is (likely) central to exa-scale computers.

As older components continue to be used and new components are developed it will be necessary to adopt component requirements on software such as:

- Version control oversight such as SVN for all components.
- Keep components buildable across multiple platforms, which will be an on-going process.
- Implement a set of physics-based regression tests for the wave and Fokker Planck solvers.

4.D. Framework requirements:

a. Analysis of the requirements for composition of the physics components (including data exchanges and algorithms)
b. Analysis of the requirements for the full workflow (task composition)

Framework requirements for composition of the physics components can be described in the context of the coupling schemes for the components. Figure WP-1 shows the coupling scheme envisioned for these

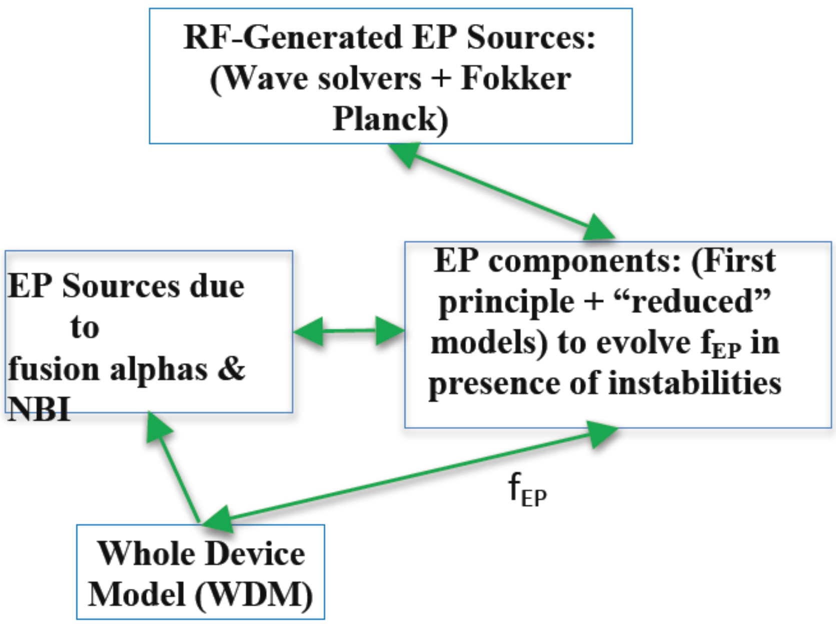


Figure WP-1: Coupling scheme for components of the wave-particle science

components over the 2-5 year time frame. Component functionality and coupling is most easily explained in terms of what physics is being done:

The Whole Device Model (WDM) (1.):

• Performs a transport evolution of the background plasma profiles for density, temperature, as well as solving an evolution equation for the poloidal magnetic field.

• Plasma profile and equilibrium information is then passed to the EP source component and EP component.

Energetic particle (EP) sources (2.):

• The RF-generated energetic particle sources consist of wave propagation models (either full-wave or ray tracing) that iterate with a Fokker Planck code to self-consistently evolve non-thermal electron and ion distributions. These coupled RF sources span the ion cyclotron (IC), lower hybrid (LH), and electron cyclotron (EC) range of frequencies.

• The other sources of energetic particles are due to fusion products such as alpha particles and fast ions due to neutral beam injection (NBI).

• The EP distribution computed by the component is passed to the EP component.

Energetic particle component (3.):

• Consists of either first principle or reduced models that evolve the EP particle distribution (f_{EP}) (in both space and time) in the presence of Alfvenic type instabilities such as Toroidal Alfven Eigenmodes (TAE's).

• It is expected that reduced physics models will be used in the EP component over the shorter term (≈ 3 years) and that first principle simulations will be employed at the mid term (≈ 5-10 years).

• The EP distribution evolved by this component is passed back to the EP source component in order to re-evaluate the wave propagation and absorption in the presence of the newly evolved EP distribution.

The coupling scheme for these components over the 10-15 year time frame is shown in Fig. WP-2. The coupling between components closely follows what was described for Fig. WP-1 except that now modifications to the plasma edge due to nonlinear effects is calculated and included in the EP source and edge transport calculations. Since the EP component now includes RF effects due to an ICRF or ECRF induced flux in the MHD equations, coupling between the EP and RF sources is now tightly coupled. Component functionality and coupling looks like the following:

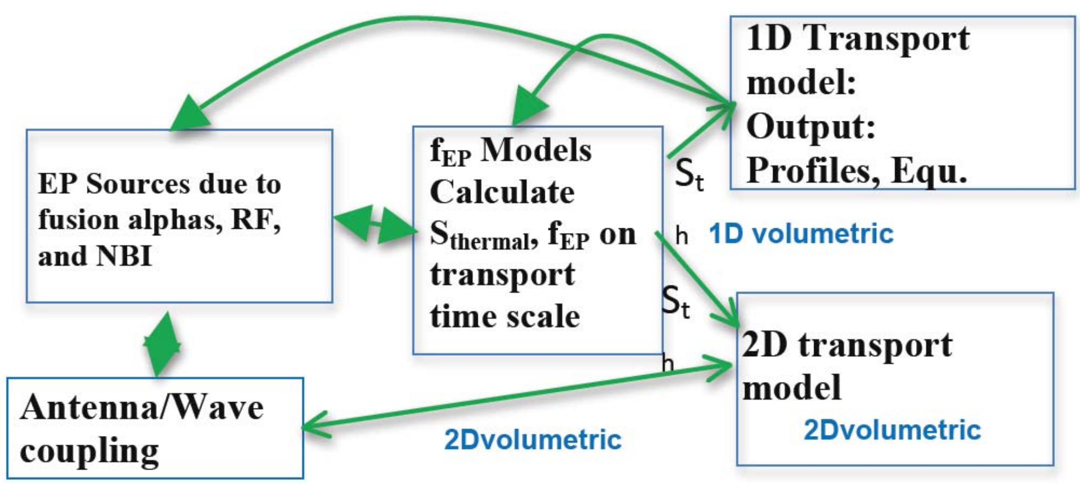


Figure WP-2: Coupling scheme for components of the wave-particle science driver assuming a 10 year time window.

4.D.1. 1D Transport Model (1.):

• Performs a transport evolution of the background plasma profiles for density, temperature, as well as solving an evolution equation for the poloidal magnetic field.

• Plasma profile and equilibrium information is then passed to the EP source component and EP component.

4.D.2. Energetic particles (EP) sources (2.):

• The RF-generated energetic particle sources consist of wave propagation models (either full-wave or ray tracing) that iterate with a Fokker Planck code to self-consistently evolve non-thermal electron and ion distributions. These coupled RF sources span the ion cyclotron (IC), lower hybrid (LH), and electron cyclotron (EC) range of frequencies.

• The other sources of energetic particles are due to fusion products such as alpha particles and fast ions due to neutral beam injection (NBI).

• The EP distribution computed by the source component is passed to the EP component.

4.D.3. Antenna / wave coupling component (3.):

• Evaluates nonlinear effects such as RF sheath formation and parametric decay instability (PDI) of the RF pump wave.

4.D.4. Energetic particle component (4.):

• Includes ICRF generated energetic particle tails in the MHD closure hierarchy so that modification of sawteeth via ICRF can be studied.

• Simulates the nonlinear evolution of EP driven Alfvenic/acoustic instabilities with macroscopic MHD in the presence of RF on transport time scales.

• Predicts fast ion transport and mode saturation levels and effects on the macroscopic MHD in burning plasmas.

• The EP distribution evolved by this component is passed back to the EP source component in order to re-evaluate the wave propagation and absorption in the presence of the newly evolved EP distribution.

4.D.5. 2D edge transport (5.):

• Includes sources of heat due to nonlinear RF dissipation mechanisms or EP losses and evolves the edge plasma accordingly.

4.E. Validation requirements:

c. Measurement requirements
d. Plans for validation of critical physics associated with the science driver

EP:

Validation is a type of stress test for energetic particle (EP) physics *models* by comparing theoretical or numerical predictions against measurements that effectively *constrain* the physics model. By "constrain" we mean the measurement of predicted quantities that are most sensitive to the model assumptions and/or input parameters. Ultimately, the "model" should be a global, nonlinear, simulation of EP instabilities and consequent phase space redistribution. At a higher level of integration, the model should also provide predictions of the effects of phase space redistribution on plasma control systems, underlying transport, macroscopic stability and the evolution of the plasma discharge.

For the FSP, the focus is primarily on the validation of physics models required for predicting burning plasma behavior. As these models must extrapolate from present experimental parameters to the burning plasma regime, validation efforts must focus on identifying the key trends needed for reliable extrapolation.

The process of validation should address *all* levels of a model from basic assumptions, underlying transport mechanisms, phase space redistribution/transport and ultimately the effects on plasma evolution. Basic assumptions are the input parameters such as the source distribution and background equilibrium properties. The underlying mechanisms are the identification of the instabilities that produce phase space resonances and energy exchange with the energetic particles. The model consequences are the effects of these mechanisms on fast ion transport, redistribution and loss.

The table below provides a hierarchy of model assumptions and predictions and some measurements that can potentially validate various levels of the model.

Table: Model hierarchy of EP physics simulation

	Fundamental Constituents	⇒			Derived Observables
Model Hierarchy	**Linear Mode Properties**	**Nonlinear Evolution**	**Phase Space Redistribution**	**Scaling Trend**	**Statistics**
Observables	Polarization, structure, frequency, threshold	spatial/temporal mode(s) evolution, bispectra, zonal flows/fields	Confined and lost particle measurements	Similarity experiment	Database
Agent/	EP spatial gradient, velocity anisotropy,	Wave-wave, wave-	Cross-phase,	Dimensionless	Inter-

Mechanism	resonances	particle interaction	relaxation	scaling	machine

Validation is intrinsically an *iterative* process. If the stress test yields poor performance, one seeks to modify the model or the quality of the measurements. One hopes that this process is convergent.

As an example, consider the DIII-D reversed-shear, beam-driven condition with many TAE and RSAE instabilities and strong central flattening of the beam distribution. The three lowest levels of the validation hierarchy must address the following issues.

(i) *primary fluctuations and source terms*, the linear modal properties including instability threshold, mode polarization, spatial structure, and frequency, and the linear coupling of RSAE and TAE modes;

(ii) *secondary fluctuations and nonlinear interactions*, which can be addressed via toroidal spectrum intensity, bispectral analysis, and secondary modes, i.e., zonal structures;

(iii) *energetic particle transport*, i.e., the perturbed EP distribution function, radial flux and redistribution.

At a higher level of the hierarchy, trends can be studies in a single device (such as the dependence of q-profile) and size scaling can be studied in "similarity experiments" between devices. For example, it is possible to operate NSTX and DIII-D with nearly identical parameters apart from the major radius, as in an earlier similarity experiment. The EP ITPA coordinates several inter-machine comparisons such as this.

While much comparison between modeling and experiment has been carried out for fast ion driven instabilities and energetic particle physics in DIII-D plasmas, these results cannot truly be called a concerted validation effort. In a comprehensive validation program, the model / data comparisons should be done over a large parameter range, typical of the expected application domain, with a well defined metric for quantifying the confidence one should have in a given computational simulation. What follows is a description of several energetic particle physics modeling / experiment comparisons that have been carried out recently on DIII-D which will form the basis of future validation efforts.

Fast Ion Driven Instabilities

For fast ion driven instability studies, current experiments are capable of probing instability structure, spectral characteristics, drive/damping, and resultant fast ion transport. Eigenmode measurements are made using a number of diagnostics that are sensitive to small changes in the electron density (reflectometers, interferometry, beam emission spectroscopy (BES)), electron temperature (ECE), or magnetic field and fast ion transport measurements are made using neutrons, equilibrium pressure reconstructions and fast ion D-alpha (FIDA). In general, comparisons between experiment and modeling are made through the use of synthetic diagnostics applied to computational predictions that mimic the instrument function of the actual experimental diagnostic.

Mode Structure and Spectral Characteristics

Successes

Improvements in the electron cyclotron emission (ECE) diagnostic on DIII-D have allowed detailed measurements of the radial mode structure of both the TAE and RSAE as well as the spatial coupling of the two in DIII-D AT discharges. Comparison with simulation is accomplished by convolving the finite RF filter width and Gaussian beam pattern of the ECE radiometer with the predicted temperature perturbation profile for a given eigenmode. Excellent agreement has been found between the ECE measured TAE and RSAE temperature perturbation with that predicted by the NOVA code in high-q, low density, L-mode plasmas typical of DIII-D current ramps. Higher radial order RSAEs as well as spatially coupled RSAEs and TAEs were also identified in mode structure measurements due to a close interaction between modeling and experiment. The introduction of Beam Emission Spectroscopy (BES) in NSTX will allow for a similar level of validation in that device as performed on DIII-D for the eigenmode structure.

Weaknesses and Future Work

Some of the specific areas in which significant disagreement with simulation has been found, for DIII-D plasmas, are in cases with large rotation or those in which the eigenmode frequency is dominated by compressibility. Similar challenges are expected in NSTX with strong rotation and for low frequency modes.

Eigenmode Drive and Damping

Successes

Recently, the stability of Alfven Eigenmodes in DIII-D plasmas was analyzed in detail for two regimes: low density, high ion temperature QH-mode plasmas as well as high-q, low density, L-mode plasmas typical of DIII-D current ramps. Historically, the stability of alpha particle driven modes in TFTR and further back in beam driven TAE experiments at low TF have been studied. In general, the calculated damping rate is of the order required to agree with observation.

Weaknesses and Future Work

A weakness of current stability calculations and comparison with experiment is the strong dependence of drive and damping rates on the exact details of the fast ion distribution function and profiles of equilibrium parameters such as q, n_e, and T_e. Experimentally, these quantities are measured with large associated uncertainty, and consequently, the accuracy of the predictions is difficult to improve.

Fast Ion Transport

Successes

Fast ion driven instabilities are a concern because of their potential for causing fast ion transport or redistribution. Measurements of confined fast ions on DIII-D and NSTX are made using FIDA, neutral particle analysis, equilibrium pressure reconstructions, and neutron emission, while lost fast ions are monitored using fast ion loss detectors (FILDs). Measurements indicate that a large redistribution of fast ions ($\delta n_{fi}(0)/n_{fi}$~50%) occurs during Alfven Eigenmode activity characteristic of DIII-D current ramp experiments (multiple modes, n~2-12, $\delta B_{max}/B \sim 5x10^{-4}$). Strong losses are observed on NSTX during sudden avalanche events.

Several attempts to explain this large fast ion transport have been made using a variety of codes such as HMGC, TAEFL, M3D-K, and NOVA calculated eigenmodes in combination with the guiding center following code ORBIT. The ORBIT calculations were carried out using a set of eigenmodes with amplitudes that were obtained by comparing NOVA calculations to ECE radiometer measurements in DIII-D. Similar calculations were made on NSTX using reflectometer data as a constraint on the magnitude of Alfvénic activity during avalanche events.

Weaknesses and Future Work

In terms of eventually developing a self-consistent set of tools capable of predicting the level of instability induced fast ion transport, there are several weaknesses with what has been done to date. The original simulations of DIII-D data were done using ORBIT coupled to NOVA calculated eigenmodes and has no predictive capability; it requires experimentally measured amplitudes. The same is also true for NSTX avalanche simulations. The HMGC, TAEFL, M3D-K and GTC simulations are more advanced, in that they self consistently calculate the eigenmode structure, frequency (real and imaginary) and evolve the mode amplitude, however neither code is currently able to incorporate the sources and sinks of energetic particles on a slowing down time scale. To truly address this problem, simulations need to be developed that are able to evolve the fast ion distribution function in the presence of multiple modes and fueling for slowing down timescales. A table of validation requirements is presented in Table 2a.

Table 2a. Validation Requirements For Energetic Particles

	Critical Physics	Measurements Needed	Important Gaps
Mode Existence & Structure	- Role of thermal ions and acoustic coupling to shear Alfven wave - Nonperturbative effects of energetic particles on mode properties - Role of Kinetic Alfven Wave coupling on mode structure	- Profiles for ne, Te, Ti, Er, Z, J(r) - 2-D fluctuations (in R,z) for ne, Te, Ti - mode polarization: B_pol, B_tor, B_parallel, on toroidal, poloidal arrays - interferometry (radial, midplane, vertical) for global survey of MHD	- 2-D internal ne, Ti not available. BES has the capability. - Mode polarization (B) not routinely measured. Key for mode identification.

		activity.	
near Drive & Damping	- Coupling to Kinetic Alfven Waves - Continuum interception - Fast Ion pressure/energy distribution/isotropy	- All the above, plus - High radial resolution of density/temperature - Collective scattering, FIDA, …	- No method has yet shown to resolve KAWs
Non linear saturation, transport, particle loss	- Sources and sinks of energetic particles, effective collision rate - Resonance overlap - Particle trapping frequency	- All the above, plus - Fast scintillator detectors, multi-channel NPAs, …	- no reliable method has been developed to measure losses in ITER - confined alpha measurementis a challenge in ITER

RF:

Validation of RF theory and simulation codes in the ion cyclotron range of frequencies (ICRF) and the lower hybrid range of frequencies (LHRF) is an important and active area of research in the SciDAC Center for Simulation of Wave Plasma Interactions (CSWPI) as well as in the base fusion theory and experimental programs. Validation of RF theory and simulation is done by comparing model predictions with experimental results at both the macroscopic and microscopic levels. At the microscopic level, simulated nonthermal ion and electron particle distributions can be used in "synthetic diagnostic codes" to reproduce the signals actually measured by diagnostics in experiments. Various moments of these particle distributions can also be computed to yield more macroscopic quantities such as driven current, plasma flows, and heating rates. Validation of these models requires theorists and computational physicists to work closely with experimentalists who are intimately familiar with their diagnostics. Below we shall give examples of these types of validation efforts specific to the ICRF and LHRF regimes.

Ion cyclotron range of frequencies:

The primary areas of concern in the ICRF regime have been in wave detection, measurement of nonthermal ion distributions, and ICRF launcher design. The Phase Contrast Imaging (PCI) technique has been used to successfully measure density fluctuations associated with short wavelength mode converted ion Bernstein waves (IBW) and ion cyclotron waves (ICW) as well as the longer wavelength fast magnetosonic wave. The signal detected by the PCI diagnostic is reconstructed numerically in a synthetic diagnostic code using the ICRF wave electric fields from sophisticated electromagnetic field solvers. This activity made it possible to identify an unexpected excitation in both the simulation and experiment, namely the intermediate wavelength ICW. Discrepancies between measured and simulated PCI data where the simulation signal amplitude is larger than in the experiment may be indicative of parasitic losses in the experiments that are not accounted for in experiment. Synthetic diagnostic codes for wave detection have also been quite useful in terms of understanding the sensitivity of the measured signal to experimental uncertainties, such as errors in minority concentration levels, sightline positions, etc.

The spatial and energy distribution of nonthermal ion distributions produced by ICRF have been measured using techniques such as a Fast Ion D-Alpha (FIDA) diagnostic and a Compact Neutral Particle Analyzer (CNPA). Nonthermal ion distributions computed with simulation models that combine full-wave (and ray tracing) calculations with Fokker Planck codes have been used in synthetic diagnostic codes to simulate the experimentally measured FIDA and / or CNPA signals. By comparing simulated FIDA and CNPA data with measured data it is now becoming possible to understand under what conditions finite ion orbit width effects are important. This type of activity therefore helps us to delineate the regime of validity of zero ion orbit width Fokker Planck solvers in describing the interaction of IRCF waves with energetic ions.

In the area of ICRF launcher design, the linear coupling of ICRF waves is simulated using 3-D electromagnetic antenna codes which in some cases are coupled to 1-D and 2-D electromagnetic field solvers. Validation of these types of coupling models is still in its infancy, however. Antenna loading and voltage "hot spots" in the launching structure are examples of useful quantities that can be compared with experiment. Validation of simulation capability to describe nonlinear processes that affect ICRF wave coupling such as RF sheath formation and parametric decay instability is also still in its early stages. Validation of linear and nonlinear coupling models requires well-diagnosed edge plasma conditions, including local probe measurements of density in the vicinity of the launching structure.

Lower hybrid range of frequencies:

In the LHRF regime extensive comparison between theory/simulation and experiment have been made by using nonthermal electron distribution functions from combined ray tracing and electron Fokker Planck codes in a synthetic diagnostic code to compute the hard x-ray emissivity associated with the fast LHRF generated electrons. Both the spatial distribution and energy spectra of hard x-rays have been compared with that measured in experiment using a hard x-ray camera. Beyond model validation, these types of comparisons have made it possible to understand under what conditions fast electron diffusivity and / or pinch effects may be important. More recently, the importance of full-wave effects in LHCD experiments has been investigated by comparing predicted hard x-ray spectra based on a full-wave / Fokker Planck model with experimental measurements. Nonthermal electron cyclotron emission (ECE) associated with LHRF generated fast electrons also offers an interesting way to validate the simulated electron distribution functions in LHCD by using those distributions in synthetic diagnostic calculations for ECE and comparing with experimental measurements.

Simulated profiles of current density (ohmic plus a nonthermal component due to LHCD) have been compared with experimentally measured current density profiles from Motional Stark Effect (MSE) diagnostic. Also, loop voltage predictions from integrated simulation models that solve an evolution equation for the poloidal field in conjunction with the nonthermal LH current density source term have been compared extensively with experiment. Very little work has been done in present day experiments to compare simulated LH wave fields with wave detection measurements, although in the past both CO_2 laser and microwave scattering were used to detect LH waves. Currently there are plans to utilize PCI and reflectometry techniques for LH wave detection and compare these measurements with LH full-wave field simulations. This should prove extremely valuable as in the past only ray tracing predictions were available for comparison with experiment.

The theory and simulation of LH waveguide launching structures (or "Grills") have been extensively and successfully validated against experiment by comparing the predicted and measured reflectivity of the waveguide array. However, two problematic aspects of these comparisons are that knowledge of the local density profile in the vicinity of the LH launcher and scrape-off-layer (SOL) is needed and second, a simple cold plasma dielectric model is typically used to represent the plasma. Also, these coupling models do not take into account the complicated edge geometry of the tokamak vessel. More recently pure finite element methods (FEM) have been applied to this problem which allows simultaneous treatment of the launcher, edge plasma, and LH wave propagation inside the plasma. Validation of these integrated coupling models will require similar measurements to those described for validating ICRF launcher models, namely detailed measurements of the local density profile in the SOL as well as voltage measurements on the launching structure itself. Finally, although slab models for nonlinear LH parametric decay instability thresholds have been compared qualitatively against experiment, there has been little work done to actually compare theory and simulation results for decay spectra, pump wave broadening, and fast ion tail formation with measurement.

The validation requirements for RF-wave particle interactions discussed above have been summarized below in Table 2b:

Table 2b. Validation Requirements For Wave Particle Interactions

	Critical Physics	**Measurements Needed**	**Important Gaps**
Coupling of ICRF and LHRF power through the SOL.	- Surface wave excitation - Power dissipation due to RF sheath formation. - Power dissipation due	- SOL profiles for ambient ne, Te, and Ti - 2-D fluctuations (in R,z) for ne in the SOL.	- 2-D SOL profile information generally not available out to the vessel wall (or well beyond antenna

	to nonlinear parametric decay instability. - Wave scattering from density fluctuations and / or blobs.	- Imaging of "hot spots" - B-dot probe measurements for surface wave detection.	strap). - Complete coupled edge-to-core simulation models not yet available to validate.
Absorption of ICRF power on energetic ions	- Importance of finite ion orbit width effects. - Effect of energetic ions on MHD stability of sawteeth, NTM's, etc. -	- Fast ion detection by FIDA or NPA diagnostics. - Edge scintillators provide a useful test of the physics when the waves accelerate some of the fast ions onto loss orbits.	- Comparison between simulated and measured EP diagnostics (FIDA and NPA) still in its infancy (metrics, etc not well-established). - Energetic particle beta not yet included self-consistently in MHD equations, so that simulating EP stabilization still not possible without using reduced model (Porcelli model).
Generation of non-thermal electron tails by LHRF power	- Spatial diffusion of fast electrons. - Effect of energetic electron tail on sawteeth and NTM's	- Hard x-ray emissivity measurements (horizontally and vertically viewing). - Motional Stark Effect measurements of non-inductively driven currents.	- Complete coupled core to edge simulation models are not yet available to validate. - Better spatially and temporally resolved profiles of LHRF current density and hard x-ray emissivity are still needed.

4.F. Connections to other work

a. Needs for collaboration with other efforts within the FSP:

For energetic particles, collaboration is expected with the whole device modeling group for integration of reduced models. Also, interaction is expected with the transport group to determine any interaction between nonlinear AE zonal flow/GAM generation and turbulence suppression. Finally, strong coupling is expected with the RF sub group for evolving the RF fields and energetic particles self consistently with the Alfvénic instabilities.

Close collaboration will be needed with the boundary group as models are developed and validated for how ICRF and LHRF power modifies the edge plasma through nonlinear ponderomotive effects, RF sheath formation, and parametric decay instability. Also the couplings discussed in Section D will necessitate close collaborations with the frameworks group.

b. Requirements for work to be accomplished outside the FSP (foundational theory, SciDAC, etc.):
The SciDAC center for Gyrokinetic Simulation of Energetic Particle Turbulence and Transport (GSEP) working on gyrokinetic (GTC and GYRO) and hybrid (TAEFL and XHMGC) codes as well as the hybrid-MHD center working on M3D-K is an essential component of a successful WPI FSP initiative. Without the availability of these codes, the verification of the efficacy of reduced models for Whole Discharge Simulation will be severely compromised.

The SciDAC Center for Simulation of Wave-Plasma Interactions (CSWPI) will need to complete the coupled core to edge RF models for ICRF and LHRF waves. This SciDAC Center is also carrying out validation work that will be incorporated within FSP. Work on coupled components is also being carried out by the FACETS and SWIM Proto-type FSP Projects that will provide useful knowledge on coupling of RF-MHD components.

4.G. Schedule and resources:

e. A projected schedule of the work to be carried over a 15 year time period
f. Realistic estimate of resources required

- Physics objective: Understand the physics of multimode induced redistribution of fast ions

  (a) Time scale of 0-2 years - (4 FTE's/yr):

  (i) Develop quasi-linear model with multiple modes, realistic sources and resonance overlap using linear eigenmode solutions - (1 FTE).

  (ii) Develop PIC code with linear eigenmode solutions and realistic sources - (1 FTE's).

  (iii) Develop nonperturbative kinetic eigenmode solver - (1 FTE).

  (iv) Include realistic distributions of energetic particles in fully nonlinear codes - (1 FTE)

(b) Time scale of 2-5 years - (4 FTE's/yr):

(i) Integrate reduced models in WDM code and validate against experiment - (1 FTE/yr).

(iii) Extend fully nonlinear simulations codes to a slowing down time scale – (2 FTE's/yr)

(iii) Integrate RF source into reduced model – (1 FTE/yr)

(c) Time scale of 5-10 years - (2 FTE's/yr):

(i) Integrate RF source into fully nonlinear models - (1 FTE/yr).

(d) Time scale of 10-15 years - (2 FTE's/yr):

(i) Integrate fully nonlinear code with RF source into RWM and sawtooth stability models and turbulence models – (1 FTE/yr)

(ii) Integrate fully nonlinear models as a replacement to the NUBEAM package (or equivalent) in the WDM code – (1 FTE/yr)

- Physics objective: Understand the effect of the edge plasma, RF launching structure, and tokamak vessel on the coupling of RF waves in the ion cyclotron range of frequencies (ICRF) and lower hybrid range of frequencies (LHRF):

(a) Time scale of 0-2 years - (6 FTE's):

(i) Develop finite element method (FEM) description of edge with linear and nonlinear boundary conditions - (2 FTE's).

(ii) Develop coupled edge to core description using a core spectral solver coupled to an FEM edge description through an admittance matrix, for example the TORIC + TOPICA codes - (2 FTE's).

(iii) Perform preliminary 3D simulations of core to edge ICRF wave dynamics utilizing spectral solvers (AORSA + TORIC) extended to a cold, linear plasma model in the edge - (1 FTE's).

(iv) Complete development of PIC codes (VORPAL) for simulating linear and nonlinear rf wave interactions with the plasma edge - (1 FTE).

(b) Time scale of 2-5 years - (5 FTE's):

(i) Use 3-D field reconstructions from spectral codes extended to edge and coupled spectral / FEM models to simulate ICRF fast and slow wave excitation including surface wave excitation and RF sheath formation in present day tokamaks (NSTX, DIII-D, and Alcator C-Mod) - (1 FTE).

(ii) Use 3-D field reconstructions from coupled spectral / FEM model to simulate LH wave coupling in present day tokamaks - (1 FTE).

(iii) Formulate conductivity operator in FEM basis in 2-D - (1 FTE).

(iv) Develop coupled core – edge FEM RF solver based on new conductivity representation and verify code against spectral solvers (AORSA and TORIC) – (2 FTE's).

(c)Time scale of 5-10 years - (5 FTE's):

(i) Use new FEM-based core-to-edge solver to assess surface and slow wave excitation in the ICRF regime using 3-D field reconstructions - (1 FTE).

(ii) Use new FEM solver to assess electric field high points on ICRF launching structures and compare with experimental measurements - (1 FTE).

(iii) Simulate long distance ICRF and LHRF coupling in ITER - (1 FTE).

(iv) Include effects of wave scattering and edge plasma variations on coupling in wave solvers - (2 FTE's).

(d) Time scale of 10-15 years - (7 FTE's):

(i) Building on existing 1-D full-wave PDI simulation experience, develop 2D / 3D full-wave simulation capability for describing three wave parametric decay instability (PDI), including finite toroidal extent of pump wave and compare simulated decay spectra with measurements - (3 FTE's).

(ii) Perform 3-D simulations of parametric decay instability using hybrid codes that employ an electron fluid description and a particle treatment for ions - (2 FTE's).

(iii) Perform 3-D simulations of RF sheath formation using hybrid codes that employ an electron fluid description and a particle treatment for ions - (2 FTE's)

- Physics objectives: Understand the role of finite ion orbit width effects and mode conversion to short wavelength modes in ICRF heating schemes:

(a) Time scale of 0-2 years - (6 FTE's):

(i) Complete integration of full-wave / Monte Carlo description of ICRF – fast wave particle interaction using statistical particle lists and 4-D quasilinear diffusion coefficient - (2 FTE's).

(ii) Validate model against experiment with synthetic diagnostics for NPA and FIDA – examine interaction of ICRF fast waves (low and high harmonic) with neutral beam ions - (2 FTE).

(iii) Use synthetic diagnostic codes for reflectometry and PCI to validate simulations of mode converted ICRF waves against experimental measurements - (2 FTE).

(b) Time scale of 2-5 years - (2 FTE's):

(i) Employ energetic particle distributions modified by the EP components in wave propagation models - (1 FTE).

(ii) Evolve EP distributions in full-wave / Fokker Planck solvers and pass back to EP component - (1 FTE).

(c) Time scale of 5-10 years - (3 FTE's):

(i) Use reduced models (full-wave + continuum Fokker Planck with finite orbit width effects) to study interaction of ICRF fast waves with NBI ions and fast fusion alphas in ITER.

(d) Time scale of 10-15 years - (4 FTE's):

(i) Use parallel framework to perform time dependent simulations where EP component, EP sources, and WDM models are iterated in time.

- Physics objectives: Understand how LHRF generated nonthermal electron tails can be used for localized control of the current profile:

(a) Time scale of 0-2 years - (2.5 FTE):

(i) Validate nonthermal electron distributions simulated by coupled full-wave / electron Fokker Planck model using synthetic diagnostic codes for hard x-ray emissivity and current density (Motional Stark Effect) - (1.5 FTE).

(ii) Develop theory for fast ion (fusion alpha) – LH wave interaction and implement in full-wave solver - (1 FTE).

(b) Time scale of 2-5 years - (2 FTE's):

(i) Compare predictions of ray tracing / Fokker Planck model against more complete full-wave / Fokker Planck treatments to determine conditions under which reduced ray tracing description is adequate - (1 FTE).

(ii) Assess interaction of LH waves with fast alphas for an ITER discharge - (1 FTE).

(c) Time scale of 5-15 years - (5 FTE's):

(i) Use parallel framework to perform time dependent simulations of LH current profile control in present day devices and in ITER.

- Physics objectives: Understand how thermal electron distributions and nonthermal ion distributions generated by ICRF and ECRF waves can stabilize of destabilize MHD phenomena in plasma.

  (a) Time scale of 0-2 years - (3 FTE's):

  (i) Finish closure theory for including driven currents due to electron cyclotron current drive (ECCD) in the MHD equations – (cases where the electron distribution is minimally distorted and the RF effect can be included through an RF flux term) – (1 FTE).

  (ii) Using a parallel framework, numerically implement this closure scheme using a ray tracing code to evaluate the ECRF – induced flux in the MHD equations - (2 FTE's).

  (b) Time scale of 2-5 years - (2 FTE's):

  (i) Validate simulation capability for NTM and sawtooth control via ECCD against experiments using the parallel framework capability developed in (a).

  (c) Time scale of 5-10 years - (3 FTE's):

  (i) Finish kinetic closure theory for including energetic ICRF distributions in the MHD moment hierarchy (case where the ion distribution function is anisotropic).

  (d) Time scale of 10-15 years - (4 FTE's):

  (i) Use a parallel framework to numerically implement closure schemes needed to include the effect of energetic ICRF tail in MHD codes.

- Physics objectives: Understand the effect of driven RF waves on plasma rotation, plasma flows, and the scrape-of-layer (edge):

  (a) Time scale of 0-2 years - (1 FTE):

  (i) Continue to validate existing theories for toroidal plasma rotation via ICRF and LHRF waves against experiment using the simulated wave fields from core wave solvers.

  (b) Time scale of 2-5 years - (3 FTE's):

  (i) Develop new theory for toroidal rotation drive and plasma flow generation via LHRF and ICRF waves if needed - (1 FTE).

  (ii) Use qualitative predictions of edge RF dissipation in coupling scheme shown in Fig.

WP-2 and simulate using a parallel framework - (2 FTE).

(c) Time scale of 5-15 years - (8 FTE's):

(i) Once RF rotation theory is developed and validated, perform time dependent simulations of existing discharges and ITER using a parallel framework - (4 FTE's).

(ii) Use parallel framework to couple the edge ICRF and LHRF wave solutions with gyrokinetic edge particle transport and stability codes (see coupling scheme in Fig. WP-2), in order to understand the interactions of RF with ELM's and to understand impurity generation from sheath interactions with the vessel - (4 FTE's).

4.H. Milestones:

g. Suggested high-level goals and milestones (perhaps at roughly the 2, 5, 10 and 15 year marks.)

Year 2:

EP Goal 1a: Demonstrate capability to simulated fast ion transport and redistribution using a reduced model analysis, both quasi-linear and PIC, on a slowing down time scale with sources and sinks of fast ions (no RF) and linear eigenmode solutions from NOVA.

EP Goal 1b: Begin validation of reduced models with experiment on DIII-D and NSTX.

EP Goal 2a: Demonstrate capability to simulate linear nonperturbative eigenmodes from NOVA-KN for inclusion in reduced models and validation of fully nonlinear codes.

EP Goal 2b: Begin verification of NOVA-KN eigenmode solver with linear mode structures generated using GYRO, M3D-K, GTC, TAEFL.

EP Goal 3a: Begin to simulate multiple Alfvénic instabilities using fully nonlinear codes (GYRO, M3D-K, GTC, GKM, TAEFL) for short durations, with realistic sources and sinks of fast ions, in order to assess whether unstable profiles will be strongly forced toward their marginal values.

EP Goal 3d: Begin verification of nonlinear code solvers on DIII-D reverse shear plasmas and on NSTX for avalanche events and transient dynamics.

RF Goal 1: Demonstrate capability to simulate linear 3-D ICRF and LHRF wave fields in the plasma edge.

RF Goal 2: Have coupled full-wave / Fokker Planck simulation capability in place to treat finite ion orbit width effects.

Year 5:

EP Goal 1a: Demonstrate capability to simulate fast ion transport and redistribution using a reduced model analysis, both quasi-linear and PIC, using nonperturbative kinetic eigenmode solvers like NOVA-KN. Continue validation effort with updated eigenmode solver.

EP Goal 1b: Integrate reduced model into TRANSP or other whole device simulation code for assessing effects of fast ion redistribution and loss on discharge evolution and vessel safety, particularly for ITER.

EP Goal 2a: Begin to simulate multiple Alfvénic instabilities using fully nonlinear codes (GYRO, M3D-K, GTC, GKM, TAEFL) for longer durations, approaching the slowing down time of the energetic particles, with accurate description of sources and sinks.

EP Goal 2b: Begin validation of fully nonlinear solvers against experiment on slowing down time scale.

RF Goal 1: Validate simulation capability for linear ICRF and LHRF wave coupling against experiment.

RF Goal 2: Validate simulation capability for core ICRF wave physics with finite ion orbit effects against experiment.

RF&EP Goal 3: Demonstrate capability to simulate coupling between EP sources and EP component (reduced models) by passing RF induced non-thermal ion distributions.

Year 10:

RF Goal 1: Validate capability to quantitatively simulate RF sheath effects against experiment.

RF Goal 2: Have closure scheme(s) formulated for including non-thermal ion distributions in MHD equations.

Year 15:

RF & EP Goal 1: Perform simulations of the coupling scheme in Fig. WP-2 using a self-consistent coupling between the EP sources and the EP component based on the closure relations formulated for the MHD equations.

RF Goal 2: Perform simulations of the coupling scheme in Fig. WP-2 using a self consistent coupling between the RF waves and plasma edge, which includes the effects of non-linear RF edge dissipation mechanisms in edge transport and stability codes.

5. DISRUPTION PREDICTION, AVOIDANCE, CONSEQUENCES AND MITIGATION

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5.A. Background and Motivation

During tokamak experimental operation, events that rapidly terminate the plasma discharge occasionally occur. The complete and rapid loss of thermal and magnetic energy in these disruptions results in large thermal and magnetic loads on the material wall. For proposed next step experiments such as the International Thermonuclear Experimental Reactor (ITER), the stored energy will be approximately 100 times greater than present day devices greatly increasing the potential damage of these events. Exacerbating the risk to the machine and increasing the engineering challenges, the disruption phenomena are often highly non-axisymmetric increasing the fluxes to the device.

This scientific driver aims to obtain an improved predictive capability for the onset of disruptions to aid in avoidance and in the development of algorithms for triggering disruption mitigation actuators, and to model the dynamics of mitigated and unmitigated disruptions in order to understand how to limit their effects. Achieving this goal would improve the viability of the tokamak as a practical energy source and enable the robust operation of tokamaks by allowing more aggressive operating regimes and by enabling faster recovery from off-normal events. The effects of disruptions include severe heat loads, JxB forces and run-away electron generation. The key scientific challenges include strongly nonlinear MHD, including kinetic effects, with large Lundquist number coupled to plasma pressure and current profile evolution; relativistic electron transport in stochastic magnetic fields; atomic physics; neutral and impurity transport; radiation transport; plasma wall interactions and an electromagnetic model of machine with its complex wall geometry, power supplies coils, control systems and diagnostics.

5.B. Goals for the Science Driver

The proposed science development roadmap was planned to enable the accurate prediction of 1) the onset of disruptions and how to avoid them, 2) the consequence of disruptions and how to mitigate those consequences. The specific questions that we wish to answer are:

1. How well can we predict the onset of a disruption and what strategies are available to avoid their occurrence?
2. How can we eliminate the instabilities that lead to the disruptions?
3. What are the effects of runaway electrons and what is the impact of operating regimes on their generation?
4. What is the impact of disruptions on the material wall, and how can we better design the first wall to handle the thermal loads?
5. What are the forces on the vacuum vessel and support forces during a disruption, and how do we improve their design?

6. How can we better design disruption mitigation systems?

Because the mechanism by which the plasma loses its energy to the wall involves long-wavelength instabilities and their nonlinear interaction, extended magnetohydrodynamics (MHD) is perhaps the dominant paradigm for answering many of the above questions. Because the extended MHD codes are less well-suited for exploring large areas of the vast parameter space and long time scales, "reduced models" are valuable to help answer these questions. For this reason, we plan on having two near-to-long term development campaigns oriented around integration efforts with whole device modeling (WDM) codes and with extended MHD codes. Because there are many unresolved physics issues in the WDM, extended MHD, material wall modeling, and models for impurity delivery systems, we will have a parallel development effort in the development of advanced components. The relationship of the physics campaigns with the development campaigns, and the needed integration that these development campaigns entail is shown schematically in Figure 1.

Summary of Integration Efforts		Development Campaigns		
Physics Campaigns		WDM Modeling	Extended MHD	
Onset Prediction and Avoidance	Transport events	Neutrals, radiation, impurities		Advanced Components
	Fast MHD Instabilities	Linear MHD codes	None	
	Slow MHD instabilites	Advanced components	Transport models	
	Feedback control	PCS	RF/MHD, PCS, 3D coil control	
Consequence Prediction and Mitigation	Runaway electrons	FP codes, reduced models	Limited FP, advanced components	
	Material wall	Material wall codes, sheath boundary conditions, neutrals, radiation		
	Structural forces	Simplified wall model codes	3D structural wall analysis codes	
	MGI, Pellel	Reduced models	Impurity delivery systems	

Figure 4. The relationship of the broad physics areas to the development campaign shows a multi-faceted approach for dealing with the problem of disruptions. Not shown are the many reduced models that are

likely to be needed for WDM-based development.

5.B.1. Disruption Onset Prediction and Avoidance

It will be desirable to operate in parameter regimes that are not prone to disruptions. The tokamak operating space is extremely large and varies according to the time profile of the activation of the many actuators, such as external neutral beam and RF sources, as well as intrinsic plasma properties such as transport, and the overall machine design. WDM codes are the most efficient means for exploring this parameter space, and are also used in interpreting the experiments, and setting up the inputs for the extended MHD, Fokker-Planck, RF, and gyrokinetic codes.

For purposes of avoidance of disruptions, the capability to predict imminent disruptions as far in advance as possible is needed. To do so, we need to simulate the plasma evolution leading up to disruptions, and the plasma response to our avoidance measures. This modeling must take into account the fact that it will never be possible to program tokamak discharges with 100% certainty -- there will be off-normal behavior of actuators, material flakes falling into the plasma, etc. Enabling this modeling capability will allow development of improved real-time capability to respond to such events appropriately. Fortunately, at reactor relevant parameters the profiles in the plasma will be changing relatively slowly. It will be desirable to have a real-time 3D equilibrium reconstruction capability that makes optimal use of current diagnostic information as well as concurrent WDM information to chart an appropriate set of actuator responses. Use of WDM information is important for modes such as RWMs, where the induced wall currents play an important role, and for locked modes, where the presence of a locked island may not be reflected in current diagnostic data.

5.B.2. Types of Disruptions

Disruptions due to ideal MHD instabilities, including external kink modes and VDEs, have been the most widely studied type of disruption. Because of the short time scales of the instabilities, these types of disruptions are considered the most dangerous because of the large sideways forces and heat fluxes generated. Ideal MHD codes have proven themselves useful for explaining many of signatures of ideal MHD instability boundaries within a factor of 10%. Due to the stiffness of the ideal MHD operator however, there is considerable sensitivity to the equilibrium, including the numerical representation of the equilibrium. To overcome this, uncertainty quantification methods for equilibria generation need to be more robustly developed. The sensitivity to the equilibrium will place a premium on the development of accurate WDM codes, and on the development of more accurate equilibrium reconstruction methods, including information from WDM codes and information from any diagnostic indicating the presence of nonaxisymmetric field perturbations. It is desirable to translate the sensitivity of the ideal instability boundary to a safety margin for operation to avoid disruption. This safety margin should be extensively tested against experimental data.

Slow macroscopic instabilities such as neoclassical tearing modes (NTMs) and resistive wall modes (RWMs) may also trigger disruptions. These modes evolve through a sequence of 3D equilibria, with the time evolution determined by transport, including flux diffusion. Because of the long time scale evolution of these modes, with saturated instabilities existing on the second time scale before disrupting, the modeling of these instabilities is extremely challenging and not amenable to large parameter studies with extended MHD codes or with current WDM codes. The evolution of these modes could be followed by a WDM code with 3D equilibria and with kinetic and flow effects included. No such code exists at present. Although the development of new components for this purpose over the long term will be desirable, significant progress in developing a simulation capability for these modes could be made in the near term by the integration of existing codes. In those cases where the disruption is triggered by a slow macroscopic instability that has been present for some time, it will be desirable to initialize the extended MHD calculation with a 3D equilibrium. For that purpose, it will be necessary to couple the extended MHD codes to 3D equilibria, and to 2.5D codes. It is also expected that the baseline and SciDAC program will also contribute to improvements in the extended MHD, and that the FSP will be able to leverage these improvements for more accurate modeling of disruptions caused by these slow growing modes.

Many of the basic features of transport-induced disruption events are well understood and the basic development needed for modeling is understood including transport models, impurity and radiation transport, and bootstrap current generation. However, the disruptions can be difficult to model due to the strong nonlinear interactions and steep pressure and current gradients that often arise. More modeling and validation efforts in these difficult regimes are strongly needed.

5.B.3. Feedback Control

Feedback control is not practical for instabilities that grow on an Alfven timescale, but has been demonstrated for slow macroscopic instabilities. If robust detection of disruption precursors is possible, then feedback control can be used in some cases to suppress or avoid the instabilities, enabling a larger operating regime. For example, feedback control using externally applied magnetic fields from coils has been successfully used to stabilize the vertical instability and RWMs. Feedback control using radiofrequency (RF) waves has successfully been used to stabilize NTMs, sawtooth instabilities, and even to affect ELM behavior. Real-time control of all systems including plasma instabilities is done by a Plasma Control System (PCS), which in the case of ITER will make use of specialized WDM codes for verification of algorithm performance and implementation. The inclusion of synthetic diagnostics in MHD models could provide previously unavailable means of optimizing the identification of disruption precursors and the triggering of feedback actuators or as discussed below, disruption mitigation actuators. Note that conventional disruption precursors indicate the presence of nonaxisymmetric components of the magnetic field, so that 3D equilibrium reconstruction becomes desirable when precursors are detected.

Disruptions are ultimately the result of crossing a plasma stability boundary into an uncontrollable region of operation. The transition to uncontrollability can occur because of poor (or intentional use of) nominal control, or can be produced by a failure of hardware or other tokamak systems. Operating with high reliability and low disruptivity is fundamentally a controllability and control robustness problem, since avoidance and many effects mitigation actions must be decided and directed by real-time control algorithms being executed by the PCS. Key among these algorithms are methods for real-time forecasting of potential or unavoidably impending disruptive plasma states. For example, given the present state and expected evolution of the plasma, the time until a given NTM becomes metastable should be predicted in real-time. To respond to and minimize the impact of tokamak system faults (e.g. hardware failures), these systems should also be monitored and their health forecasted to a reasonable degree. For example, this forecasting mission typically involves monitoring such system characteristics as the local heating and field amplitude states within superconducting coils, and thus likely falls outside the scope of FSP.

In order to provide quantifiably high confidence in low disruptivity operation, a real-time disruption prediction system must include high accuracy reconstruction of the present plasma state, determination of that state's proximity to relevant stability boundaries, and a look-ahead, or forecasting capability for probable disruption onset. Forecasting generally includes direct projection based on algorithms such as neural nets or extrapolation in time with a linear response model, or actual faster-than-real-time simulation (FRTS). The former requirement can often be provided with simplified models derived from complex FSP components. The latter is often envisioned as a form of WDM configured for FRTS execution. FRTS forecasters will likely operate by being reinitialized or state-corrected at periodic intervals to incorporate accumulated diagnostic knowledge in real-time. All of these computational algorithms must be able to execute in real-time rapidly enough to provide reconstruction, stability boundary assessment, and prediction of disruption onset sufficiently before a controllability boundary is crossed to allow the proper control action. For example, detection of a growing NTM island may provide less than a second of time before it reaches a potentially disruptive saturated amplitude in ITER, while a corrective action such as reducing the plasma beta will require a confinement time of several seconds. Prediction of impending NTM instability prior to crossing of the stability boundary may provide sufficient time to respond by lowering beta. On the other hand, direct detection of NTM growth may provide enough time for enabling and aligning ECCD deposition with the appropriate resonant surface to stabilize the mode. Navigating these kinds of decision trees and executing the necessary control action will require sophisticated control algorithms.

The final goal of the Disruption Science Driver in the area of control for disruption prediction/avoidance is development of tools for verification of performance and implementation of control algorithms. As will be the case with nominal scenario real-time PCS control algorithms, the complex algorithms required to traverse the disruption decision trees will themselves require verification of performance and implementation using WDM codes capable of simulating off-normal and disruptive events. These WDM codes must be capable of running offline to verify performance of the algorithms, and must also be interoperable with real-time software (perhaps hardware) to enable verification of the actual implementation of real-time algorithms prior to operational use.

5.B.4. Consequence predictions and mitigations.

If disruptions due occur, then studying the consequences of disruptions would enable more robust designs of machines that are able to withstand disruptions. We break the consequences further into 3 areas: 1) runaway electrons, 2) material wall interactions, and 3) structural materials. We note that the danger of runaway electrons is their damage to the material walls, and that their currents contribute to the large structural forces; however, the specific challenges of understanding this phenomena is great enough to call out as a separate challenge. Finally, in addition to designing better machines for withstanding disruptions, active mitigation techniques have been experimentally developed and improving these techniques is an important part of this effort.

5.B.5. Runaway electrons

The strong electric fields generated by a disruption can accelerate electrons to relativistic energies, called runaway electrons that have dangerous consequences for the integrity of the machine. A complete model of these effects is quite difficult because of the need to model relativistic electrons in a stochastic magnetic field. Because the currents generated by the runaway electrons are significant, self-consistency between the electron transport and magnetic field is needed for a complete description. The difficult of this problem means that a hierarchy of models is needed as well as significant theoretical developments of mathematical formulation enabling numerical approaches for solving this problem.

Runaway electrons have been modeled in several ways. One model is use a model equation for the evolution of the runaway electron current within a WDM code with the runaway electron current acting as a source in the Ohm's law. Another model is to use the Fokker-Planck code CQL3D with crude models for radial transport due to stochastic field but a complete model of electron equations of motion. The final method is to integrate a simplified electrons equation of motion in extended MHD code with three-dimensional magnetic fields and no feedback of these electrons on the MHD dynamics. F-P codes require the input of an Ohmic electric field, which is typically calculated from a simple Ohm's law. A more sophisticated model would require coupling with an MHD/transport code with a self-consistent Ohm's law taking into account the energetic electron population. In the near term, theoretical development is required to produce a computationally tractable model for runaway electron feedback onto the MHD equations similar to that used for energetic ions. These models would take magnetic fields from MHD simulations for use in the Fokker-Plank codes. On a similar time scale, development could start on developing models suitable for integrating runaway electron modeling into transport codes through parameterization of magnetic fields for various disruption scenarios. Other reduced models are possible (e.g., Zakharov's Kadomtsev-Pogutse shell model extensions). For the longer term, it will be necessary to solve for the distribution function of runaway electrons in 5D space using the drift kinetic equation (DKE) and to integrate this into other elements of the calculation.

5.B.6. Plasma Material Interactions

As the disruption progresses, the entire plasma energy is deposited onto the material walls in a sub-second time scale. This represents orders of magnitudes larger increases in heat flux than the steady-state operation of tokamaks due to the short time scale and because of toroidal localization of the forces and heat loads. In current devices, this can result in extremely large plasma outgassing, dust generation, and wall ablation. For ITER, these issues are even more dangerous with difficult-to-predict implications for tritium retention, wall integrity, and subsequent shot performance if the machine does survive a disruption. Modeling of the plasma wall interactions is a significant issue even in steady-state, and the focus of another FSP science driver, but for disruptions the issues are significantly larger due to the higher heat fluxes.

The extended MHD codes have primitive wall interfaces compared what is available in the edge community and the most developed PMI model, HEIGHTS, which has less sophisticated fluid codes. To begin bridging the gap, a collaboration between the WDM and extended MHD communities with the boundary physics community is needed to implement sheath boundary conditions and reduced wall models, developed as part of the boundary physics science driver, into the disruption codes and verify the implementation. At the same time, wall models to improve/verify their plasma-wall physics would use fluxes from MHD simulations. In the longer term more complete integration of these models would be carried out. Many detailed physics issues, for example, implementation of "kinetic boundary conditions" have similarity to developments needed by the edge transport community.

Even during a disruption, while the plasma still has significant energy, the plasma can interact with the wall and inject impurities into the plasma. The subsequent impurity transport and radiation losses can have a significant impact on the disruption evolution, thus modeling of disruptions with WDM or extended MHD codes requires the ability to model neutral, impurity, and radiation transport. Integration of MHD with models for impurity radiation and transport are necessary to calculate heat loads from the thermal quench and to simulate runaway electron mitigation. A first step would be to create standardized libraries for the relevant atomic physics cross-sections with a uniform API for use by MHD and PMI codes. This should be a cross-cutting area useful to several science drivers. Standardized verification and validation cases will need to be developed in collaboration with members of the edge community and experimental teams.

5.B.7. Structural walls

Interactions between a disrupting plasma and a structural wall will involve mass, thermal energy, magnetic energy, and momentum. The material wall codes will provide information on the interactions of mass and thermal energy. The interactions through magnetic energy and momentum will need additional information, including the geometry and material properties of structural components. In general, many MHD-like dynamics perturb magnetic fields at the location of structural components. The shape of structural components and their electrical conductivity influence the path and diffusion of eddy currents. Besides the direct response of eddy currents of the same harmonic content as the MHD perturbation, asymmetric structures will induce other harmonics that will feedback on the plasma, possibly through further changes to stability or through changes to magnetic topology and its influence on transport. If the plasma is rotating, the interaction will also induce torques. Many studies of plasma rotation and locking due to magnetic perturbations emphasize the importance of torques from error fields and from magnetic perturbations that penetrate imperfect conductors. Magnetic field that has both a normal component and a tangential component along a surface admit a tangential force. If the surface is not toroidally symmetric, its surface normal direction will have a toroidal component, so magnetic pressures will also lead to torques on the plasma. Efforts have begun in calculating these forces with simplified wall models, but improving the accuracy of these models, especially for complicated walls like that of ITER, is needed.

Active Disruption Mitigation

While every effort will be made to avoid the parameter regimes that lead to disruptions on large reactor-scale devices, it is considered essential to have a realistic and reliable strategy for detecting the conditions leading to disruptions and either stabilizing them as discussed earlier, or actively mitigating the effects of disruptions when they do occur. Having the plasma deposit its energy to the wall via radiation instead of heat conduction is preferable as it would result in more evenly-distributed heat loads. To enable this, rapid and large injections of impurities upon the detection of a disruption precursor has successfully been used mitigate the effects of disruptions. Modeling of these effects also requires neutral, impurity, and radiation transport as well as models for the impurity delivery systems such as gas injection systems or pellet injection. Standard physics-based models for penetration/ablation of impurities given fixed plasma profiles should be developed (at least in 1D or ideally 3D). Integration into MHD codes would require the models to respond to profile changes that can occur ahead of the pellet/jet front due to MHD-related changes in transport. A serious concern with using gas or pellet injection for disruption mitigation is the possibility of runaway avalanche due to large-angle "knock-on" collisions between runaway seed electrons and thermal electrons. Theoretically, density increase above the Rosenbluth limit would suppress the runaway avalanche. Quantitative modeling of the density increase from gas or pellet injection could be integrated with CQL3D, which has the "knock-on" avalanche physics, to evaluate the efficacies of the various proposed disruption mitigation techniques.

5.C. Components

5.C.1. Functional requirements for components

As discussed in Section B, two primary development paths are planned organized around whole-device modeling-based models and extended MHD-based models. At this level, the distinction between components and frameworks can become blurred due to the types of coupling (in-memory/file-based) and how the underlying code is developed. Here, we treat WDM and extended MHD codes as components although the integration with other codes might require a very tight coupling. This is discussed further in the frameworks section.

5.C.2. WDM component

WDM codes have successfully been used for modeling many features of disruptions caused by VDEs. By including models for the non-axisymmetric factors, large areas of parameter space can be explored. Because of the dynamic nature of disruptions, the key features of WDM codes used for disruption control are accurate modeling of free boundary equilibrium along with current evolution equations and plasma control systems. The integration of WDM codes with 3D equilibrium codes might also require substantial upgrades due to different interfaces required.

5.C.3. Linear MHD component

Linear ideal MHD codes have proven to be useful in explaining many features of fast MHD phenomena including external and internal kinks, and peeling-ballooning modes. Because the codes can be run relatively quickly, they are a key component in exploring stability regimes in predictive simulations. Key to understanding their usage however is their sensitivity to the underlying equilibrium. Because of the stiffness of the ideal MHD operator, the resultant stability is sensitive to slight perturbations of the equilibrium. For this reason, the spatial requirements for the equilibria in the WDM codes are greatly increased to obtain converged solutions. This step can be done by recalculating the equilibrium on a refined mesh and using this as input to the linear MHD codes. Also, to help with the uncertainty quantification, creating a "cloud" of equilibria is needed to understand the proximity to the ideal stability boundaries.

For slow MHD modes such as NTMs, linear codes have been less useful for predictive capabilities. This is due to the lack of such codes (with PEST-III and MARS being the only available), the nonlinear onset mechanisms that are often experimentally observed, and in the lack of linear codes which take into account the additional physics known to be important such as energetic particles, two fluid effects, and Landau damping. To some degree, it is possible to use the extended MHD codes as linear instability codes which enables the significant investments into their development to be leveraged for accurate exploration of parameter space. Extensive development validation is required for their reliable use within WDM codes however.

5.C.4. Three-dimension equilibria component

A 3D equilibrium code is needed as a component for constructing a 2.5D WDM code, and also for 3D equilibrium reconstruction. Tokamak equilibria typically have multiple rational surfaces with low mode numbers, and this implies that a 3D equilibrium code for tokamaks must be capable of handling islands and stochastic regions. A 2.5D code will use a set of transport equations to calculate the time evolution of the pressure and current profiles, and it is necessary that the 3D equilibrium code be capable of solving for equilibria having specified pressure and current profiles on the good flux surfaces as well as the interior of the large islands.

The code must be able to handle free-boundary equilibria. That is, it must be able to solve for a 3D equilibrium with the boundary condition that the magnetic field goes to zero at infinity, and with coils specified outside the plasma. The code must be able to handle realistic coils. The boundary of the plasma will be determined by the presence of a limiter or divertor, and the code must be able to handle both cases. The Pfirsch-Schlüter currents may exhibit local structure in the neighborhood of magnetic islands, and this localized structure can play an important role in determining island widths. The code must demonstrate a capability to resolve this structure. Finally it will be desirable to incorporate kinetic and flow effects in the equilibrium solution. It will be desirable to have a path forward to incorporate these effects through coupling with existing codes rather than through a massive development effort.

5.C.5. External Source (RF and neutral beam) components

The modeling of the RF and neutral beam sources is an important part of controlling the plasma to operate in the desired operating regimes. A complete description of how these components are used includes their integration with the Fokker-Planck codes (described below) and the Plasma Control System (PCS) as well as the various models. This integration is described further by the WDM and energetic particle Science Drivers. Of particular interest is the implication of these components beyond the typical transport modeling that is needed for disruption modeling. The neutral beam and RF sources are able to produce energetic ion distribution functions that have a dramatic effect on the stability of the plasmas. To calculate this energetic particle distrubition function, Fokker-Planck components are used and are discussed in the next section.

The electron cyclotron radiofrequency (ECRF) sources are distinguished by other sources by their slight modifications to the electron distribution function and the localized currents that they generate. The spatial localization enables their use for the alteration of the stability boundaries for instabilities that are sensitive to the magnetic shear and for stabilizing tearing modes that have already begun their relatively slow growth. The modeling of this type of stabilization requires integration with the extended MHD codes as well as integration with PCS models.

5.C.6. Fokker-Planck component

Fokker-Planck codes are critical for modeling the deposition of energetic particles and RF power into the thermal plasma and are extensively used in other science drivers. Accurate modeling of the linear stability boundary frequently requires the accurate calculation of the ion distribution function and the accurate conveyance of this information to both linear stability codes (e.g., NOVA-K) and extended MHD codes that have the energetic ion closure. Because the stability depends on the derivatives of the distribution function rather than moments of the distribution function as needed for transport code, the accurate conveyance of this information is still an open research topic due to weaknesses in the underlying components and mathematical issues in the coupling of discrete codes to continuum stability codes.

For the study of disruptions, F-P codes are also used for studying runway electrons due to the accurate electron equations of motion for runaway electrons include relativistic effects and "knockon electron" source terms as described previously. The only code at present that includes the complete equations of motion for accurate velocity space dependence, CQL3D, is only one-dimension spatially and includes reduced models for the transport due to stochastic fields. Despite the limitations of the magnetic field transport model, this code has been extensively used for modeling the effects of runaway electrons and has successfully explained many features of the experiment.

5.C.7. Plasma Feedback (PF) component

Design of control algorithms to execute the appropriate control actions requires models of relevant plasma and system responses (which may be simplified models derived from complex

FSP components), and the ability to verify the performance of the resulting algorithms (which typically requires WDM simulations interoperable with design codes and ultimately with real-time PCS code). Detection of a potentially disruptive event, or prediction of high probability of disruption in the near future will force a choice among actions such as active mode suppression, switching to an alternate operating state, recovering the original operating state, or proceeding to rapid shutdown. The models needed for design of the controllers for navigation of the decision tree and execution of the complex actions along the way are envisioned as key results of FSP under the disruption science driver. An example of such models is a computational description of how the plasma burn state will respond to various proposed burn control actuators, including edge impurity puffing, fueling regulation, active regulation of NTM island size, non-axisymmetric applied fields, and auxiliary heating systems. We envision that the FSP will develop a component to encapsulate the algorithms and allow these algorithms to be used by multiple codes to avoid redundant coding and common development of algorithms. The relationship of the FSP-develop PF components and the new PCS systems being developed for ITER remains to be determined.

5.C.8. Extended MHD component

Considerable development has been invested in the magnetohydrodynamic codes under the Center for Extended Magnetohydrodynamic Modeling (CEMM). The key requirements for an extended MHD component may be summarized as follows:

1. Even for fast instabilities such as VDEs and ELMs, implicit methods are required for overcoming the time step limitations of the MHD waves, and for slow-growing NTM simulations these methods are critical. The two-fluid terms add dispersive terms that make implicit methods more difficult to implement, but even more critical to resolve.

2. Implementation of an anisotropic heat conduction model is critical for obtain many of the important questions for disruptions such as energy confinement times. To study anisotropic heat conduction in non-symmetric fields, including fields that are fully stochastic, requires the use of high-order spatial discretization schemes. Although grids aligned with the zeroth-order magnetic fields help reduce the grid requirements, it is not a requirement as it is with second-order methods such as those used by the edge transport codes.

3. An axisymmetric thin resistive wall model is the minimally required model for obtaining qualitative agreement with the experiments for VDE-induced disruptions. This model is currently the state-of-the-art in calculating the forces due to the disruptions.

4. Quantitative modeling for many modes requires a sophisticated closure treatment, including integration with sources of non-Maxwelling distributions functions such as those from RF and neutral beams.

Each of the areas listed above represents an area that is still under active research by the base theory and SciDAC communities. Production level codes that have achieved most of the above requirements are expected to be the primary base for the FSP.

5.C.9. PMI codes

The integration of PMI codes with WDM codes requires the same development as required for the boundary SD. As part of the integration efforts in the integration of core/edge/wall tranport has been the development of the WallPSI code for implementation as a wall component. This component implementation has the advantage of being relatively simple, fast, and easy to implement.

A complete discussion of the variety of codes available for modeling plasma-material wall interactions are beyond the scope of this science driver given that they are extensively discussed in the Boundary Science Driver. Of greatest relevance to the discussion for Disruption SD is the HEIGHTS package that has already been used to model the effects of disruptions on the material walls including the nonlinear effects of ablation on subsequent plasma behavior. The MHD codes used in this integration effort do not have the level of physics fidelity of the extended MHD codes considered in the next section, but offer a solid basis for the FSP integration efforts.

5.C.10. Plans for legacy components and Development of advanced components

As discussed in previous sections, we plan to have a range of physics models of varying physics fidelities. Even our best simulations at present lack the level of physics fidelity that we desire. Our goal is to reuse the existing components to the extent possible to exploit the advantages of integration in exploring new physics. Where needed, we will also investigate the development of new components that will enable a new level of physics fidelity and quantitative predictions.

5.C.11. Summary of components status and needs

The upgrade for the components is motivated by the needs for integration so most of the requirements are discussed in that context. Here we summarize the results of those discussions, with the notable exception of the extended MHD codes which have requirements not easily summarized, and the new codes which are discussed next.

Component	Development required
WDM – 2D equilibrium	Robust, free-boundary equilibrium for extended MHD codes. Ability to refine and perturb equilibrium for linear MHD
F-P codes	Ability to easily take in magnetic perturbations from other codes. Provide high-resolution distribution functions for

	accurate MHD stability analysis
Plasma Feedback Component	New component that needs to be developed.
External sources	Work with F-P code. ECRF codes need to interact with extended MHD codes

Table 1. Summary of components and likely upgrades required for the planned disruption studies

Extended MHD codes

The extended MHD codes have made significant progress in understanding the numerical requirements needed for advancing the two-fluid model in simulations extending from the core to the wall. As the simulations are run for longer times, and for a wider range of applications, effects that were relatively unimportant become increasingly important.

In the modeling of disruptions, current simulations rely on relatively simple boundary conditions, both for the magnetic boundary conditions at the vacuum vessel, and the plasma (density, momentum, thermal energy) boundary conditions at the material wall. As discussed in the section on integration, plans for improving the models for interaction these boundary conditions is an important part of this effort. For the integration of the material wall, not only are incoming fluxes for the bulk plasma species is needed, but the influx of impurities and neutrals is needed as well to explain many of the observed features such as the amount of energy loss due to radiation. Although the two-dimensional edge transport codes have had such physics, the three-dimensional extended MHD codes have not and will need to be upgraded for the proper integration to take place.

For slow saturated modes such as NTMs or RWMs, the modes evolve on a transport time scale and as the capability to include sources and transport models for these time scales increasingly become important. For ECRF stabilization of NTMs, the localized source causes a movement of the rational surface, which requires a complete description of transport processes, and a way of controlling the ECRF sources in the same way as the experiments is required.

5.C.12. Development of new components

Impurity delivery systems

Current models of gas jet injection are fairly simplistic and while more complicated models for pellet and gas jet deliver exist (P. Parks) they are difficult to implement. More tractable models will need to be developed and verified. Calculations for gas mitigation may require integration with standard CFD (computational fluid dynamics) codes. At present, the current models are hard-coded into individual codes. A needed step is to abstract these models and provide an individual component that other codes can reuse. As this development takes place, the possibilities of more accurate modeling can be investigated.

Advanced kinetic/MHD hybrids

Other FSP science drivers expect further improvements in fundamental plasma and wall models as part of the base theory and computation programs and. This raises the question whether there is something about the physics of disruptions that requires more accurate models. For example:

- Will electron transport in a stochastic field be well-described by the drift-kinetic equations (DKE)?
- Will ion transport in a stochastic field be well-described by DKE? (Because of orbit size, this is more problematic, especially for energetic particles).
- What is the best model for disruptions beyond an extend MHD model? For example will it be necessary to develop a kinetic-MHD hybrid code.

The issues are quite detailed and are still under considerable development by the theory community. We expect this part of the disruption plans to evolve as the FSP planning progresses, and that validation will further illuminate the need for better theoretical and code development in this area.

5.D. Framework Requirements

5.D.1. WDM Framework requirements

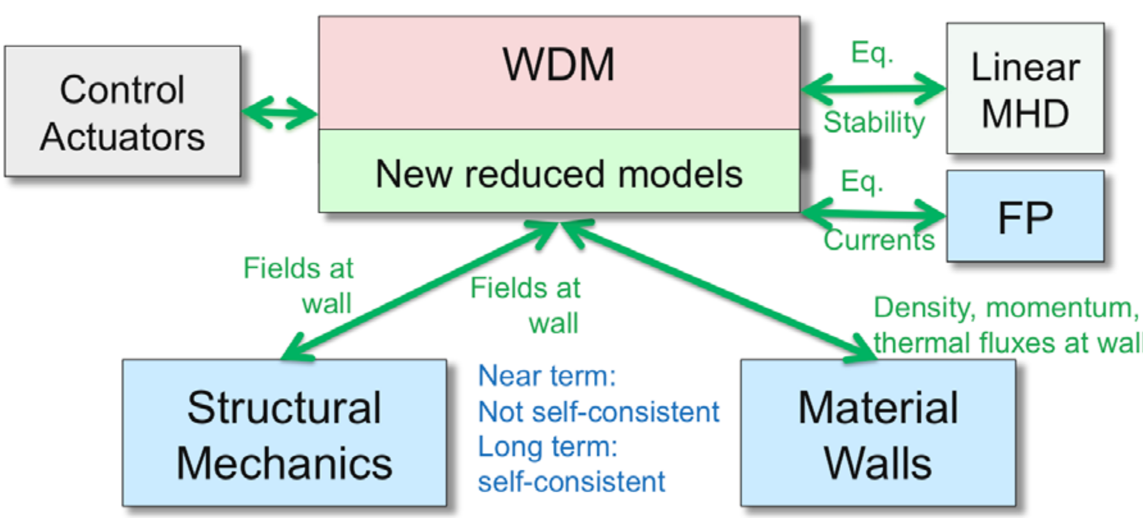

Figure 5. Schematic showing the integration planned for the WDM-based integration plans.

In the context of disruption control, whole device modeling has the following requirements:

1) In order to develop operating scenarios with a relatively low risk of disruptions, WDM require the capability to predict imminent disruptions hence the ability to simulate the plasma evolution leading up to disruptions, and to simulate the response of the plasma to our avoidance measures.
2) In order to accurately calculate the nonlinear evolution of unmitigated and mitigated disruptions, accurate calculations the initial conditions at the onset of the disruption are needed.
3) Validation efforts require the ability to use WDM codes in analysis mode, including accurate equilibrium reconstruction.
4) Non-axisymmetric effects for slow MHD events such as RWM sand NTMs are required. Inclusion of these effects can be either due to reduced models or components for calculating three-dimensional equilibria.
5) Reduced models that capture the bulk nonlinear effects would be beneficial for performing large parameter studies for scenario development, and for modeling regimes that are difficult to model with extended MHD codes.
6) In those cases where macroscopic instabilities lead to transient events rather than to disruptions, restarting the simulation in the post-relaxation phase, either via a reduced model of the non-axisymmetric evolution or via restart from an extended MHD code is needed.
7) Given models for the non-axisymmetric flux deposition onto the wall, calculation of the impacts on material properties of the wall, and the subsequent interaction of impurities and plasma fueling on plasma behavior, including behavior of subsequent discharges, is of critical importance. These issues overlap extensively with the goals of the Boundary Science Driver with the exception that the fluxes during a disruption are much higher.

Because the Grad-Hogan equations are an averaged form of the MHD equations, many similarities between the two development plans exist. However, because disruptions are a three-dimensional phenomena, any use and development of a whole-device models requires extensive development of reduced models, and many caveats for its use in modeling disruptions. We expect the greatest use of the WDM-developments to be in the use of onset prediction that is needed for understanding the tokamak operating space; however, because the extended MHD codes have difficult simulating all the way into the current quench regime, we expect that WDM developments also play a role in the studying of disruption consequences.

5.D.2. Integration of linear MHD codes

Approximately 10 codes exist in the community that is eligible for use as linear instability components for integration with WDM codes. All of these codes take the MHD equilibria as their input. The mechanism for transferring the data from the equilibrium codes is currently done via files using a "mapping code"; i.e., the general structure is:

[GS Code] $\Rightarrow$ [Mapping code] $\Rightarrow$ [MHD Code]

Because the MHD perturbations are small compared to the terms in the MHD equilibria, small errors in the GS code and in the mapping code can cause substantial error in the solutions of the MHD solution. For this reason, the equilibria that are used in inputs for the MHD codes are usually recomputed on a much finer grid. In addition, because of the stiffness of the ideal MHD operator, the linear solutions are sensitive to unknowns in the underlying equilibrium. To ameliorate these issues, a statistical approach to the equilibrium is needed to quantify all of the uncertainties associated with the linear stability. Because the vast majority of these codes assume that the equilibrium is axisymmetric, the instability of each toroidal mode number (from a Fourier decomposition) is independent of other toroidal mode numbers. Thus, calculating the complete instability boundary requires a set of trivially decomposed computational tasks for each generated equilibrium. By creating a "cloud" of equilibria, a statistical assessment of the stability boundary may be ascertained given sufficient number of computational resources.

In addition to requiring the MHD equilibrium as an input, some linear MHD codes are able to use information on the energetic particle distribution as inputs. In this model, the energetic particles are treated as a separate ion species and the modifications to the stability boundary occur because of modifications to the momentum force balance equations. Because the stability effects are sensitive to derivatives in velocity space of the distribution functions, the accuracy requirements for MHD stability on the Fokker-Planck components are generally much more stringent than a typical transport calculation which requires only velocity and spatial moments of the distribution function. There is also a significant difference in the numerical accuracy of the coupling depending on whether the F-P codes are Monte-Carlo based, or whether they are continuum based. Because of the increased accuracy requirements, any development of a new F-P code should take into account the best mechanisms for coupling to the linear MHD codes.

5.D.3. Integration of Fokker-Planck codes

There are a number of Fokker-Planck codes within the fusion community that have large user communities based on the particular strengths that the code has. For example, NUBEAM has a large user community because it has the best ionization sources as well as the most accurate modeling of the slowing down physics. CQL3D has found wide usage for modeling of electrons, and for ions where its speed and accurate RF physics is valued over its less accurate neutral beam sources and ion equations of motion.

For disruption modeling, CQL3D's accurate equations of motion for the modeling of runaway electrons are a critical feature. CQL3D has already been integrated with WDM codes using the SWIM IPS framework. In this coupling, CQL3D has been used to study runaway electron generation during startup in addition to more typical use in the modeling of the RF deposition. This coupling was performed as an explicit, file-based coupling. Because of the relatively long time scales of the slowing down time compared to the evolution of the underlying plasma equilibrium, this coupling seems adequate for the couplings envisioned in this science driver.

5.D.4. Integration of Material wall codes

Integration of material wall codes with edge transport codes has occurred to varying degrees over the past 10 years but is not routinely used for analysis of fusion experiments. For WDM modeling, the integration of the WallPSI component with UEDGE edge component using the FACETS framework provides an instructive look at the issues with the coupling. Because the goal of transport modeling is to perform long time scale simulations, an implicit coupling mechanism is needed to obtain accurate, self-consistent fluxes between the edge and wall components. WallPSI is a serial code that models the wall as a 1 dimensional domain with that domain being into the wall; thus, each wall segment is functionally independent of the neighboring wall segment. Because WallPSI is a serial code, this enables the framework to treat each wall segment as trivially parallelized code. This technique is currently being planned for transport modeling, and can easily be used for reduced-model WDM disruption simulations. The method is relatively trivially parallelized to three-dimensions as well.

The material wall codes in the HEIGHTS package are more complex and sophisticated in their treatment of the material wall including detailed modeling of coolant channels, and wall geometry. Because this sophisticated modeling does not make the independent wall segment approximation of WallPSI, the interfaces and mechanism for coupling to the plasma physics codes will have to be generalized. Because of the complexity of this coupling, in the near term only a loose coupling is envisioned whereby more accurate flux distributions can be used as inputs into studying the impact

5.D.5. Integration with Plasma Feedback Component

As discussed in Section C.1.f**,** the Plasma Control System's used in experiments can be quite complex requiring their own verification and validation efforts. The complexity of the systems and that many of PCS components are written in MATLAB hinders a close integration with most WDM codes. An alternative approach is to enable the PCS system to control the WDM code. This approach has been done with the CORSICA code for example. To date, the development of simplified versions of these systems, which we denote as PF components, have been performed as one-off developments with no encapsulation of efforts. To facilitate V&V activities and the integration with newly-developed PCS systems, the FSP should develop a standalone component and have it integrated with WDM and extended MHD codes.

5.D.6. Integration with Three-dimensional equilibria codes

The evolution of NTMs and RWMs is sufficiently slow that the inertia term in the momentum equation can be neglected. The long time scales on which these instabilities grow, and the fact that saturated instabilities can persist for substantial periods of time, pose a great challenge to codes that retain the inertial term. (One "hybrid" scenario being proposed by the DIII-D group for ITER has a persistent 3/2 NTM as a required feature.) High performance experiments will run 100 times longer than those in current devices. The substitution of a 3D equilibrium solver in the 1.5D algorithm for the simulation of slow macroscopic instabilities would enable long time scale simulations of the effect of non-axisymmetric effects. Such codes are sometimes called "2.5D" codes. A 2.5 code has been developed previously as using the VMEC code, solving flux-surface-averaged equations for the flux diffusion. This was the first code of this type to use a 3D equilibrium solver, although the VMEC code does assume nested flux surfaces, and therefore cannot be used for NTMs.

Another relevant development was the work of Edery et al on magnetic island growth. Although their calculation was analytical, they showed that it is possible to monitor the magnitude of the neglected inertial term in the momentum equation when solving for the slow evolution of a magnetic island. In this way, they determined the narrow regions where the approximation brakes down, and constructed a boundary layer solution in those regions. This work is relevant to WDM modeling in that the same method can be used to monitor the magnitude of the neglected inertial term in 2.5D codes, with a transition to an extended MHD code becoming necessary when the term does become non-negligible. Slow macroscopic instabilities could be simulated using a 2.5D code, but magnetic islands, kinetic and flow effects need to be included. No such code presently exists, but considerable progress in the development of such a simulation capability could be made by the integration of existing codes.

The existing 2.5D WDM code can provide the needed framework, to be supplemented by integration with other existing components. The VMEC equilibrium code, which assumes good flux surfaces, must be replaced by a 3D equilibrium code that can handle magnetic islands and stochastic regions. Kinetic and flow effects would be incorporated by integration with a neoclassical gyrokinetic code, which would be used to intermittently calculate corrections to the component of the current perpendicular to the magnetic field from the particle drift trajectories. Incorporating a more complete set of flux-surface-averaged transport equations from a 1.5D code could make further improvement.

5.E. Extended MHD Framework Requirements

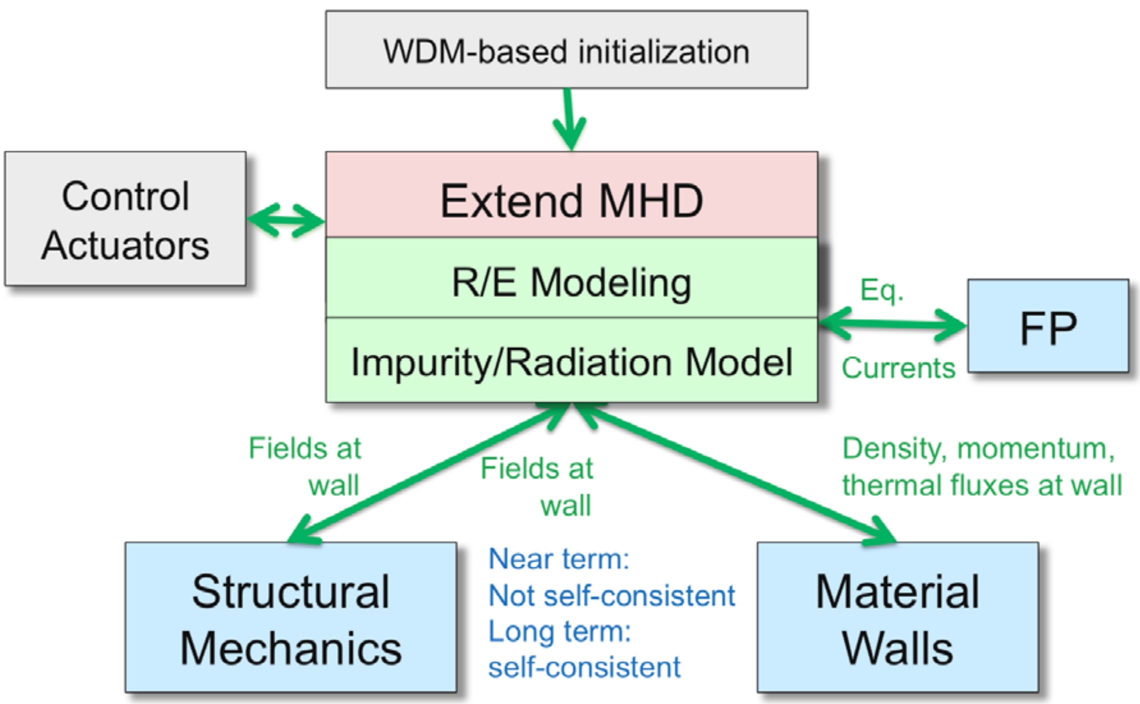

Figure 6. Schematic showing the integration planned for the extended MHD-based integration plans.

Extended MHD modeling has the following requirements:

1) For fast MHD instabilities, develop validated predictive understanding of their onset, and the conditions under which they cause a full disruption.
2) For slow MHD instabilities, understand the conditions by which such modes arise, how they evolve, how they can be controlled, and the conditions under which they lead to full disruption.
3) Allow calculation of structure forces from simple models using axisymmetric, thin-wall approximation of resistive walls to more complete detailed models of experimental structures.
4) Calculate the effects of disruptions on material walls, and the results of plasma – material wall interaction on the subsequent evolution and disruption behavior.
5) Understand how the role of runaway electrons on the nonlinear evolution of disruptions.

5.E.1. Integration with actuators

Extended MHD codes have traditionally used extremely simplified models for sources with the most common being sources designed to the solutions in perfect steady state. Because most extended MHD simulation occurred on the 10 msec time scale, the details of the sources profiles are not important for studying the details of the instability dynamics. As the extended MHD codes run for longer time scales, more accurate modeling of the sources, and including sub-grid models for the small scale turbulence increases in importance.

Integration of feedback control is also likely to be important in the quantitative calculation of VDE instability dynamics. Because modern experiments operate in a regime where the plasma is often stabilized by the plasma control system, inclusion of a stabilization method is required for free-boundary transport simulations, or in the understanding of how the VDE becomes unstable in extended MHD. There is also some experimental evidence that the PCS can make the disruption actually work and inclusion of this must be included when modeling VDEs.

This modeling is especially important for simulations of electron cyclotron radiofrequency (ECRF) stabilization of NTMs. Because these modes grow and saturate on a 100 msec ime scale, accurate modeling of the source and transport becomes increasingly important. In addition, because the ECRF source modifies the electron cyclotron distribution function, including the RF sources in a manner consistent with the closure calculations required for the neoclassical tearing mode physics. Also, because the RF source modifies the location of the rational surface, quantitative simulations of ECRF stabilization requires a model for feedback control of the RF source based on detection of the MHD mode.

5.E.2. Integration of Fokker-Planck codes

The accurate calculation of runaway electron transport in the presence of MHD fluctuations requires two inputs from Fokker-Planck codes: an energy distribution that can be used to generate an appropriate test population for orbit integration, and a time-dependent runaway electron current distribution that can be incorporated into the MHD equations. The Fokker-Plank code requires as input the time evolution of the electric field, which can be obtained from the

MHD code. Full integration of the two codes is therefore needed for a fully self-consistent model. However, the feedback of the Fokker-Planck code on the MHD evolution is only significant late in the CQ when the RE current becomes a large fraction of the total current. Thus, a useful first step would be to first run the MHD code to obtain the E-field evolution, then run the Fokker-Planck code. Orbits for a runaway test population based on the F-P predicted distribution function can then be integrated on the 3D fields produced by the MHD code to obtain transport predictions.

5.E.3. Integration of Material wall codes

The integration of the material wall codes is similar to that done for whole device modeling with some important differences. First, because the fundamental time scale for extended MHD codes are much shorter than WDM codes, the time discretization issues are easier and it is likely that explicit coupling is probably satisfactory for this coupling. Second, because the wall model would have to include the entire interior surface of a tokamak, codes that model the wall with a three-dimensional domain will need to cover a larger domain than what has been covered to date. In the near term, performing loosely-based coupling that are not self-consistent provides beginning studies to learn about the requirements for more self-consistent couplings. In the intermediate term, coupling with the reduced models such as WallPSI provides the easiest mechanism for performing self-consistent coupling.

5.E.4. Integration of Structural mechanics codes

Free-boundary WDM models have been used to calculate the forces on the wall assuming models for the toroidal peaking factor. Using the thin-wall approximation, extended MHD codes have also calculated the forces due to disruption. More complete modeling of the response and diffusion of eddy currents on asymmetric structures has been modeled with codes like VALEN, which uses finite elements to model structural components with the thin-shell approximation. The finite-element representation is coupled to plasma responses through a Green's function approach with plasma perturbations represented by effective surface currents on an imaginary control surface that surrounds the plasma. In general, some form of coordinate and component transformation is required between a plasma model and electromagnetic codes. Many structural finite-element codes have options for modeling magnetic diffusion through structures. If structural engineering models already exist for an experiment, developing transformations to couple magnetic perturbations from WDM or extended-MHD to these models can, in principle, also provide electromagnetic feedback information from eddy-current diffusion. This approach would aid direct assessment of forces on structures. Structural finite-element computations require pressures and tractions over nodes of the expansion along surfaces. Here, they are the magnetic pressures and tensions noted earlier, which need to be determined through coupling of MHD perturbations with magnetic-diffusion modeling in the structures. The most tightly coupled modeling conceivable would include feedback from the inductive effects of deforming structural components on MHD disruption dynamics. While this may be superfluous, the inductive effects may influence the outcome of worst-case scenarios with respect to the integrity of tritium breeding modules or other nuclear components. The computational practicality of coupling engineering finite-element models, as opposed to specialized codes like VALEN, with WDM and extended-MHD computations needs to be assessed. In the near term, improvements in the Green's functions codes to be able to handle better non-axisymmetric terms, double walls, and more poloidal variations would add a dramatic improvement into the modeling.

5.F. Validation requirements and plans

We present here some of the issues related to validation of specific aspects of disruption modeling. For a more detailed list of the issues related to the different causes of disruptions, see Appendix 1 and more detailed list of the diagnostics. We note that an important aspect of experimental validation is the availability of high quality equilibria coming from equilibrium reconstruction. Ways of improving these equilibria, especially in including information coming from non-axisymmetric perturbations, is needed and should be considered as part of the FSP, but no development plan is included in this document other than the investigation of the use of 3D equilibria.

5.F.1. Disruption Prediction and Avoidance:

Extensive experimental data sets in the form of time-evolving equilibrium reconstructions incorporating relevant kinetic profiles already exist for code validation. These data sets should initially be used for testing the ability of various levels of simulation capability to predict the observed stability thresholds and the plasma dynamics early in the disruption for a range of instabilities including sawteeth, classical and neoclassical tearing modes, and resistive wall modes. Such comparisons would establish the degree to which more sophisticated models could be reduced while still post-predicting experimental observations. Once instability onset and evolution models have been validated, simulation can be utilized to find possible nearby equilibrium states which can avoid instability onset – for example the experimental equilibrium state prior to instability onset. Importantly, the ability of available control actuators (such as heating, current drive, and momentum sources) to access the stable equilibrium states can be numerically assessed, and dedicated experiments testing the models of plasma stability response to the actuators can be performed. A near-term example of this process would be systematic time-evolving non-linear simulation and validation of NTM stabilization by ECCD. Similarly, simulations of RWM stability thresholds, mode dynamics including flow damping from the RWM itself, and avoidance by modifications of the q profile and/or rotation profile by NBI current-drive and momentum input should be validated.

5.F.2. Consequences of disruptions

Generation of Runaway Electrons:

Operation of reduced density plasmas in existing experiments could provide a reproducible means of generating runaway electron plasmas for model validation. Such experiments may provide the most accessible scenario for a wide range of facilities to measure the fast-electron population generation, evolution, and energy distribution - using for example hard X-ray cameras - and then compare to simulation. If performed routinely, such experiments are potentially operationally dangerous, and it will be imperative for the experiments to have developed reliable means of runaway plasma control, runaway suppression, or other safe-shutdown techniques. For these sustained runaway equilibria, plasma densification, the application of 3D fields, and impurity gas puffing all provide means of controlled tests of runaway suppression for comparison between experiment to simulation. To extend this validation activity to the plasma disruption phase, improvements in the equilibrium reconstructions during the thermal and current quench (including high time resolution kinetic profile measurements) would prove very valuable in validating models of the internal electric field evolution during the quench and thus for validating predictions of runaway generation in conditions more directly applicable to disruptions.

Plasma Material Interactions:

Measurements of the plasma surface response to incident plasma heat, particle, and current flux have increased in number and capability in recent experiments. For example in-situ measurements of sputtering, retention, and recycling in the tokamak divertor are becoming more routine. However, measurements of the material surface response to disruptions (and ELMs) are much more limited. These measurements should be extended to enable validation of models of the disrupting plasma exhaust into the scrape-off layer and plasma facing components, and the liberation of impurities from the plasma facing components into the plasma. The placement of these disruption-induced impurity liberation diagnostics would be guided by a combination of present experimental observations and expectations/predictions from the simulations.

Several different types of disruptions can be experimentally generated to modify the thermal and current quench rate and the location of the disruptive plasma-wall interaction. These variations will modify how impurities are generated and transported into the plasma. Similarly, massive gas injection can be assessed as a function of gas species, gas delivery rate, and delivery location. Diagnostics with sufficiently high time and spatial resolution to measure local power deposition on the first wall, impurity liberation including a multitude of species and charge states, and the rapid transport of impurities into the plasma must be further developed to enable model validation.

Structural Effects:

As progressively larger tokamaks are built (in particular ITER), the structural integrity of major components of the device including the first wall, blankets, vacuum vessel, and vessel supports can be threatened by large electromagnetic loads on electrically conducting elements. More extensive measurement of 3D currents flowing in the structure of present devices combined with more systematic implementation of force measurements (such as accelerometers, strain gauges, displacement measurements, etc) should be implemented to validate the force calculations. The placement of these diagnostics should be guided by a combination of structural analysis modeling and MHD simulation expectations. These validated models are quite important for the design of ITER components, and for the design of future fusion facilities including DEMO.

Modeling of Delivery Systems for Disruption Mitigation:

Extensive experimental data sets are available for assessing the time between disruption precursor observation and the time for disruption quench onset. These data sets should be utilized to assess the viability of various disruption mitigation systems to react in time to influence disruption evolution. The plasma response to mitigation techniques such as massive gas injection has already been measured in several devices and compared to simulation.

However, improved diagnostics are needed to better measure the impurity penetration rates into the plasma and the plasma response to the impurities. For other means of disruption and/or runaway suppression such as 3D fields (either externally applied or generated by the plasma), additional diagnosis of the 3D plasma magnetic topology could enable fast 3D equilibrium reconstructions and could substantially improve model validation.

Feedback Control:

As in the case of disruption prediction and avoidance, it is essential that the disruption effects simulations and mitigation response models developed in the FSP project are sufficiently well-validated against operating experiments. Since disruption effects simulations tend to guide machine design efforts more than they are applied to control design, the required accuracy of these simulations is somewhat lower than the models on which controllers are based. However, control algorithms that act as part of the mitigation system must have quantifiable performance, and thus typically require high accuracy models. For example, specialized control that must be enabled when a large runaway current channel is produced by a disruption (mitigated or otherwise) will require accurate validated models of seed runaway production, runaway avalanche, growth in response to applied electric fields, collisional damping (and thus impurity transport), etc. Development of high-fidelity models must ultimately impact machine design and operation to improve robust tokamak performance.

5.G. Connection to other work

Extensive interaction with other science drivers is expected as similar personnel, components, and development tasks are envisioned. The entirety of the Whole Device Modeling development path needs to be performed in conjunction with that science driver with the emphasis on the modeling shots that lead to disruptions.

The integration of material wall interactions into WDM codes and extended MHD codes is obviously closely related to the integrated SOL, edge, wall Science Driver. We expect a great deal of overlap in components.

The control of MHD via RF is also an issue for the Energetic Particle Science Driver. Although not extensively discussed, the accurate calculation of the linear instabilities depends can be sensitive to the presence of hot particles. Fokker-Planck codes are extensively used to calculate hot particle distributions, and this represents the most dominant common component between the two groups.

The development of an kinetic/MHD advanced component is a goal shared by the "Turbulence on Transport time scales" science driver which has mesoscopic physics such as gyrokinetic turbulent transport in the vicinity of a magnetic island as one of its goals. The Pedestal Science Driver also shares this goal because it needs an integration to handle the compression of time scales that occurs in the pedestal region. We expect that as the FSP planning progresses, further collaboration on plans for this advanced component will occur.

5.H. Schedule and resources

The tasks will given in this section includes tasks that for experimentalists, computationalists, analysts, and theorists, and although these roles are denoted, close cooperation, including inclusion into the code design process, will be required for the success of this endeavor. We also make note of the milestone that each task can address.

1. **Y1.** Develop experimental database of disruptions and make data available to FSP analysts using FSP-developed standards for data storage and access (all milestones).
2. **Y1.** Analyze database to study how the consequences and effects of disruptions differ for the various types of induced disruptions (all milestones)
3. **Y1.** Use WDM to simulate onset of VDE in extensive scan of experimental database. Benchmark instability and controllability threshold and early growth rate against linear stability calculations and experiment (M2.a.)
4. **Y1-2.** Improve validation of extended MHD codes by comparing with more localized measurements of plasma quantities for cases within experimental database (M2.b.)
5. **Y1-2.** Develop a PF component capable of reuse by existing codes.
6. **Y3-5.** Integrate WDM codes and extended MHD codes with PF component to study interaction of feedback system on dynamics of disruption.

7. **Y1-3.** Extend MHD component capabilities to include improved ability to model impurities, radiation, and simplified wall models.
8. **Y1-2.** Enable WDM codes to refine and perturb equilibrium as simulation progresses.
9. **Y2-3.** Enable WDM code to launch ideal MHD codes for multiple toroidal mode numbers and analyze stability boundaries.
10. **Y2-3.** Statistically analyze the results of simulations of WDM with linear MHD analysis when applied to the experimental database.
11. **Y2-3.** Perform initial extended MHD simulations of cases and validate against experiments on a subset of cases performed in Task 10 including studies of effects of impurities.
12. **Y1-2.** Using the capability of generating refined and perturbed equilibria, enable calculation of localized measures of plasma parameters and calculation of stability parameters, develop and analyze parameters for tearing mode onset.
13. **Y2.** Apply the capability developed in previous task to experimental cases and analyze the predictive capability of reduced models.
14. **Y1**. Couple neoclassical gyrokinetic code to 3D equilibrium solution with magnetic island. Incorporate self-consistent bootstrap current from gyrokinetic code. Begin work on coupling of $\mathbf{j}_{\perp}$ from gyrokinetic code to 3D equilibrium solver to incorporate kinetic and flow effects in the equilibrium. Allow for localized currents near rational surfaces due to shielding effects of flow.
15. **Y2.** Complete code modifications needed to couple $j_{\perp}$to 3D equilibrium solver to incorporate kinetic and flow effects. Begin validation of modified equilibrium solver against saturated NTM's, using pressure and net current profiles consistent with experimental data.
16. **Y2-3.** Replace VMEC equilibrium solver with a 3D equilibrium solver that can handle islands and stochastic regions in the Strand-Houlberg 2.5D code, using transport equations for flux diffusion outside and inside islands. Initially use constant-ψ approximation in islands.
17. **Y3-5.** Improve handling of kinetic effects and flow in 3D equilibrium.
18. **Y3-6.** Incorporate effects of turbulence in 3D equilibrium using gyrokinetic code that can handle turbulence. (This assumes that there is a parallel effort in the core transport group to couple gyrokinetic codes to equilibria with magnetic islands. If not, this will be moved back in time, and will be completed in FY10.)
19. **Y3-5**. Incorporate the improved 3D equilibrium in 2.5D code. Incorporate sources and transport model, including models for NTM triggers and momentum transport with NTV, in 2.5D code.
20. **Y1-5.** Validate extended MHD components against measured rotation evolution of bulk plasma, and also propagation frequency and dynamics of mode observed in experiment, including validation of ECCD feedback stabilization simulations using

extended MHD models. Study rotation of TM/RWM with external perturbations for cases with large perturbations and fast slowing down times in extended MHD codes.

21. **Y2.** Simulate gas-jet penetration and pellet ablation in 3D in the pre-TQ phase, including radiation and parallel heat transport and validate TQ onset time against experiment.
22. **Y2.** Perform WDM simulations integrating in disruption mitigation techniques.
23. **Y5.** Perform nonlinear simulations of TQ with 3D jet/pellet model and validate mixing/assimilation fraction versus species against experiment with improved impurity models.
24. **Y5.** Perform WDM simulations integrating in disruption mitigation techniques
25. **Y1.** Determine verification and validation metrics for F-P, WDM, and extended MHD simulations of runaway electrons, and ability to share data.
26. **Y1-2.** Simulate thermal energy and particle transport and RE formation during thermal quench. Compare the global confinement properties of F-P simulations against extended MHD simulations. Compare/validate against experiment – explore effects of 3D fields, massive gas injection, etc.
27. **Y2.** Using existing models, investigate the generation of REs in low-field device as possible means of explaining why runaways are generally not observed in low-field ($B < 2T$) tokamaks.
28. **Y1-5.** Model RE confinement/transport during current quench – in particular transport of RE during successive transitions from stochastic to (partially) closed flux surfaces during q-evolution and evolving island overlap.
29. **Y1-5.** Model non-linear evolution of thermal plasma current converted to RE current, simulate equilibrium profiles of RE plasma, and ability to control RE plasma equilibrium and validate against experiment for both WDM and extended MHD.
30. **Y1-2.** Define interfaces between structural wall codes and WDM/extended MHD codes.
31. **Y1-3.** Provide data from WDM/extended MHD disruption simulations to more detailed PMI and structural analysis codes and perform initial assessment and validation of effects of disruption on the wall.
32. **Y1-2.** Improve existing wall component to enable three-dimensional wall effects, gaps, double-walls, and blankets. Use new component to define new interfaces to more complete codes such as VALEN.
33. **Y2-5.** Interface extended MHD codes to more complete wall models, including newly developed components, and more detailed analysis.
34. **Y2-5**. Use newly developed capability to compute currents and forces induced in realistic 3D conducting structure, utilize reduced models of plasma material interaction to compute surface damage, impurity generation
35. **Y4-6.** Validate 2.5D code for full time-evolution of NTM, including trigger threshold and momentum transport (including NTV terms).

36. **Y6-7.** Validate 2.5D code against RWM time-evolution.

5.I. Milestones

The milestones for years 2 and years 5 are presented. Year 10 milestones are presented afterwards.

Disruption onset and avoidance

1. *For all types of disruptions***:**
    a. Have experimental database of disruptions cases along with the data available to FSP analysts using FSP-developed standards for data storage and access. The experimental database will include control or comparison cases.
    b. An analysis of the effects of disruptions given the different causes of disruptions will be provided to the computational and theory community to aid in assessing issues that can be addressed by FSP capabilities.
2. Vertical instability induced disruption
    a. **Y2.** Provide validated WDM capability for enabling predictions of VDE onsets with the uncertainties in the modeling quantified through validation.
    b. **Y2.** Quantify the limitations of extended MHD for calculating the forces due to the nonlinear evolution of a VDE disruption.
    c. **Y5.** Provide capability for WDM and extended MHD components to model the effects of feedback control through integration with PF components.
    d. **Y5.** Provide numerical analysis of role of impurities in the nonlinear evaluation of VDEs.
3. Fast MHD induced disruptions
    a. **Y2.** Provide validated capability for using linear ideal MHD codes to predict the onset of fast MHD induced disruptions with the uncertainties in the modeling quantified through validation.
    b. **Y2.** Quantify the limitations of extended MHD for calculating the forces and fluxes due for fast MHD induced disruptions.
    c. **Y5.** Investigate the extent to which impurities affect the nonlinear dynamics of the disruption.
4. Slow MHD (Tearing modes and resistive wall modes)
    a. **Y2.** Couple free-boundary, 3D equilibrium code with islands to neoclassical gyrokinetic code. Gyrokinetic code provides: self-consistent calculation of bootstrap currents in NTM; $j_\perp$ from cross-field drifts for purpose of incorporating kinetic and flow effects in the equilibrium.
    b. **Y2.** Begin validation of previous development against saturated NTMs.

c. **Y3.** Replace VMEC equilibrium solver with a 3D equilibrium solver that can handle islands and stochastic regions in the Strand-Houlberg 2.5D code. Initially use constant-ψ approximation in islands. (In general geometry, this corresponds to the approximation that $\mathbf{B}\cdot\nabla\psi/\mathbf{B}\cdot\nabla\phi$ is constant across the island. This is generally a reasonable approximation, even for relatively large islands, as long as the equilibrium is not close to marginal stability for an ideal mode.)
d. **Y2.** Provide summary of the ability of the extent to which WDM can predict TM/RWM onset using linear codes combined with reduced models.
e. **Y2.** Using NTV rotation models with other momentum transport models, simulate rotation dynamics of RWM/TM including resonant, non-resonant, and wall torques on mode. (Y2 – something into 1.5WDM code)
f. **Y5.** Use 3D equilibrium codes (perturbed ideal MHD, stellarator codes) + transport codes to model thermal and particle transport in presence of island(s) and compare to non-linear kinetic MHD simulations
g. **Y2.** Provide quantified analysis of extended MHD ability to predict ability to model rotation evolution of bulk plasma, and also propagation frequency and dynamics of mode observed in experiment in the presence of external perturbations and ECCD feedback stabilization simulations.
h. **Y5.** Sources and transport model incorporated in 2.5D code.
i. **Y6.** Validate 2.5D code for full evolution of NTM, including trigger threshold and momentum transport (including NTV terms).
j. **Y6.** Begin validation of 2.5D code against RWM time evolution.
k. **Y5.** Improve validation of TM/RWM simulations by using energetic particle and CEL-DKE closures. Include interaction with other modes such as AEs.

5. Disruption mitigation
    a. **Y2.** Provide validated capability to model gas-jet penetration and pellet ablation in 3D in the pre-TQ phase, including radiation and parallel heat transport and validate TQ onset time against experiment.
    b. **Y2.** Provide WDM capability for modeling gas jet injection.
    c. **Y5.** Provide quantified analysis of the ability to model the injection of jet and pellets, especially to describe the mixing/assimilation fraction.
    d. **Y5.** Provide quantified analysis of WDM capabilities for modeling disruption mitigation experiments.

Consequence prediction and mitigation

6. Runaway formation threshold and RE confinement:
    a. **Y2.** Report on quantified analysis of the uncertainties in the WDM, F-P, and extended MHD approaches to modeling RE damage for the various

disruptions above, include regimes where REs are not observed such as low-field devices.

   b. **Y5.** Model RE confinement/transport during current quench – in particular transport of RE during successive transitions from stochastic to (partially) closed flux surfaces during q-evolution and evolving island overlap.

7. Material wall consequences:
   a. **Y2.** Provide report on the quantified effects of disruptions on materials walls as a function of time from disruption onset to the end, and compare with simple models of walls in extended MHD codes versus more detailed models of material walls.
8. Structural forces consequences
   a. **Y2.** Provide quantified analysis of difference in computed forces using simplified models axisymmetric models of 2D walls and the calculation of forces with 3D structures using the forces provided by extended MHD codes using the simplified walls.
   b. **Y2.** Deliver new component for more accurate calculation of the effects of non-axisymmetric walls, but using the Green's function approach. Deliver a design document outline plan for integration with more detailed wall models.
   c. **Y5.** Provide report on the quantified differences of extended MHD results using more realistic wall models and the simplified wall models.

Year 10 Milestones

Provide validated software for modeling disruption onset, mitigation, and consequences using the WDM modeling via integration with linear MHD, plasma feedback, external source, material wall, and structural wall components.

Provide new 2.5D WDM software for enabling the study of the slowly evolving MHD instabilities where the inertia is small.

Provide new ability for studying the nonlinear, three-dimensional evolution of the instabilities that lead to disruptions, the consequences of the disruptions, and ways to mitigate their consequences.

Appendix 1. Phenomena Identification and Ranking Table (PIRT) for Disruption Studies

Issue	Critical Physics	Measurements Needed	Important Gaps
Fast MHD-induced disruptions (VDEs, ideal MHD)	-Stability of low-n modes -Non-linear VDE evolution -Uncertainty quantification of stability boundaries -Control of actuators for stable equilibria access -Thermal effects on walls including ablation, dust generation, … -Magnetic interactions with walls and subsequent evolution	•Fast measurements for mode structure identification & growth rate •Measurements for high quality equilibrium reconstruction •High-frequency plasma measurements near the wall as plasma scrapes off the wall •Identification of signatures of near-stability regimes •Measurements of heat and particle flux on walls (in situ measurements, IR measurements, …)	•Robust free-boundary equilibrium codes •Feedback control techniques have yet to be tested in a wide range of plasma conditions •Modeling of 3D effects of conducting structures and halo currents •Detailed physics models of PMI during disruptions •Development of reduced models for WDM analysis •Synthetic diagnostics for aid in determining experimental signatures of precursors •Modeling of controllability •Time-dependent measurements

Issue	Critical Physics	Measurements Needed	Important Gaps
Disruption mitigation (separate issues specific to this issue)	-Delivery of impurities into the impurities and their subsequent transport	•Detailed spectroscopy of impurity transport	•`Modeling of impurity injection systems •Impurity/radiation/ neutral transport •Synthetic diagnostics for aid in determining experimental signatures of precursors

Issue	Critical Physics	Measurements Needed	Important Gaps
Runaway electron formation threshold and relativistic electron confinement	-Thermal energy and particle transport and RE formation during thermal quench -Role of velocity space instabilities driven by fast electrons in transport -RE confinement transport during current quench -Nonlinear evolution of magnetic topology when RE current is significant fraction of total	•Explore effects of 3D fields, MGI, pellets, etc. •Fast electron velocity measurements in configuration space •Parallel electric field measurements •Fluctuations during RE generation •3D magnetic field measurements and equilibrium reconstruction (?) •Fast electron interactions with first wall •EM forces on plasma fall	•`Ability to obtain plasma data approaching and during the quench phase •Rigorous models for self-consistent RE and plasma descriptions •Validation of reduced models •Correlation of RE deconfinement and 3D magnetic structure •Synthetic diagnostics for aid in determining experimental signatures of precursors •Modeling of controllability

Issue	Critical Physics	Measurements Needed	Important Gaps
Tearing mode-induced disruptions	-Accurate closures for MHD equations including energetic ions -Evolution of tearing modes on transport time scales including rotation dynamics and interaction with external structures -Threshold physics of neoclassical tearing modes	•Highly localized diagnostics near the tearing layer during onset. •Measurements enabling 3D equilibrium reconstruction •Rotation measurements near the tearing layer •Identification of signatures of near-stability regimes	•`Validation of 3D equilibrium reconstruction •Modeling of controllability •Measurement of plasma modification due to 3D magnetic fields •Fidelity of NTV model and 3D field induced rotation •3D magnetic field effects on particle and heat transport •Synthetic diagnostics for aid in determining experimental signatures of precursors

Issue	Critical Physics	Measurements Needed	Important Gaps
Resistive wall mode	-Accurate closures for MHD equations including energetic ions to accurately capture RWM stability -Evolution and control of RFA on transport time scales including rotation dynamics and interaction with external structures	•Measurements enabling 3D equilibrium reconstruction •Measurements of mode structure •Identification of signatures of near-stability regimes	•`Validation of 3D equilibrium reconstruction •Modeling of controllability •Measurement of plasma modification due to 3D magnetic fields •Fidelity of NTV model and 3D field induced rotation •3D magnetic field effects on particle and heat transport •Synthetic diagnostics for aid in determining experimental signatures of precursors

6. WDM

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6.A. Background and motivation

The whole device modeling of tokamak discharges involves the integration of different spatial and time scales for modeling of all discharge phases starting from discharge startup to discharge shutdown. High fidelity predictive whole device modeling should accurately account for scrape-off layer physics, plasma wall interactions, core transport, heating and current drive, fast particles, pedestal physics, ELMs and impact on the divertor, 3D MHD modes, as well as other physics issues. The success of a new WDM tool is strongly dependent on careful coupling of different physics components. Due to interrelation among physical effects, strong coupling of the physics components becomes essential. The interplay between different physics components introduces a new level of physics fidelity and leads to discovery of new effects that are not available when physics components are considered in isolation.

There are four overall thrusts that can shape the successes of the WDM. These thrusts are:

- High fidelity science components;
- Reliable and flexible framework that set standards for coupling of science components in the WDM suite of codes. The framework should be flexible enough to allow the coupling with 1d, 2d, or 3d components, explicit and implicit coupling, dynamic parallelism, flexible data exchange and storage;
- Verification and validation (V&V) of individual physics components and WDM tool in general. The V&V activity will include the establishment of V&V metrics, set of synthetic diagnostic tools, development of interfaces to experimental data, and legacy transport codes;
- Data visualization, analysis, transport, and storage.

Since the WDM science driver is in an unusual position of receiving physics modules from other science driver areas, it is important to understand what are the specific activities that are uniquely the responsibility of WDM. A list is being developed of anticipated responsibilities for the WDM group within the FSP, however that is constructed. These include the primary role of supplying the equilibrium/transport solver package and describing the required "plasma state" like data, but also includes the large range of additional physics modules for which there may be no responsible group. The device description aspects (structures, coils, etc.) and the experimental interpretation functions (like TRANSP) are also primary roles for the WDM.

The kinds of physics problems that will be addressed with FSP WDM suite of codes will include the following:

- Predict the plasma confinement, transport and plasma profiles in tokamak discharges. Currently, there are a variety of transport models that yield different predictions for confinement and fusion power production in burning plasma tokamaks such as ITER. In the future, there must be a convergence in the transport predictions based on high-fidelity turbulence and particle orbit computations.

- Predict the onset, frequency and consequences of macroscopic instabilities including the plasma disruptions. Comparisons will be made with experimental data for the frequency of sawtooth oscillations and for the effect that each sawtooth crash has on the plasma profiles. The onset of neoclassical tearing modes and their resulting magnetic island widths will be simulated and compared with experimentally measured data. The onset, frequency and width of edge localized modes are critically needed information for high-power burning plasma experiments. There is a need to predict the onset of disruptive instabilities and their nonlinear evolution in order to avoid or mitigate disruptions of tokamak discharges.

- Predicting the plasma boundary conditions from plasma-wall interactions through the scrape-off-layer and the H-mode pedestal. All of the plasma profiles are strongly influenced by the evolution of the plasma boundary. Some WDM codes are also used to compute interactions between magnetic coil currents and plasma currents.

- Predicting the sources and sinks that drive all of the profiles in plasma discharges. Sources such as neutral beam injection, fusion reaction products, and radio frequency heating and current drive all involve the computation of fast particle distributions and their interaction with the thermal plasma profiles. Predictions are needed for the effect of fast ions on macroscopic instabilities such as sawtooth oscillations.

Some critical physical issues relevant to WDM as well as important gaps and experimental measurements that are needed to address these physical issues are given in the Table below.

Table 1. WDM physical critical issues

Issue	Critical Physics	Measurements Needed	Important Gaps
2.5-3D free-boundary equilibrium generation and discharge evolution	– Model field errors, magnetic islands, applied magnetic perturbations – Diagnostic location – Evolution of plasma and machine parameters – Breakdown processes – Dist. functions in 3D space – Self-consistent treatment of EPs from NBI, ICRF, and fusion products	– 3D arrangement of magnetic probes; preferably also MSE points – Profile measurements	– Effective flexible fast 2.5-3D eq code – Model for internal transport barriers and momentum transport – Mag islands consistent with diagnostics or MHD model – Source models in non-axisymmetric equilibria
Evolution of plasma profiles from boundary to core	– Coupling of validated models for microturbulence, EP modes, MHD activity and their effects on transport	– Turbulence in density, Te, Ti, B – Profiles and gradients – EP sources and dist. functions – Precise measurements of current density profile	– Validated component models – Model for interaction between physics models – Synthetic diagnostics – Nonlinear saturation models for EP and MHD modes – Model linking MHD activity to flux evolution
Prediction, control, and mitigation of instabilities	– Onset, growth rate, and nonlinear saturation for sawteeth, ELMs, RWMs, TMs, NTMs – How these modes affect plasma evolution–transport and poloidal flux	– Internal mag field fluctuations and structures – 3D arrangement of mag probes	– Validated component models – Model for interactions between models – Effect on profiles and equilibrium – Effect on sources
Interaction of boundary with plasma core	– Effect of heat flux on the boundary and of the boundary on the heat flux	– Profiles and dist fns in the pedestal and SOL – Impurity generation at wall – 2D radiation profile – Radial electric field and bootstrap current in	– Validated reliable component models for SOL and PSI – Validated model for density transport in boundary and core – Effects on discharge and PSI of ELM control

		boundary region	techniques – Impurity transport

It is expected that different elements of the WDM tool (different combinations of components) will be progressing at different rates, delivering different levels of physics fidelity. So although it is true we may not reach the "full" fidelity model of an ITER discharge in 20 years, we would have brought all aspects that we were targeting to some level of fidelity that was 1) verified, 2) validated/compared to experiments, 3) assessed in its predictive capability toward future tokamaks, and 4) applicable to ITER discharges. Of course, by then we will have ITER discharges for comparison as well. The ongoing project on predictive modeling of ITER scenarios provides an example of WDM approach. Different physics components that are used in this project are listed in Appendix A. Each component describes an individual physical effect. Individual components, by themselves, cannot be used to answer questions about ITER performance and to optimize the ITER scenarios. These problems can be addressed only when all physical components are used together in the dynamic whole-device simulations.

The WDM group has constructed four high priority research areas along these lines:

- 2.5D equilibrium and transport solver;
- Self-consistent fast particle treatment for neutral beam, ion cyclotron, and alpha heating and current drive sources;
- Incorporation of turbulence simulation into transport time-scale simulation;
- Self-consistent, coupled core-edge dynamics.

These four research areas are being developed from the point of view of deliverables in each given year, incremental progress in physics/code capability, demonstration of specific physics. While these research topics do not cover the whole spectrum of research problems associated with WDM, progress in four identified areas will significantly enhance the predictability of whole-device modeling of tokamak discharges.

A series of observations within the group by members provides some perspective that may not be fully developed yet.

- More than one approach to the framework may be required for the FSP to accommodate phases in its development.
- WDM will likely be faced with making components work in time-dependent simulations after they are validated in individual time-slices by the responsible group. This task includes recognizing all integration time-scale issues.

- Fleshing out a group of whole device modeling users should help to direct the needed structure of the WDM tool.
- The experimental data connection will be critical for the WDM tool. The goal is to make this connection as uniform as possible allowing multi-machine comparisons of models.
- Legacy codes are needed to 1) verify new tools developed, 2) facilitate access to interpretation of experimental data.

6.B. Goals for Whole Device Modeling in FSP

The goals for Whole Device Modeling (WDM) are congruent with the goals for the Fusion Simulation Project as a whole — to provide a comprehensive predictive simulation capability for magnetically-confined plasmas that integrates the knowledge from key multi-scale physical processes to continually improve fidelity. This capability is needed to maximize exploitation of fusion experiments, especially ITER, and to establish the scientific basis for an economically and environmentally attractive source of energy. In particular, FSP WDM software must be designed to meet the following needs:

- Scenario modeling to plan new experimental champagnes in existing tokamaks or to extrapolate to planned future devices. Scenario modeling is used to optimize discharge parameters, such as maximizing fusion power production in burning plasmas, and to maximize the effectiveness of planning new experiments.
- Analysis of experimental data to compute the time evolution of plasma profiles that are not measured and to resolve discrepancies between different ways of measuring experimental data.
- Validation or calibration of theoretical models by comparing simulation results with experimental data. Theoretical models are used to compute sources, sinks and transport of heat, particles, momentum or current density as well as the equilibrium shape, plasma-wall interactions and the effects of macroscopic instabilities in tokamak discharges. WDM provides self-consistent simulations that can be used in the validation of individual physics models.
- Development of discharge control techniques
- Production of self-consistent simulation results that are passed on to other more specialized computer codes.

Fundamentally, there are three kinds of challenges faced by WDM suite of codes:

1. Coupling between different regions of the plasma — such as the coupling between core and edge plasma regions.

2. Coupling between different physical phenomena — such as the coupling between transport and large-scale instabilities.

3. Bridging the gap between short and long time scales, or between microscopic and macroscopic space scales. An example of this last kind of integration would be the simulation of turbulence, which grows on microsecond time scales and sub-millimeter space scales, resulting in transport across the plasma and the evolution of plasma profiles over tens of seconds in a tokamak with dimensions of several meters.

The required whole device modeling capabilities involve self-consistent simulations of the entire plasma discharge that include all of the relevant physical phenomena. Depending upon the requirements of each simulation, the user should be able to choose from a spectrum of models for each physical process including high physics fidelity modes based on first-principles computations or reduced models for more rapid computations and validation or empirical models. Full-featured WDM simulations should be capable of simulating the entire time-span of the discharge, from start-up to shut down, and the entire spatial scale from the magnetic axis to the interaction between the plasma and the first wall and magnetic coils. There should be seamless access to experimental data or the results from previously-run simulations.

Most of the existing WDM codes are limited to axisymmetric plasmas with simply nested closed magnetic surfaces. There are needs to further develop WDM codes for the open magneric field region at the plasma edge, including plasma-wall interactions, and to couple the closed magnetic surface regions of the plasma with the open magnetic surface regions. There is also the need to include the three-dimensional effects that result from the formation of magnetic islands, magnetic ripple, resonant magnetic perturbations and macroscopic instabilities in tokamak discharges. Future WDM codes must include more kinetic modeling — as opposed to fluid approximations — and there must be a closer coupling between fast particle distributions and the more thermal part of the distribution function. A WDM suite of codes must be developed to bridge the gap between high-fidelity turbulence simulations on microsecond time scales and the resulting transport on multiple-second time scales. The WDM software must also be able to incorporate high-fidelity simulations of macroscopic instabilities such as sawtooth oscillations, neoclassical tearing modes, resistive wall modes, edge localized modes and, ultimately, disruptive instabilities. There must be an integration between fine-scaled kinetic and large-scale macroscopic physical phenomena in order to produce a fully self-consistent simulation capability.

6.C. WDM Components

As described in Sec. I, the WDM code will ultimately model the tokamak discharge from start-up to shut-down, from the magnetic axis of the core plasma to all externally driven and passive conductors and to the material surfaces which interact with the relatively cold edge-plasma. The components needed for whole device modeling to solve physics problems include the following:

- Modeling of plasma profiles and levels of turbulence in MHD-quiescent core and edge plasmas using gyro-kinetic turbulence simulations within a full-featured WDM framework is essential to predict the plasma confinement. Ultimately, the following components will be needed: 1) Gyro-kinetic or gyro-fluid modules that are designed for use within WDM suite of codes to compute transport fluxes and turbulence spectra in core and edge. In addition, options should be available for reduced models that are calibrated by gyro-kinetic simulations. 2) Modules to compute sources and sinks of heat, particles, momentum and current; 3) Modules to set boundary conditions; 4) Free boundary equilibrium modules to compute the shape of magnetic surfaces within the core and edge plasma.

- In order to compute edge plasma conditions and plasma-wall interactions, such as power deposition to the first wall and recycling of neutrals, all coupled to the core plasma, the following additional components are needed: 1) Modules to compute transport in the scrape-off-layer region along magnetic field lines as well as across magnetic surfaces including gyrokinetic or gyroturbulence turbulence effects; 2) Modules to compute neutral particle density and flow; Modules to compute recycling of neutrals from the first wall; 3) Modules to compute the formation and evolution of the H-mode pedestal.

- In order to compute the effects of macroscopic instabilities, the following additional modules will be needed: 1) Modules to compute the triggering of sawtooth crashes and the effects of each sawtooth crash on plasma profiles; 2) Modules to compute the formation and evolution of magnetic islands and stochastic regions driven by neoclassical tearing modes as well as externally applied non-axisymmetric magnetic fields. 3) Modules to compute resistive wall mode amplitudes and their effect on the plasma profiles; 4) Modules to compute edge localized mode frequency and their effect on the plasma; 5) Additional modules will be needed to compute macroscopic instabilities that are driven by fast particles.

- In order to compute the onset of plasma disruptions and to mitigate their effects, the following additional components will be needed within the WDM framework: 1) Modules to compute the instabilities that trigger plasma disruptions as the plasma profiles evolve; 2) Modules that compute the non-linear evolution of the disruptive instability.

Multiscale methods will need to be employed in order to exploit the disparities in time and spatial scales and the different dimensions characteristic of the underlying phenomena. This is true not only for routine simulation with models of reasonable fidelity, for which reasonable computational turn-around time is required; it is also true for the infrequent highest-fidelity runs performed on super-computers; and we expect this to remain the case for the foreseeable future.

The most basic of the scale separations for WDM's, underlying almost all the transport-timescale codes in the U.S. and abroad, is that between the (fast) compressional Alfven time, on which the

MHD equilibrium is established and responds, and the (slow) transport time. The “engine” of the WDM consists then of an equilibrium component (a 2D, axisymmetric elliptic solver, for present tokamak WDM codes) coupled to a 1D diffusion-equation component simulating the transport across magnetic surfaces. The approach, developed by Grad and Hogan, is customarily referred to as “1&1/2D.” We will adopt this approach for the FSP WDM and, as one of our thrusts, extend it to the case of 3D toroidal equilibria: 2.5D (1.5D plus one additional dimension for the equilibrium). All the remaining physics enters as components, dependent upon the equilibrium geometry and (to lowest order) 1D plasma profiles, either plugged in as transport coefficients (from the simplest models to 5D turbulence codes, or taken from experiment) or sources (again, with a range of options at various levels of fidelity) or serving as boundary conditions to the core-plasma engine (an edge-plasma component). On the one hand, the Grad-Hogan approach introduces complexity: many ingredient pieces and algorithms, including multiple algorithms coupling various modules together, in play at once; on the other hand, it lends itself to modularity of the physics (as well as, of course, the code design) and therefore customizability—what physics to include at what expense—by the user.

To manage the complexity of its many interacting components, it is particularly important for the WDM driver that a carefully chosen list of requirements on components be drawn up and that the components adhere to them. The requirements on physics components in the FSP framework are decribed in Sec. IV. In Sec. III.1, we identify the physics components needed for each of the four WDM thrust areas set forth in Sec. I. The wide array of components needed for the WDM code as a whole is surveyed in Sec. VI.

6.C.1. Physics components needed for the four WDM thrust areas

6.C.2. 2.5D equilibrium and transport solver.

The 2.5D solver requires a menu of 3D equilibrium code options, which can be supplied by one or more components. The simplest and first needed component will assume nested, closed magnetic surfaces with prescribed boundary-conditions. Higher-fidelity equilibria will include magnetic islands and will calculate free-boundary solutions. The most capable equilibrium component must be capable of computing regions of stochastic magnetic field and must couple to external 3D error or applied fields from coils. A component describing the external active conductors, passive conducting material, and non-conducting hardware (divertor plates, limiting walls, etc.) for the machines of major interest is needed in both 3D and axisymmetrized versions. This will be developed by the FSP itself. (Present free-boundary 1.5D codes obtain this data via non-modularized features of their equilibrium components, which require the data in order to compute the free plasma/vacuum interface.) A component, or perhaps a sub-component of the 1D diffusion-equation component, is needed to provide stable implicit coupling of the 3D equilibria to the diffusion solver. In addition, an array of 1D transport coefficients (or fluxes) and surface-averaged source components are needed (as for 1.5D, but taking into account the 3D as opposed to 2D underlying geometry). Highest-fidelity simulations will involve coupling algorithms (components or sub-components) not encountered in 1.5D, such as coupling to a non-turbulent gyrokinetic component to simulate neoclassical tearing mode evolution; experience and algorithms, if not ready-to-go components, for these might be available from SciDAC projects within the next few years.

6.C.3. Self-consistent fast particle treatment for neutral beam, ion cyclotron, and alpha heating and current drive sources.

Fast-particle computations include components that model the effects of neutral beams, alpha fusion products, and ion-cyclotron (ICRF) and high-harmonic fast-wave (HHFW) sources. These sources can heat, fuel particles, and drive rotation and current in the plasma. Components are needed for all these, at various levels of fidelity. These components plug into the WDM framework or a currently functioning 1.5D code. Simpler fast-particle models are needed for routine analysis and for relatively quick predictive scoping surveys. High-fidelity models are needed to study each fast-particle distribution itself, as it evolves self-consistently under the combined action of multiple sources and evolving background plasma profiles.

6.C.4. Incorporation of turbulence simulations into transport time-scale simulations.

The first line of development of this WDM thrust entails paramaterized or reduced models derived from micro-turbulence simulations. This effort requires a 1.5D code as described above (under the FSP framework or a currently functioning 1.5D code), with the full spectrum of currently available transport-model and source components. The goal of this effort is to significantly improve the assessment of currently available models with respect to experiment — to improve or select models — in order to provide better confidence in predicting transport for ITER or other proposed large machines. (This effort is detailed in Sec. VII.)

The second line of development of this WDM thrust addresses the direct incorporation of micro-turbulence simulations into the core-edge plasma transport equations for highest fidelity predictions of profile evolution on the transport timescale. The initial implementation will treat only energy transport. It will require the basic 1.5D engine described above. It will not require the full complement of transport and source/sink models; but it will require an additional, simple thermal transport component to set a reasonable floor for the 1D temperature diffusion equation.

The turbulence-simulation component for the initial implementation will be a 5D gyrokinetic (GK) module in the local approximation, i.e., simulating turbulence in localized flux-tubes across the plasma. Multiple copies of the component will be run to obtain the turbulence-driven energy flux at points across the minor radius. The next step instead couples a global GK module, which not only permits the inclusion of non-local physics, but, for some problems, can be computationally more efficient than running multiple local simulations. First-principles edge turbulence can be included in the WDM either through an extension of these techniques to the edge, or by coupling to an edge turbulence components.

Successive steps will generalize the coupling to multiple channels of transport — density, momentum, and magnetic field — and will bring in the full array of transport and source models for best-physics prediction and comparison with experimental data.

The next step is a proposed coupling of 3D fluid micro-turbulence models. Such a coupling would have a significant computational advantage due to its reduced dimensionality relative to GK codes, while it can potentially capture much of the physics. While there is an appropriate 3D code (BOUT) for proceeding with the approach for edge plasmas, the development of gyro-Landau fluid codes needed for the core plasma has stalled. Knowledge obtained from the global gyrokinetic simulations can help development of the gyro- fluid codes.

Coupling algorithms (possibly componentized) are needed. While algorithms have been demonstrated for single channel coupling when turbulence and transport timescales remain disparate, development is needed for coupling at the later stages. Work in this area by the FACETS and CPES projects is currently in progress. In addition, development of the GK codes is needed; e.g., to accommodate changes in the equilibria; to compute surface-averaged fluxes for more channels of transport; to satisfy the requirements for robust components. The GK formalism should be reviewed for its applicability to transport timescales: there is some controversy as to whether or not present GK formulations are correct with respect to collisions and there are accumulated changes in the distribution functions over long time scales.

In the longest term, given successful results in 1.5D, an extension of turbulence coupling to 2.5D can be considered. This would require additional development of GK codes, most of which currently assume axisymmetry in their coordinates and/or geometric coefficients.

6.C.5. Self-consistent, coupled, core-edge dynamics

As discussed in Sec. VII, advanced models of the edge region and of first-wall interactions are less mature than the models for plasma regions. The development of boundary and pedestal physics will be carried out in separate FSP science drivers, and full-physics components are expected only as that research proceeds. Nevertheless, we identify this a thrust area for WDM due to its importance and due to the need to prepare for coupling to the edge models. The 1.5D approach to WDM permits modeling the boundary with various degrees of accuracy; we will begin with the currently available reduced models. In the simplest treatments, boundary conditions are supplied to the 1D core transport equations at some outer flux surface; these conditions can be either prescribed or computed by an edge code. In the latter case, the edge transport code might be 0, 1, or more dimensions (surface-averaged if needed), and the coupling between the core and edge might be advanced explicitly or implicitly, which has the advantage that at each step the solution has consistent fluxes and values in each component. The FACETS project is presently exploring such core/edge coupling using the axisymmetric 2D UEDGE fluid transport code as its edge model. Further core/edge coupling techniques might overlap over a finite band in radius, e.g., to assure uniform overlap in the mathematical sense or for efficiency with expensive boundary plasma models if some fields need only a 1D treatment near the core. A longer term core/edge coupling scheme includes global whole volume modeling from core to edge across the magnetic separatrix surface without boundary between them.

The WDM components needed for any of these boundary-plasma models include, apart from the boundary-plasma model itself, the standard 1.5D WDM framework components and a coupling algorithm as indicated by the selected boundary-plasma. For the more substantial coupling algorithms, the coupling itself should be componentized.

6.C.6. Plans for adapting older components and developing new WDM components

We propose to establish an FSP Components Committee whose functions will be: to assess and prioritize the module needs of the WDM project and the state of codes in the fusion community that might meet those needs; to review and revise the required standards for FSP components; to review components with respect to the required standards; and to commission and monitor the development of new components (e.g., 1D solver, coils description) as needed.

6.D. Framework Requirements

The overarching goal of the Whole Device Modeling science driver is to provide the FSP with a comprehensive model of tokamak discharges from the magnetic axis to the wall, in part by drawing from existing modeling capabilities that handle various aspects of the physics with differing degrees of fidelity. The integration of such existing capabilities along with newly developing models that span a wide spectrum of temporal and spatial scales makes necessary an FSP-WDM framework that can allow these different models to interoperate in a way that supports the critical tasks of model verification and validation. It is recognized that more than one type of approach to such a framework may be needed to satisfy all the requirements of WDM through its various phases of development, transitioning from mainly legacy codes and models to new physics models created specifically in response to the FSP science drivers. Nevertheless, we can outline the requirements for success of an FSP-WDM framework by examining two critical aspects of whole device modeling: composition of multiple physics models to form a complete tokamak discharge simulation, and management of a workflow that represents the various computational tasks needed to execute such a simulation study from start to finish.

6.D.1. Requirements on physics components

The long experience with 1&1/2D modeling codes on the part of both the theoretical and experimental U.S. fusion programs has provided us with a well-developed view of the requirements necessary to place on constituent modules for the successful execution of integrated physics simulations, for meaningful verification and validation of such simulations, and for efficient maintenance, debugging, and continued development of an integrated WDM code. The Modules Library committee of the National Transport Code Collaboration codified and published on its web-site the first widely-used requirements and guidelines lists in the mid 1990's. The more recent proto-FSP projects have developed their own standards, updated to include issues such as object-oriented code designs and incorporation of modules running on massively parallel architectures.

At the FSP March Planning Workshop, physics components requirements were discussed in the context of some of the individual science drivers. From these discussions (which drew upon the experience just mentioned) a number of generic, cross-cutting requirements emerged; these were summarized in the Workshop Summary. Given that WDM is by its nature comprehensive and cross-cutting, the requirements apply directly to the WDM driver, and we present the list on components here.

- Components should come with documentation of sufficient detail so that component users can determine equations solved, solution methodology, order of error in discretizations, limits of validity, and parallel capabilities. Component internals should be documented sufficiently that modifications needed for physics composition can be made if needed by someone other than the component developer. For the most part this is a matter of dedicating time to providing the needed information. In the case of order of error in discretizations, this may or may not be known to the component developers, and may be difficult to assess purely from analysis for complex algorithms, in which case convergence studies are required.

- Components must be "componentized": they must be provided with an agreed-upon interface that provides, for a given component type (functionality), agreed upon ingredients:
    - Common input and output data quantities
    - Common input and output variable names
    - Common methods

In addition, there must be agreed-upon definitions for what constitutes a component; in particular, the agreed-upon level of granularity. In particular, an agreed answer must be provided to the question, "is it a sub-component of another component, or a component" — which will typically depend on the reusability of the (sub)component in question. For existing (legacy) components, conforming to an agreed-upon interface can be achieved through the use of wrapper code (as done for legacy components in the SWIM and FACETS projects) or through rewriting of interfaces. New components should be written to adhere to the agreed-upon API. The coarsest level of component granularity is mainly set by obvious considerations of physics functionality (we need components for core microturbulence, RF sources, data analysis tools, etc.) and at a finer level (sub-components) by mathematical functionality and reusability (for example, linear and nonlinear solvers).

1. Components should be provided in source form so that they can be modified as needed for bug fixes or to fit within the physics composition framework, whether the framework requires minimal modifications (e.g., changes to I/O) or more extensive modifications. This should simply be stated as a requirement for inclusion of a component.

2. Components should come with a suite of test problems for each component along with accepted results. Tests for individual components should exercise the features of the component, along with results. Tests should be repeatable at the numerical precision level, thus implying at minimum control over message patterns and quasi-random number sequences. This control must be exposed to the framework; in particular, a component should be able to accept a specified seed from the framework to enable insensitivity of coupled simulations to small parameter changes (see composition software requirements in Sec. IV). We note that the maintenance of what would otherwise be strict continuity

when Monte Carlo components are included in a simulation is not possible in general (for example, a neutral-beam particle deposited near the edge of the plasma will at some point, as all other parameters change continuously, fail to be trapped in the plasma, leading to a discrete jump); nevertheless, by employing seed control significant improvements in insensitivity can be achieved, which in turn improves reproducibility and facilitates debugging of complicated codes. There is no technical obstacle here, but a fair amount of work may be required for a legacy code to expose control over quasi-random number sequences and message patterns to the framework.

3. Components should provide for a mode in which their results are insensitive to small changes of initial parameters. In the case where a component has multiple chains of random events in a component, a technique must be provided to ameliorate the consequences of possible changes in the number of random number invocations in a particular chain. This is generally not done in magnetic fusion energy (MFE) codes and so is a gap. An example of a solution technique is combing [Monte Carlo Methods, Vol. I, Mal Kalos and P. Whitlock, Wiley-Interscience (1986)]; we need to determine if there are alternatives.

4. Components should provide provenance, i.e., sufficient information to achieve reproducible results, including source code version, versions of external libraries, and compilers and their versions. This is a matter of supplying the necessary effort.

5. Components should be able to check-point restart and integrate forward precisely as if they had not been restarted. This requirement also applies to component suites used in a physics composition. Most but not all components in the MFE community have such a capability. This capability is new or in development for the proto-FSP's. A substantial amount of work may be required to implement this capability where it does not exist.

The following grouping of requirements involves no fundamental technical obstacles, but many candidate components fail to provide one or more of these; some effort is required to remedy:

1. Components should be able to revert to the state prior that that of the current time step (as needed for implicit coupling). This requirement requires saving prior-state information.

2. Components should be able to exit gracefully and provide an error code.

3. Components should allow for specifiable input and output file names.

4. Components should not have hard-wired input/output; in particular there should be settable log files (versus sending output to stdout, for example).

5. Components should have any embedded graphics disabled, but with data necessary to produce component graphics included in what is available to the framework.

6. Physics component precision should not be set by a specification on its compilation line; rather, precision should be specified in the source code.

7. Components need to work on a common set of (preferably multiple) platforms and come with a cross-platform build system for building them on multiple platforms. This is in some cases a gap; some codes in the MFE community are customized to a very limited set of platforms. Remedying can entail substantial effort.

6.D.2. Requirements on composition software

The composition software itself is expected to fulfill the following requirements:

- Provide the infrastructure to enable various types of code coupling, including the sort of "tight", in-memory coupling that is inherent to strongly coupled codes, including implicit coupling;
- Make coupling algorithms, which support multiple types of code coupling, available as services;
- Make available conservative data interpolation services between different grid representations;
- Support verification testing of components both individually and in composition;
- Provide efficient transfer of data between models with differing parallel decomposition (MxN problem);
- Support orchestrated checkpoint/restart of individual components and complete WDM code;
- Provide access to experimental data for model validation tests or use within WDM;
- Provide documentation of the supported types of physics composition, coupling algorithms, and data interpolation methods, as well as the component execution models, parallel decomposition, and data interfaces (quantities and units).

Due to the wide range in fidelity and capability of the physics models that will be brought together in WDM, it is understood that the complete WDM simulation will require coordination of many different computational tasks involving multiple types of computing resources. For example, 3D particle-based turbulence models will be run on the largest parallel computing platforms available, while a reduced dimension transport model or an eigenmode analysis tool may operate sufficiently on a workstation. Surrounding the operation and interaction of such models are additional tasks such as input file creation and validation, file transfers, data analysis and reduction, and data visualizations. A scientific workflow can help to orchestrate these tasks and manage the allocation of computational resources, while also providing opportunities for reuse across multiple applications. Thus, it is anticipated that the FSP-WDM framework should possess several key attributes in support of task composition, including the following:

- Universal workflow software, in the form of either a scientific workflow system such as Kepler or a script-based solution (such as shell scripts or Python), or perhaps some combination of these;

- Ability to record provenance data on physics models, computer system, compilers/libraries, etc.;

- Input file preparation, staging, and validation (especially in the context of coupled models);

- Efficient and flexible I/O libraries with rich metadata to support large-scale physics components;

- File migration between parallel computing facilities and integrated data management systems;

- Non-interactive data analysis and visualizations via scripted tools or services (such as IDL or Visit);

- Interactive simulation monitoring and data analysis through web portal or dashboard systems that can drive graphical analysis tools and display results in real time.

6.E. Validation requirements

Validation of the integrated whole device model (WDM) against experimental data is an essential but extremely challenging part of the FSP project. It is essential because it builds confidence and credibility in the predictions of the model, and challenging because it involves so many component models working together. It is recognized in the code development community that validation in the strictest sense cannot be done for a complete model, but rather for a range of model problems in a range of parameters characteristic of the problems the code is expected to address. Here we describe some of the processes that contribute to the validation.

6.E.1. Validation of component models

Validation of the component models that together form the whole device model is an absolutely key first step. Models for transport, for example, must be validated in detail before validation of the WDM can proceed. Transport models, for example, are now in the process of being extended and validated in tokamak experiments that attempt to isolate transport effects for this purpose. Discharges without MHD activity, like sawteeth, ELMs, tearing modes, and Alfven eigenmodes, are used to simplify the test that the fluctuations calculated by the transport model are in fact what is driving the transport. Quantities like density and temperature fluctuations and their cross-phase distribution are being measured as a way of testing each model at a higher level than simply the gross transport effects. The key parameters to which the model is found computationally to be sensitive are varied keeping the other dimensionless parameters fixed, and the results are compared with experiment. If this is done successfully over the range of dimensionless parameters – like normalized Larmor radius, collisionality, elongation, T_e/T_i, beta, safety factor, and so on – then the model can be considered valid over that range. This conclusion, however, is limited to the types of discharge for which the comparisons were made.

Metrics for validation need to be determined. Quantifying and evaluating partial success at predicting phenomena is a key part of validation. If a transport model predicts fluctuations and transport consistent with experiment at a normalized minor radius rho=0.5, but with poor agreement at rho=0.75, to what extent can the model be considered validated and used with confidence in a very complicated WDM?

The component model validation is well advanced in some topical areas, including 2D equilibrium reconstruction, ideal MHD instability, and some heating sources like neutral injection and electron cyclotron heating. In most other areas there is a great deal of component model development and validation to be done before validation of a complete WDM can be completed. Much of model validation at this level can be and is being done using today's 1.5D transport codes.

6.E.2. Validation of simplified combinations of models

A tokamak discharge may have a large number of physical processes occurring simultaneously. First, the equilibrium must satisfy ideal MHD stability requirements and include possible nonaxisymmetric effects like magnetic islands driven by native and applied magnetic perturbations. Near the axis, the discharge may exhibit the relaxation oscillations called sawteeth. In the plasma core, there will be neoclassical transport and other neoclassical effects like Neoclassical Toroidal Viscosity (NTV) as well as turbulent transport mediated by the density and temperature gradients and shear in the magnetic structure and toroidal and poloidal flows. The core may also be affected by energetic particle modes and classical or neoclassical tearing modes (NTMs). In the pedestal region calculations of turbulent transport and MHD stability are computed by other models, and periodic ELMs must be assessed for their effects on the whole discharge. The connection between the pedestal and the Scrape Off Layer must be modeled, and interactions with the wall, especially in the presence of ELMs, must include the generation of impurities and their transport into the plasma with attendant radiation losses and their flow into the divertor. Add fueling and heating and current drive in a not-fully-axisymmetric system, and time dependent effects like relaxation of poloidal flux on the resistive time scale, and the resultant whole device model can be seen to be extremely complex with many interactions between models. An example suggests the nature of the interactions: energetic particle modes affect the background microturbulence, and the microturbulence affects the transport of energetic particles and hence the energetic particle modes, so the WDM must address this combination of phenomena self-consistently.

It is clear that WDM validation in a fully complex tokamak discharge is extremely difficult. Even if all the component models have been validated in the regime of interest, it would be very difficult to identify the nature of a discrepancy with the model in such a discharge. But the FSP WDM has an advantage over models like those for world climate: we can devise experiments in which as few of these phenomena are occurring as possible, with as simple as possible controlled conditions, the validation can be carried out piecemeal.

So the second phase of the WDM validation procedure will entail comparisons between the model predictions for simplified situations. For the example cited above, of turbulent transport in the presence of energetic particle modes, experiments could be performed in discharges without any MHD activity like sawteeth or tearing modes or ELMs that would affect the core transport. Another example would be poloidal flux transport in the presence of NTMs, which would involve the interacting models for resistive poloidal flux transport and resistive MHD stability. These validation studies would be done first in a time-independent way, where that makes physical sense, and then in a time-dependent mode.

A very large number of relatively simplified interactions between models can be devised. Many of these represent physics problems important to the fusion community, which would be addressed even outside the context of the FSP. Progress on these physics tasks will support the FSP WDM validation process.

It is important to note that much of the validation process can be done using simplified or reduced models for phenomena considered not immediately relevant to the particular study. For example, a calculation of core turbulence and its interaction with energetic particle modes may be judged to not require a sophisticated model for the SOL and plasma/surface interaction. Use of a simplified model for the SOL would, in this case, greatly simplify the calculation procedure with probably little effect on the conclusions.

6.E.3. Addressing the WDM Goals

Over the long term of 5 to 15 years, a successful conclusion of many of these "somewhat simplified" validation activities will establish the plausibility of calculations in fully complex conditions. The third phase of the WDM validation process would be testing the model against experimental data for the challenge faced by the FSP: self-consistent simulations of the entire plasma discharge evolution, including all of the relevant physical phenomena from the axis to the wall with high fidelity component models.

6.E.4. Requirements on Experimental Data

During the course of the validation process, it will be necessary to have data from a broad range of plasma diagnostics and other physical measurements. Generating the data that can be compared with the model usually involves complicated analysis. The derivation of physically meaningful values might involve fitting a curve to measurements (e.g., deriving the electron temperature from the slope of the scattered photon wavelength distribution), performing inversions of chordal measurements, or subtracting polluting contributions. These kinds of processes and many others introduce uncertainties in the value of the data points. Data points are then frequently fit to a curve for use as profiles in the model, and this fitting introduces further uncertainties. So it is extremely important in the validation process that these uncertainties in the experimental data be evaluated correctly and fully propagated in the calculations.

Likewise, development of "synthetic diagnostics" in the code models is essential in the correct interpretation of experimental data. Synthetic diagnostics interpret the calculated quantities in terms of what specific diagnostics would measure, given the specific diagnostic's characteristics.

6.F. Connections to other work

Whole Device Modeling (WDM) requires input from every other part of the Fusion Simulation Project (FSP) as well as input from the rest of the fusion community. WDM requires a complete collection of modules for equilibrium, sources, sinks, transport, turbulence, onset and consequences of macroscopic instabilities, fast-particle distributions and plasma-wall interactions. All aspects of the integrated modeling framework are needed for WDM simulations. Close and seamless connections are needed with experimental data and other simulation results in order to validate and verify WDM simulations. Improvements to WDM will require a close collaboration with the rest of the fusion community to develop improved theoretical models and to provide detailed experimental tests of WDM simulation results. The SciDAC projects will provide input to WDM in the form of improved models and framework, as well as using the output of WDM simulations in order to carry out more detailed simulations of individual physical phenomena in a post-processing mode.

As it is illustrated on Fig. 1, the WDM will provide output to the other science drivers by:

- Validating specific physical components that are derived in other science drivers or in the SciDAC projects. Such validation is often possible only in content of whole device modeling codes;

- Deriving reduced models that would describe effects that are associated with interaction between multiple physics components.

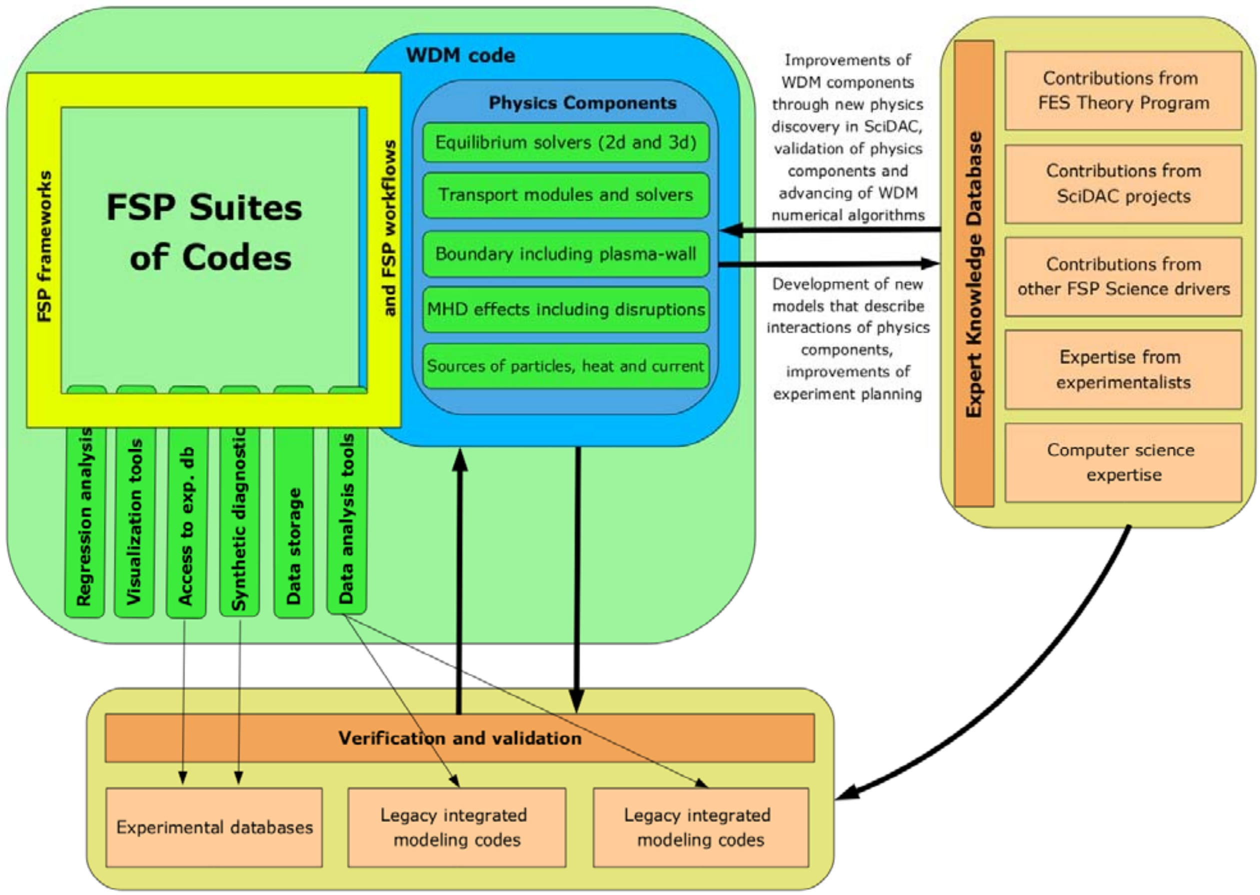

Fig. 1. WDM code as a part of the FSP suites of codes.

The most immediate WDM connection will be to the wide range of components that will be required for nearly every WDM simulation. The required components include the following:

- Sources of heat, particles, current and momentum: Many of the source modules have reached a relatively high level of maturity. Monte Carlo computations of neutral beam injection (NBI), for example, provide high-fidelity results for all channels of the NBI source as a function of radius and poloidal angle within the core plasma. Fokker Planck computations of radio frequency heating have matured considerably for low-frequency full-wave calculations and for high-frequency ray tracing. Existing modules for NBI and RF sources can be adapted to the FSP WDM framework while those modules are being incrementally improved.

- Atomic physics and nuclear reactions: Relatively mature tables of atomic and nuclear cross sections are available and the algorithms for using these cross sections are currently employed in WDM codes. Three-dimensional Monte-Carlo computations of the interactions between neutrals and tokamak plasmas have been developed over decades.

These modules are needed to compute radiation and charge-exchange losses from the plasma as well as sources of ions resulting from edge neutrals and neutral beam injection.

- Equilibrium plasma shape: Many equilibrium modules have been developed over the past six decades and they are constantly being improved. Free-boundary and prescribed boundary 2-D axisymmetric equilibrium modules are currently used in all WDM simulations. Free-boundary equilibrium computations include calculations of the interactions between the plasma current and magnetic coil currents, including eddy currents in all of the conducting structures of the tokamak. Three-dimensional equilibrium modules — which include the effects of magnetic islands, stochastic magnetic field regions, externally applied resonant magnetic field perturbations and non-axisymmetric magnetic ripple — are available, but 3-D equilibrium modules need to be hardened for use in WDM codes and the WDM framework needs to be developed in order to make effective use of 3-D equilibria.

- Transport and turbulence: Most existing WDM codes use reduced models for anomalous and neoclassical transport. There has been a considerable effort to improve reduced transport models over the last few decades but, currently, different transport models that agree with experimental data about equally well produce different results in simulations of future burning plasma experiments. There have been several successful research efforts aimed at producing self-consistent simulations of turbulence and transport using gyro-kinetic codes. Turbulence codes will be merged in with WDM codes using an appropriately tight coupling for self-consistent turbulence-transport simulations in order to bridge the gap between the microsecond time scale of turbulence and the multi-second time scale of transport. Gyro-kinetic codes will also be used within WDM simulations in order to compute neoclassical transport with finite banana orbits extending out to the first wall. Improved 2-D transport modules must be developed for simulations that include the scrape-off-layer plasma. Ultimately, 3-D transport modules must be developed to compute the interaction between transport and macroscopic instabilities, including slowly evolving magnetic islands and resistive wall modes.

- Episodic macroscopic instabilities: Improved modules are being developed in order to compute the frequency and consequences of periodic macroscopic instabilities such as sawtooth oscillations and edge localized modes (ELMs). These reduced modules are currently being used in WDM simulations and they can be adapted readily to the FSP WDM codes. In addition, high-fidelity computations of sawtooth and ELM crashes are being carried out by various SciDAC projects in an effort to improve the fundamental understanding and reduced modules of these phenomena.

- Slowly evolving macroscopic instabilities: Reduced modules are available to predict some aspects of neoclassical tearing modes (NTMs) and resistive wall modes (RWMs), which can evolve on transport time scales in tokamak discharges. SciDAC projects are investigating these modes in detail using high-fidelity computations. It is anticipated that both reduced modules and high-fidelity computations of slowly evolving macroscopic instabilities will be needed within the FSP WDM framework.

- Disruptive instabilities: The onset of those disruptive instabilities driven by NTMs has been computed in WDM simulations, but that capability is currently not available in the major WDM codes. Implementations of modules designed to predict the onset of disruptive instabilities, which terminate the tokamak discharge, are a high priority for the FSP WDM codes. Nonlinear extended MHD codes have been used to follow the evolution of disruptive instabilities. Those simulations involve the close interaction between macroscopic instabilities and the enhanced transport and resulting profile changes that the macroscopic instabilities produce.

- Fast particle effects: Macroscopic instabilities are observed to be influenced by the distribution of fast ions and electrons. Fast ion distributions are computed by NBI and RF source modules, but only some moments of the fast ion distributions have been used to compute the onset of sawtooth crashes. A more complete connection must be developed to reproduce the effect that fast charged particles have on the instabilities observed in tokamak discharges.

- Plasma-wall interactions: Rudimentary recycling models are used in existing WDM codes to compute the influx of neutrals from the first wall in tokamaks. Significant progress is needed to improve the plasma-wall recycling and power deposition modules for use within the FSP WDM codes. Modules are needed to compute the impurity influx rate as well as the complete interactions with the scrape-off-layer plasma.

- Connection to experimental and simulation data: A close collaboration will be needed between FSP and the experimental and SciDAC communities in order to produce a seamless connection with experimental data, to set up simulations and validate results, and with the larger simulation community, in order to verify FSP WDM modules and to hand off FSP simulation results to more specialized computer programs.

6.G. Schedule and Resources

The FSP Whole Device Model (WDM) schedule is broken down into four thrusts plus the central team and production system :

- 2.5d WDM & transport solver (3d equilibrium, 1d transport).

- WDM components for fast particle evolution and sources which take into account RF coupling to fast ions created by neutral beam injection and/or fusion reactions.

- WDM components for evaluation of plasma turbulent transport on transport time scales.
- WDM that couples in edge and wall models (with successive fidelity).
- WDM "central team" and production system.

For each of these, estimates are made of:

1. Projected schedule of work to be carried out over a 15 year time period.
2. Realistic estimate of resources required.

6.G.1. Background considerations:

1. *Need for multidisciplinary teams*. The key physics models needed for advanced FSP components will come out of physics research carried out in the base program (and perhaps with additional direct FSP support in years to come). These are generally codes written by research physicists working in theory and computation. But, as indicated in section V "Software Integration and Support" of the March 2010 FSP planning workshop report, the technical requirements on FSP components are very demanding. These go far beyond what is normally or traditionally produced within MFE theory/computation oriented research programs. In addition, WDM use imposes a reliability constraint on components far greater than is needed in single physics research prototypes: a 99% reliable package called 99 times has a 73% chance of failing at least once. Significant *computational engineering* labor will be needed to bridge these gaps, and, FSP will need to pay for it. For WDM it is vital that this issue be addressed appropriately, as the ability to integrate components is critical to WDM construction. To meet this requirement, computational engineers will need to be requisitioned and assigned to work closely with physicists, roughly one for each major component supplier research group. In addition, WDM will have responsibility for integration of necessary components not covered by any FSP science drivers—MHD equilibrium solvers, for example—and this will necessitate an FSP WDM multi-disciplinary core team combining physicists and computational scientists and engineers.

2. *Need for engineering support*. No user of a multi-physics WDM is expert in every component. Support for use of physics components by non-experts is what drives several FSP component requirements. Meeting these requirements, as well as the purely technical requirements of portability and build systems, involves demanding tasks that do not in themselves contribute directly to publication-ready research in any field. There needs to be staff that is rewarded simply for getting the necessary work done, and not penalized for lack of peer reviewed publication, i.e.: engineering staff. It is not customary for theory

and computation projects in OFES or OASCR to support non-research staff—nevertheless there is a pressing need.

3. *Staffing considerations*. Management presentations for U.S. SciDAC projects as well as overseas projects (e.g. the European ITM—Integrated Tokamak Modeling initiative) frequently point out the inefficiency of the assignment of small fractions of people to work on projects. In fact the practice is disastrous—in terms of accountability it is a nightmare and generally the fractionally assigned person is unavailable for close collaboration when urgently needed. Nevertheless small fraction assignments are widespread. This is partly because past theory and modeling project funds have been too thinly spread across too many institutions due to "political" considerations. It is also due to the fact that such projects have in the past been funded by raiding the theory base program, such that both institution by institution and OFES program wide, new program initiatives have not in fact justified any hiring or staff expansion. This has meant that assignment of project tasks had to fall to senior staff already committed to multiple pre-existing projects and only available at low fractional levels in any case. To meet its goals FSP must do better. It is supposed to have the requisite resources (if it does not, it should not proceed). In its internal planning, ITM does not even count staff assigned at less than the 50% level and FSP should do likewise.

4. *Schedule considerations*. The requirement of FSP to bring on new skilled staff (whether computational engineers or physicists or computational scientists) implies a *likely* delay of one year for any project milestone dependent on the new staff hires. This is because it takes up to 6 months just to make such a hire, and in many cases an additional 6 months or more to effectively integrate new staff into a project which is involved with every aspect of magnetic confinement plasma physics.

5. *Special implications of reduced physics models*. It frequently happens in the use of WDM codes that reduced models are needed to approximate certain physics, in order to allow WDM studies to be carried out in a timely manner on such computational resources as may be available for a given project. WDM use considerations drive the need for reduced models, but their strong simplifying approximations can be problematic from the standpoint of verification and validation. Collaboration between WDM central team staff, specialists from the non-WDM science driver teams, V&V teams, and user groups will be needed to determine appropriate treatments; schedule and resource requirements will be affected.

6.G.2. Schedule and resources for four high priority thrusts

6.G.3. 2.5d WDM MHD equilibrium, stability, and transport solver.

This WDM thrust entails integration of 3d MHD equilibrium codes with transport solvers and models adapted (at least initially) from existing 1.5d legacy codes. It also includes the development or use of software for detection of MHD instability, and a data output capability to provide initial conditions for detailed non-linear 3d MHD modeling (e.g. of disruptions). It is likely that transport effects of slowly evolving 3d MHD phenomena will need to be represented with reduced models for some time to come.

The effort needs to address design strategy issues early, in particular the nature of the 3d MHD equilibrium geometry to be used as the fundamental basis for modeling, and, the strategy for modeling the interaction of 3d magnetic islands with transport and sources. This is likely to involve a need for theory development, the outcome of which could affect schedule and resources. However, there is already considerable experience in the community with use of standalone 3d models; it is possible to articulate near term goals and resource requirements. Applications of this thrust will rely also on the development of core plasma transport models.

In what follows, schedule years denote time from start of project. For types of staff the following acronyms are employed:

- PI – Principle Investigator, lead physicist (research staff)
- PD – Post-doc or staff physicist below level of lead (research staff)
- CE – Computational Engineer (engineering staff)
- CS – Computational Scientist or applied mathematician (research staff)
- Year 1:
    - PI assigned; available 2.5d equilibrium codes assembled and tested standalone: VMEC, PIES, …
    - 2 CEs hired.
    - Probe 2.5d model problems with prototype code.
    - Plan and start the FSP componentization of VMEC (prescribed boundary equilibrium, nested flux surfaces).
    - Plan and start the FSP componentization of PIES (islanded free boundary equilibrium with prescribed boundary option).
    - Inventory of reduced models needed for basic equilibrium and transport evolution.
- Year 2:

- Complete FSP componentization of VMEC (0.5 FTE CE).
- Computation in place for flux surface averages needed for 1d transport equations (as derived from the 3d MHD equilibrium).
- Provide Flux diffusion calculation in 3d equilibrium [Strand and Houlberg, Phys. Plasmas 8, 2782].
- 1d transport equations working with simplified sources and boundary conditions and reduced transport models.
- All reduced models in place for basic equilibrium and transport evolution.
- First 2.5d simulations with prescribed boundary 3d equilibrium and closed flux surfaces; benchmark with TASK 2.5d.
- Inventory of reduced models needed for MHD stability assessment and effects of slowly evolving MHD island structures.

- Year 3:
    - Complete FSP componentization of PIES (1.0 FTE CE).
    - Reduced models in place for MHD stability assessment and MHD island representation.
    - MHD stability assessment working; ability to output 3d initial condition data to non-linear 3d MHD stability code.
- Year 4:
    - Source models (NB, RF, fusion alphas) adapted for 3d.
    - 2.5d prescribed boundary simulation including magnetic island evolution, with adapted reduced transport models.
    - 2.5d free boundary simulation with nested flux surfaces in the confinement region.
    - Coupling to non-turbulent gyrokinetic code, simulations of neo-classical island evolution.
- Year 5:

- Model ready for detailed validation against observed 3d effects in tokamaks and stellarators. Universal applicability of reduced models not expected.
- Production deployment for validation studies.

- Year 10:
  - 3d edge/SOL/wall coupling – if deemed feasible.
  - Core transport models specifically adapted for 3d.
  - Core model useful for prediction of 3d effects in experiments, using input data for boundary conditions.
- Year 15:
  - Core/edge combined model useful for prediction of coupled core edge system behavior.

Resources:

- Years 1-2: {PI, 2*CE, PD}
- Years 3-5: {PI, 2*CE, 2*PD}
- Years 6-15: {PI, 2*CE, 3*PD, CS} – if core/edge coupling is attempted; otherwise continue at year 3-5 level; an additional CE may be required if core model production deployment results in wide use. Complexity of core transport in 3d equilibrium might also require addition PD labor resources.

6.G.4. RF coupling to fast ions.

This project can leverage ongoing efforts of the RF SciDAC and SWIM FSP prototype SciDAC projects to address physics that is observed in current experiments. In particular, the RF-SciDAC has a milestone for FY-2013 Q3, to validate NUBEAM/AORSA against observations of RF resonant fast ions in NBI+ICRF experiments in JET and NBI+HHFW experiments on NSTX and DIII-D. Nevertheless, a push will be needed to make the product of these efforts available for a wide user base in deployed WDMs. This project represents an opportunity for FSP to make important contributions to the wider OFES program, within 2-3 years.

The project involves interaction of ICRF or HHFW fields with non-Maxwellian fast ion distributions f and there are two main strategies based (a) on continuum representation of f (e.g. codes such as CQL3D), and (b) particle representations of f (e.g. codes such as ORBIT-RF or NUBEAM). For verification and validation purposes both approaches should be integrated into a shared WDM framework and made available for detailed comparison against each other and (with diagnostic simulation) against measurements over a range of plasma scenarios.

Due to a targeting of early deployment, one or more legacy WDMs will be used. However, any component installations will be based on coupling methods that are sure to be reusable in future FSP WDMs. As these couplings do not involve tight non-linear interactions at short time scales this is expected to be practical.

- Year 1:
  - PI assigned (preferably an RF physicist in the SWIM or RF SciDAC projects).
  - CE assigned or hired.
  - CE familiarized with important codes relevant to this work: TORIC, AORSA, NUBEAM, CQL3D, ORBIT-RF
  - Legacy WDMs (such as TRANSP or ONETWO) identified as target for deployment; CE familiarized.
  - NERSC port of selected legacy WDMs by CE.
- Year 2:
  - Verify componentization of important codes; improve as required.
  - Install RF code / CQL3D combination in legacy WDMs.
  - Install RF code / NUBEAM combination in legacy WDMs.
  - Test using RF-SciDAC identified shot data.
- Year 3:
  - Production deployment and support.
- Year 5:
  - Production deployment and support in high performance FSP WDM.

Resources:

- Years 1-3: {0.5*PI, CE} – experienced RF physicist connected with SciDAC if available. If not additional resources may be required for RF physicist training.

- Out years: {0.5*PI, CE} for production support; integration with FSP high performance WDM frameworks.

This relatively short term FSP project should serve as a demonstration of the ability of the FSP effort to put tools in the hands of researchers in the wider OFES/MFE community.

6.G.5. Plasma turbulent transport on transport time scales.

There are two main lines of development, the first using reduced transport models, and the second developing ways to make more direct use of first principles transport models at transport, confinement, or whole discharge time scales. Since the turbulence codes are more advanced in the plasma core region than in the edge region at the present time, fidelity of the reduced transport models is expected to be higher in the core region in the earlier phase of the project, until the edge turbulence codes are more advanced. Two approaches are desirable. FSP WDM can include both core and edge, as is done in some legacy WDMs and as described here, and it can separate the core and edge plasmas into two components with a spatial coupling between them, as described in VII.2.4.

For the development using reduced transport models, n the past there have been separate, insufficiently funded efforts, associated with each legacy WDM (1.5d transport code), to address turbulent transport by means of coupling of reduced transport models (e.g. GLF-23, MMM, TGLF, installed or attempted in PTRANSP, ONETWO, TSC, Corsica). The FSP WDM effort can have an impact here by providing adequate resources to a unified effort. It should be noted that progress in componentization of models means that such an effort can go forward without prior selection of a legacy WDM as a basis. Three promising efforts are currently in progress: (a) FMCFM in the FACETS SciDAC, (b) a SWIM SciDAC Plasma State based approach being developed and expected to be tested in TSC, SWIM, and PTRANSP, and (c) reduced-dimensional kinetic based WDM approach in the CPES SciDAC, which uses reduced transport models (*e.g.*, GLF-23, MMM, and TGLF) for transport time scale plasma profile evolution while keeping the background kinetic effects such as the particle orbit dynamics and the neoclassical polarization effect. 4d Cogent and XGC0 can be used as WDM basis. Approaches (b) and (c) may require higher computational resources than (a). A fully funded FSP effort leveraging reduced models would include enhanced engagement with research groups developing and applying first principles models, by more fully supporting step (1) and particularly step (3) of the three-step process around which the reduced model methodology is organized:

1. Reduced models derived from parameter scans of first principles models;

2. Reduced models applied at transport time scales in WDMs;

3. First principles models applied to time slices of WDM results for verification.

Finally, WDMs using the reduced models with verified and accepted solver methods would be broadly employed in validation efforts against the wide range of available experimental results. This would be done with the understanding that for fundamental reasons the reduced models are incomplete and that their predictive capability will by no means cover every experimental situation.

For the second line of development, first principles codes can be coupled to a reduced WDM at time intervals to increase its fidelity. Existing examples are neutral bean and RF modules in PTRANSP, turbulence , MHD and other modules can also be coupled to a reduced WDM, as being developed in the SciDAC projects as WDM basis. There are existing mathematical techniques for such couplings (e.g., Gear-Kevrekidis equation-free method and Jacobian-free Newton-Krylov method). In this development, large amount of data may need to be coupled between the reduced WDM and the first-principle codes. CPES EFFIS or FACETs approaches can be used for efficient in-memory or in-file couplings in such a WDM framework. This framework will be a large-scale computing component of FSP WDMs.

The most ambitious direct applications of first principles models face major challenges. The March 2010 FSP workshop report (section IV-D) makes clear that "new theoretical and numerical formulations" will be needed for global GK simulation methods, coupled with models for overlapping time-space scale MHD phenomena, to reach transport time scales. Although it is not possible to schedule application of methods faced with such fundamental open research questions, there may be scope for direct application in situations where overlapping MHD effects are negligible. Where feasible, such applications would still be expected to have accuracy advantages over indirect approaches based on reduced model approximations or fits.

- Year 1:
  - Experienced PI assigned (presumably from prototype FSP SciDAC project).
  - Survey and assessment of existing WDM transport capabilities including results of FSP prototype projects.
  - CE hired or assigned.
- Year 2:
  - Development of at least one componentized solver module with access to all reduced transport models embedded.
  - Numerical and performance issues of solver/transport component understood in context of reduced models.
  - Componentized solver installed in legacy and/or FSP prototype WDMs, verified and available for production use.
  - Establish kinetic-based reduced WBM with MHD perturbuation included.
- Year 3:

- Framework for verification of WDM time slices by first principles models.
- Design for extension of solver/transport component to incorporate 1st principles transport models in both fluid-based and kinetic based reduced WBMs.
- Production deployment for reduced model validation.

- Year 5:
  - Transport time scale 1st principles simulation validated when overlapping MHD not present.
  - Design for turbulence time scale 1st principles simulations embedment into WDM.
  - All core transport components deployed in new high performance FSP WDM(s) as these are developed. Deploy available edge transport components.

- Years 6-10:
  - Verification and validation of transport time WDMs, with space-time embedded turbulence-time-scale first principles gyrokinetic codes.
  - Development and testing of coupling techniques to 1st principles gyrokinetic turbulent transport components, as transport-timescale gyrokinetic formalism becomes available.

- Year 10:
  - Wide production use of transport-timescale WDM using 1st principles turbulent transport models.

- Year 15:
  - If research results allow, combined 1st principles transport and MHD, at transport time scales.

Resources:

- Years 1-2: {PI, CE, CS, PD}
- Years 3-5: {PI, CE, CS, 3*PD}

- Years 6-15: {PI, 2*CE, 3*PD, 2*CS} – expansion of FSP effort if warranted by results of base program core transport theory/computation efforts.

6.G.6. Self-consistent, coupled, core-edge dynamics

While many of the physics component efforts in this area are necessarily very long term, it is possible within the first few years to bring forth a coupled, core-edge capability in the first few years of FSP. This will, of course, be only as reliable as the underlying physics components, which must model extremely complicated behavior. Indeed, beyond the coupling to the edge are internal transport/turbulence couplings within the edge and coupling to the wall. We do not further call these out here, as they are being considered by a separate science driver (Boundary Layer).

However, there are already appearing models for the edge region and wall, and these will only improve as the FSP progresses. In the first few years, it is reasonable to expect coupling to physics based static (time-averaged) pedestal models, such as EPED, which predicts pedestal heights parametrically, or to XGC0, which predicts (2D) pedestal buildup due to neoclassical or prescribed diffusivities. In the out years one can expect coupling to fluid turbulence computations, such as those provided by BOUT++, and subsequently to kinetic models, such as those provided by COGENT and/or XGC1. In all cases tight coupling to the edge region is required in a WDM scenario where the core and the edge are considered to be two separate components. Therefore, the development of coupling capabilities now will allow the incorporation of early models and their successors as they become available.

While there are many uncertainties, staffing is needed for addressing the coupling issue as well as for componentization of existing static models based on pedestal buildup saturated by at the onset of linear instability.

Because of urgency of modeling applications which can account in some manner for core-edge dynamics, there will be considerable interest in reduced model approaches. It is likely that WDM staff will be engaged in the prototyping, testing, and deployment of promising reduced model approaches.

- Year 1
    - Staff assigned {0.5*PI, 0.5*CE}
    - Initiate testing of edge coupling in existing efforts.
    - Initiate componentization of linear static Pedestal:
        - Address robustness, error handling and automation issues.
        - Address documentation and portability
- Year 2

- Linear static Pedestal component completion
  - Work with Boundary Layer effort on wall coupling.
  - Installation in FSP WDM coupling computational applications.
  - Support for production and validation applications.

- Years 3 and on
  - Explore reduced model methods for incorporating additional core-edge dynamics.
  - Incorporate higher fidelity pedestal components, including full turbulence models.

Resources:

- Years 1-2: {0.5*PI, 0.5*CE}
- Out years: at a reduced level, continued support for production and validation applications. Ramp up staff as edge/wall components mature to readiness for WDM deployment.

There would appear to be formidable challenges of integration, for Pedestal, ELMs, SOL and 1st wall components to work together even without a core plasma coupling. Indeed, such integration could well be of greater difficulty than the construction of *entire* core plasma oriented WDMs and would need to be resourced accordingly. The general considerations of component requirements and need for CE staff applies in this area even in its pre-WDM stages.

6.G.7. WDM "central team" and production system.

The March 2010 FSP Workshop Report section IV-G (Whole Device Modeling) includes a list of typical desirable physics models or components. The following is a subset of this list that is not clearly covered by other science drivers, and therefore likely to fall to the WDM central team for development and support:

- 2d/3d MHD equilibrium solvers—this is the locus of failure of many if not most current day WDM simulations!
- Development of 1d transport solver capable of robust, accurate solutions of stiff transport models.
- Neutral beam heating and torque and current drive.
- Neutral beam, pellet, gas injection, and recycling particle sources in the core, with associated atomic physics.

- Neoclassical resistivity and bootstrap models; poloidal field diffusion equation.
- Radiation (Bremsstrahlung, line, cyclotron).
- Fusion reactions and fusion fast ion source.
- Free boundary MHD equilibrium coupling to PF coils, conducting structures, and tokamak feedback systems.

This list should be supplemented with these necessary items (alluded to in the report text):

- Access to experimental data.
- Diagnostic simulation, with associated atomic physics.

The WDM central team would likely need to be involved with extraction of best models from legacy WDM transport codes, as recommended in the report.

Within the FSP program, the WDM central team and production systems support staff would have strong interaction with all teams responsible for components, frameworks, and validation, as well as science drivers.

As the WDM central team will likely include first adopters of new components, it would be appropriate for the WDM central team to play a role in assessing whether candidate codes meet FSP developed component standards. This activity would revive and extend the "NTCC modules library standards committee" efforts of the late 1990s and early 2000s. Experience shows that a formal process for component assessment clearly benefits software quality. It is expensive in labor, but effective FSP software integration absolutely requires a software quality assurance process. This has also been shown by the experience of the more recent FSP prototype SciDAC projects. It is important to note that for component development teams to be able to respond to componentization standards review recommendations, they will need CE support. This is expensive, generally lacking in traditional MFE computational physics efforts, it is a resource gap that must be filled by FSP if the program is to be successful. Every major FSP component provider will need FSP financed CE support.

The WDM central team will also need to be involved in the development and extension of data repository components and standards to facilitate inter-component data sharing and communication. This would entail evaluation and planning on adoption of tools such as the SWIM SciDAC "Plasma State", or, possibly, the "Consistent Physical Objects" (CPO) of the European ITM program. This area also encompasses standardization of machine hardware description: coils, antennas, neutral beams, vacuum vessel, etc. Many of these data items have to be shared across multiple components and codes, and the standardization of their representations will greatly aid software integration processes. The "Plasma State" effort has made a beginning on addressing such needs but further development is needed. Data standards will affect software component development strategies, so, these need to be established early in the project.

As many users will access FSP capability through execution of WDM models, it is logical for the WDM core team to be involved with the development and support of production systems, and the support of research teams using the models for FSP and component validation exercises. Even for validation focused on individual components, an WDM is likely to be needed in order to couple to the experimental data—experiments being performed in whole devices.

The WDM central team would need to be involved in evolving a design for usability standards and organization of data management and handling and support of production systems. This group would need to deal with all aspects of FSP, i.e.: framework, components, and validation, not just science drivers. It is likely that user feedback would come back to FSP through this group, and this should affect planning and development of at least the engineering aspects of FSP.

- Year 1
  - Assignment of PI from experiment or validation community.
  - 2 CEs assigned or hired.
  - Establishment of software component standards review process.
  - Development of data standards planning group:
    - Plasma State or successor.
    - Machine Description, Shot Configuration.
    - Access to Experimental Data.
    - WDM control input data.
    - WDM time dependent output data.
  - Development of plan for extraction of components from legacy WDMs:
    - Inventory.
    - Prioritization.
  - Establishment of NERSC-based production system for legacy WDMs:
    - Collaboration with base program funded legacy WDM teams.
- Year 2
  - WDM validation capability on NERSC

        - This may include SciDAC FSP prototypes {SWIM, FACETs, CPES}, and the FSP frameworked WDM.
        - Prioritization based on demand of research/validation user groups.
    - First FSP component installation in legacy WDMs:
        - Collaboration with base program funded legacy WDM teams.
    - 3rd CE hire.
    - Production system documentation and user support.
    - Code development to assist users (portal access, dashboards, etc.).
    - Troubleshooting.
    - Establish governance by research user groups.
- Year 3
    - Testing/development of high performance FSP WDM prototypes.
    - FSP component review, installation, and testing.
    - Production system documentation and user support.
    - Code development to assist users.
    - Troubleshooting.
- Year 4
    - Testing/development of high performance FSP WDM prototypes.
    - FSP component review, installation, and testing.
    - Production system documentation and user support.
    - Possible 4th CE hire.
    - Code development to assist users.
    - Troubleshooting.
- Year 5

    - First production use of high performance FSP WDM.
    - FSP component review, installation, and testing.
    - Production system documentation and user support.
    - Code development to assist users.
    - Troubleshooting.
- Out years
    - Priorities set by experimental and validation research user groups.
    - FSP component review, installation, and testing.
    - Production system documentation and user support.
    - Code development to assist users.
    - Troubleshooting.

Resources:

- Year 1: {PI, 2*CE}
- Year 2 and out years: {PI, 3*CE} – possibly expanded based on demonstrated user requirements. If FSP tools see wide use, a very substantial expansion of CE support might be needed.

This activity needs to have strong direction and governance by validation research user groups. This entire activity could be considered part of the validation activity of FSP (rather than counted as falling under the WDM Science Driver).

The staffing estimates made in this section are conservative. FSP will need to have the flexibility to expand staff as warranted.

6.H. WDM Milestones

The goals for WDM are to provide comprehensive predictive simulation capabilities for magnetically confined plasmas that integrate the knowledge from key multi-scale physical processes across the whole device with progressing levels of physics fidelity. Four high priority physics topics have been identified to support WDM research toward these goals: 2.5D equilibrium and transport solver, self-consistent fast-particle treatment of heating and current-drive sources, incorporation of first-principle gyro-kinetic turbulent simulations into transport time-scale simulations, and modeling of ELMs with pedestal, SOL, divertor, and first-wall interactions. Additionally, to support WDM verification and to make efficient use of resource as well as to engage the fusion community, legacy WDM tools and related SciDAC FSP prototype projects useful for WDM will need to be identified and integrated into the WDM framework early in the project phase and used as starting points for development.

A set of high-level milestones and deliverables based on the planned research activities in these areas to meet the WDM goals is given below. These are organized into 2, 5, 10, and 15-year marks and separated into two groups. In Section A, the overall milestones and deliverables to provide comprehensive predictive simulation capabilities across the whole device with progressing levels of physics fidelity and their validation and applications toward a full ITER discharge simulation is given. The milestones start from legacy WDM transport codes and SciDAC WDM prototypes and move forward toward a set of comprehensive predictive FSP WDM tools with increasing physics fidelity and parallel architectures. In parallel with the development effort, device description aspects and experimental interpretation functions will be established. This is then followed by validation of the physics components against experiments with increasing levels of interactions among crucial physical processes, and demonstration of integration of these components toward ITER applications will be performed.

In Section B, a short list of high-level milestones and deliverables for the four WDM support thrusts are given.

6.H.1. A. WDM predictive capability and validation milestones

Near-Term 2-3 Years

- Identification and establishment of candidate FSP WDM frameworks
- Identification of candidate legacy WDM 1.5D transport codes and related SciDAC WDM prototype codes for FSP WDM applications
- Componentization of physics modules from legacy 1.5D transport codes and SciDAC WDM prototype codes. Integration of the components to the FSP WDM framework. Establishment of device description and experimental interpretation function under WDM framework
- Establishment of validation metrics
- Identification of candidate test cases for verification and validation
- Validation of component models from legacy WDM 1.5D transport codes and SciDAC WDM prototype codes
- Validation of simplified combination of component models in legacy WDM 1.5D transport codes and related SciDAC FSP prototype WDM codes

- Demonstration of selected ITER applications under WDM framework with legacy WDM 1.5D transport codes and SciDAC WDM prototype codes
- Identification of gaps in component models to meet WDM goals

5-8 Years

- Installation of selected FSP components from WDM thrusts and other FSP areas into legacy WDM transport codes and SciDAC WDM prototypes as they become available
- Establishment of FSP WDM prototypes with parallel architectures
- Demonstration of high performance FSP WDM prototypes under WDM framework
- Verification and validation of component models in high performance FSP WDM prototypes
- Establishment of plausibility of validation in complex conditions
- Verification and validation of combination of component models with progressing levels of complexity in high performance FSP WDM prototypes
- Optimization for WDM parallel architectures
- Demonstration of selected ITER applications under WDM framework with high performance FSP WDM prototypes
- Establishment of production system on high performance computing system and documentation
- Deployment of production system on high performance computing system
- Identification of gaps in component models to meet WDM goals
- Establishment of development plan to meet gaps in component models

10-15 Years

- Installation of selected FSP components with more physics fidelity into FSP WDM codes as they become available
- Validation of combination of component models under more complex conditions over the entire discharge evolution in high performance FSP WDM codes under WDM framework

- Demonstration of selected ITER applications under complex conditions over the entire discharge evolution with high performance FSP WDM codes under WDM framework

6.H.2. B. Milestones and deliverables for four WDM support thrusts

6.H.3. 2.5D Equilibrium and Transport Solver

Near-Term 2-3 Years

- Identification and establishment of 3D equilibrium solvers for WDM applications
- Integration of 3D equilibrium solvers into WDM framework
- Verification and validation of 3D equilibrium solvers
- Adaptation of 1D transport equations in 3D magnetic geometry

5-8 Years

- Adaptation and assessment of reduced transport models and simplified source and loss models in 3D magnetic geometry
- Identification and development of 2.5D transport solvers for WDM applications
- Integration of transport and 3D equilibrium components into 2.5D transport solver under WDM framework
- Verification and validation of 2.5D transport solver against legacy WDM codes and experiments under WDM framework with and without 3D magnetic effects
- Demonstration of selected ITER applications with 2.5D equilibrium and transport solver under WDM framework with and without 3D magnetic effects
- Optimization of 2.5D WDM transport tool for WDM parallel architectures

10-15 Years

- Installation and integration with 3D core and pedestal transport models when they become available
- Installation and integration with 3D SOL, divertor, and wall interaction models when they become available

6.H.4. Self-consistent fast-particle treatment of heating and current-drive sources

Near-Term 2-3 Years

- Identification and establishment of essential beam, RF, and alpha-particle physics components for WDM applications
- Evaluation and development of algorithms for integration with WDM tools

5-8 Years

- Installation and Integration with WDM simulation tools
- Verification of validation under WDM framework
- Optimization for WDM parallel architectures
- Demonstration of selected ITER applications
- …

6.H.5. Incorporation of gyro-kinetic turbulent simulations into transport time-scale simulations

Near-Term 2-3 Years

- Identification and evaluation of first-principle gyro-kinetic turbulent transport simulation tools for WDM applications
- Evaluation and development of algorithms to integrate first-principle turbulent transport tools with WDM simulation tools

5-8 Years

- Installation and Integration of first-principle turbulent transport tools with WDM simulation tools
- Verification of validation of first–principle turbulent transport models under WDM framework
- Optimization for WDM parallel architectures
- Demonstration of selected ITER applications with first-principle turbulent transport models under WDM framework
- …

6.H.6. Self-consistent, coupled, core-edge dynamics

Near-Term 2-3 Years

- Identification of reduced pedestal, SOL, divertor, and first-wall interaction physics component(s) for WDM applications
- Installation and integration of these components into WDM
- Verification and validation of these components under WDM framework
- Demonstration of selected ITER applications under WDM framework

5-8 Years

- Installation and integration of components with more physics fidelity
- Optimization for WDM parallel architectures
- Verification and validation of these components under WDM framework
- Demonstration of selected ITER applications under WDM framework
- …

6.I. Appendix A: Whole Device Modeling for ITER discharge simulations

Several multi-institutional projects on ITER scenario modeling that are funded by the ITER organization give perception of physics components that will be needed for robust modeling of ITER discharges for realistic transport times. These simulation efforts are based on the best available components that are implemented in two most widely used integrated modeling codes in US, PTRANSP and TSC. By exercising these two codes in different plasma parameter regimes and by comparing different transport models and components for heating and equilibrium, strengths and weaknesses of these components become more apparent. The components that are currently available for the ITER scenario modeling in PTRANSP and TSC are listed below.

6.I.1. Existing capabilities

-
    - Prescribed and free-boundary 2D equilibria
        - Free boundary has PF coils, conductors and feedback systems
    - 1D transport solver

- various representations, serial and parallel (FACETS)

- varying levels of integrated source models (NB, LH, EC, IC, alpha)
  - fast particle treatments are generally simplified, eq Maxwellian
- varying transport channels are solved (j, Te, Ti, n, v-phi, v-theta)
  - empirical, semi-empirical, and reduced fundamental models for transport coefficients
- impurities generally treated as fractions of ne
- varying levels of He treatment
- some pedestal models, more generally prescribed
- varying sawtooth models, Porcelli with hyper-res & chi-enhance reduced model
- varying bootstrap models, single ion and NCLASS
- can include B2-Eirene derived correlations for divertor-separatrix parameters
- varying radiation models for bremsstrahlung, cyclotron, and line
- PF coils, conducting structures, force analysis, super-conducting coil limits
- Fast particle treatments include equivalent Maxwellians, slowing down models, and Monte Carlo treatments
- Range of impurity treatments
- Edge plasma models range from none to 0-D through 2-D (UEDGE) implementation with fully kinetic (electrostatic so far) 3D turbulence computations (XGC1, COGENT).
- Connection to ideal MHD stability, with some feedback to transport simulation
- Existing links to MDSplus experimental database for discharge interpretation

6.I.2. New components that will enhance the robustness of ITER modeling

- Prescribed and free-boundary 3D equilibria, capable of treating islands and stochastic regions
- 2D transport solver (improve SOL coupling)
- access to hierarchy of increasing physics fidelity models for each source
    - accurate treatment of all fast particle species (FP)
- transport models include hierarchy of increasing physics fidelity, increasing number of channels treated, including access to gyro-kinetic like treatment that treat fluxes rather than coefficients
- ideal MHD model for sawtooth crash and nonlinear evolution of post-sawtooth plasma
- impurity transport included
- inclusion of MHD stability based pedestal model, with ELM crash evolution
- inclusion of 2D-3D SOL plasma model(s)
- inclusion of neutrals model(s)
- inclusion of plasma-wall interaction model(s)