

# Center for Simulation of Wave Interactions with MHD (SWIM)

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## PSACI PAC Meeting June 7-8, 2007

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**R. W. Harvey** – *CompX*, **D. Schnack** – *U. Wisconsin*, **J. Ramos, P. T. Bonol, J. Wright** – *MIT*

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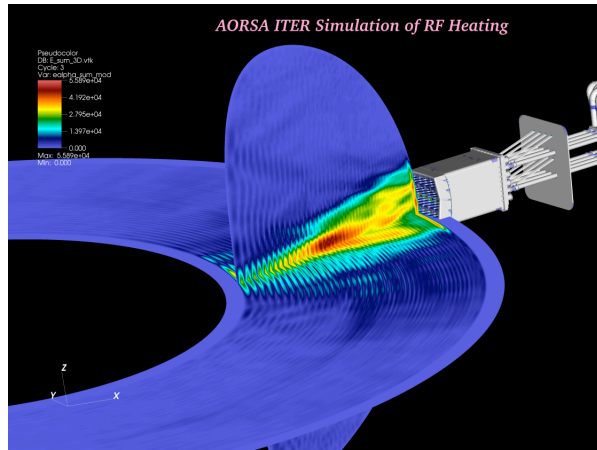
- **What is this project? (for non-fusion types)**
- **Progress on scientific goals**
- **Role of collaborations**
- **Role of leadership-class computing resources**
- **Plans to address 3-year project goals**



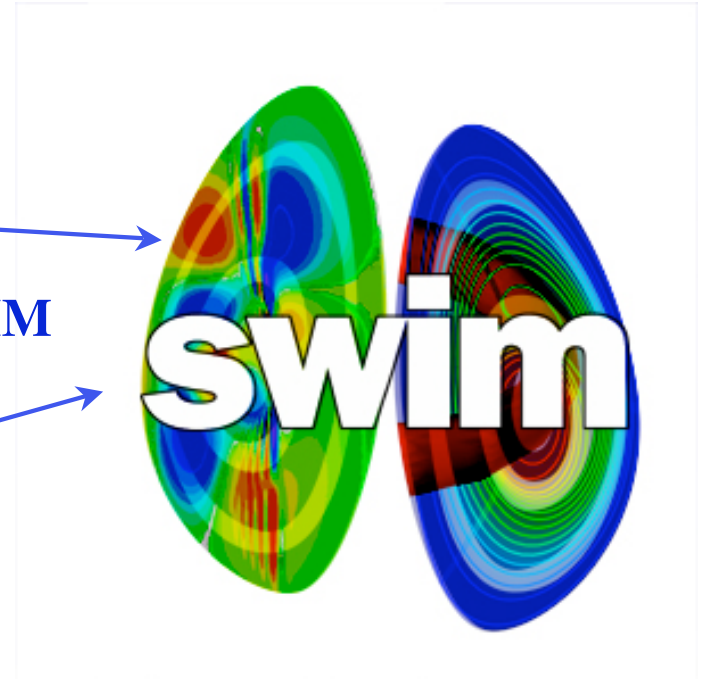
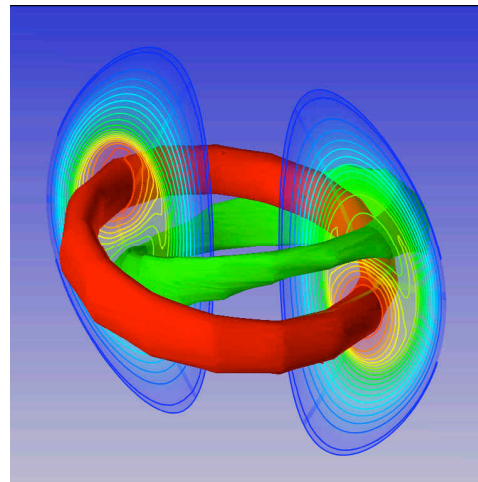
*See our fun website at: [www.cswim.org](http://www.cswim.org)*

# SWIM brings together two mature fields of fusion computation

## High power wave-plasma interactions – CSWPI



Extended MHD – CEMM

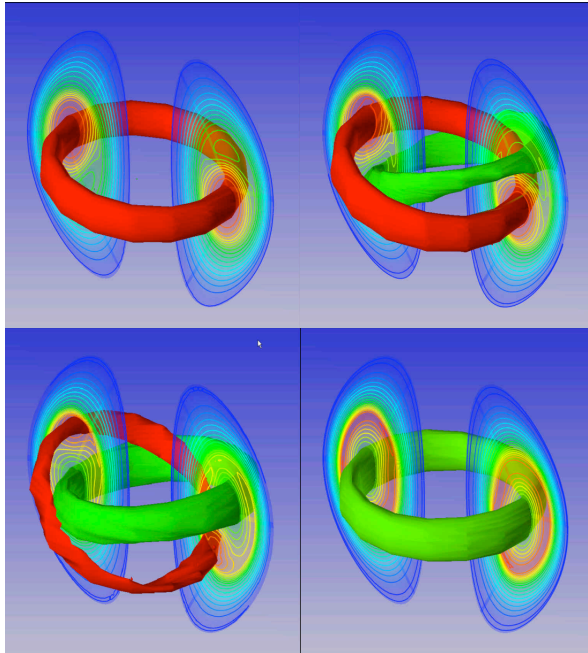


Partnership of DOE OFES and OASCR under the SciDAC

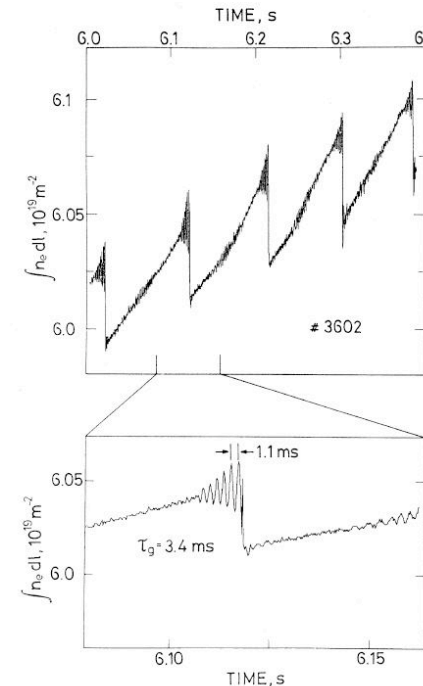
### Why couple these particular two disciplines?

- Macroscopic instabilities can limit plasma performance
- RF waves can mitigate and control instabilities

# Sawtooth oscillations can *limit* plasma performance and represent one of the greatest uncertainties for ITER



**M3D simulation for CDX-U  
of internal reconnection event**

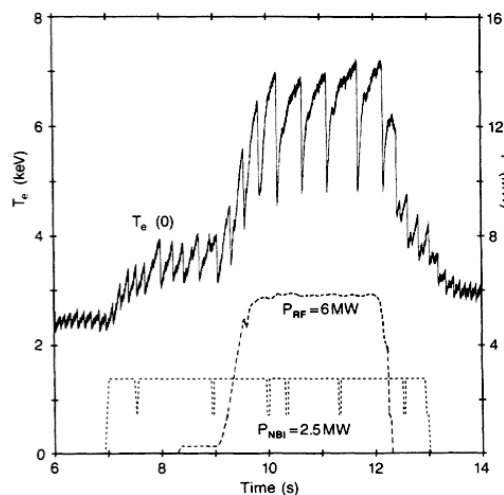


**Crash phase is several orders of  
magnitude faster than growth**

- **Sawteeth can directly limit plasma performance – particularly when energetic particles (e.g. fusion alphas) produce large amplitude oscillations**
- **Sawteeth are correlated with other instabilities**
  - Neoclassical tearing modes – provide seed island
  - **Disruptions**

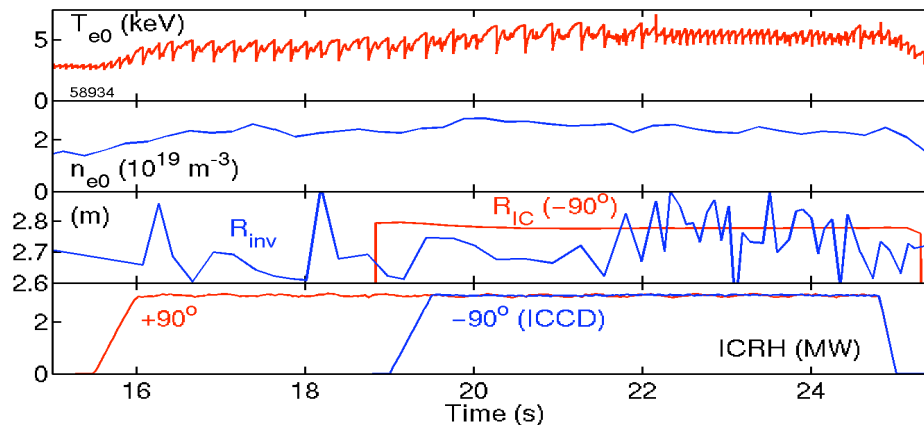
# There are several experimentally demonstrated mechanisms by which RF waves can control sawtooth behavior

## ICRF stabilization on JET



- ICRF heating can produce “monster” sawteeth – period and amplitude increased
- Likely stabilization mechanism – energetic particle production by RF

## Sawtooth control on JET with Minority Current Drive on JET

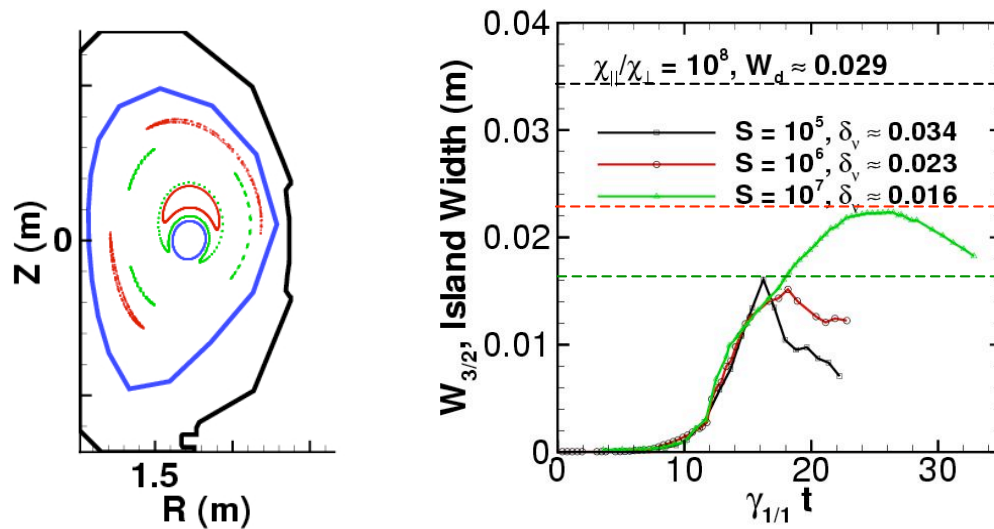


- ICRF minority current drive can either increase or decrease period and amplitude
- Likely stabilization/destabilization mechanism – RF modification of current profile

- Sawteeth can limit plasma performance themselves, or can trigger other instabilities – disruptions, neoclassical tearing modes
- Many physics processes interact – *qualitative* understanding exists but *quantitative* verification and *prediction* is lacking

# Neoclassical Tearing Modes (NTMs) are a major concern for ITER. They can *limit* plasma pressure in tokamaks and can lead to *disruption*

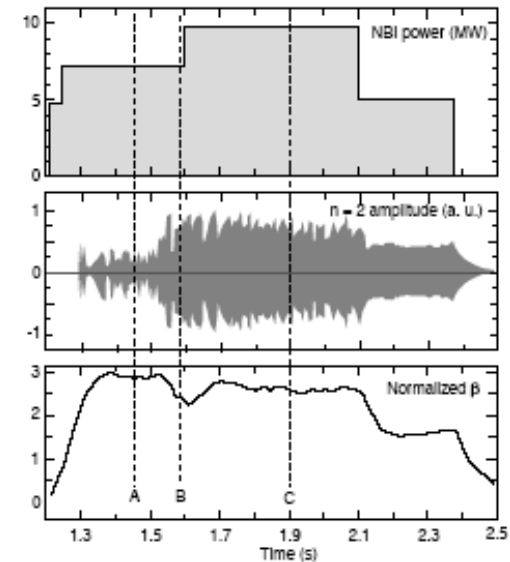
## Simulation with NIMROD



Sawtooth and secondary islands

Secondary island growth  
Varying S

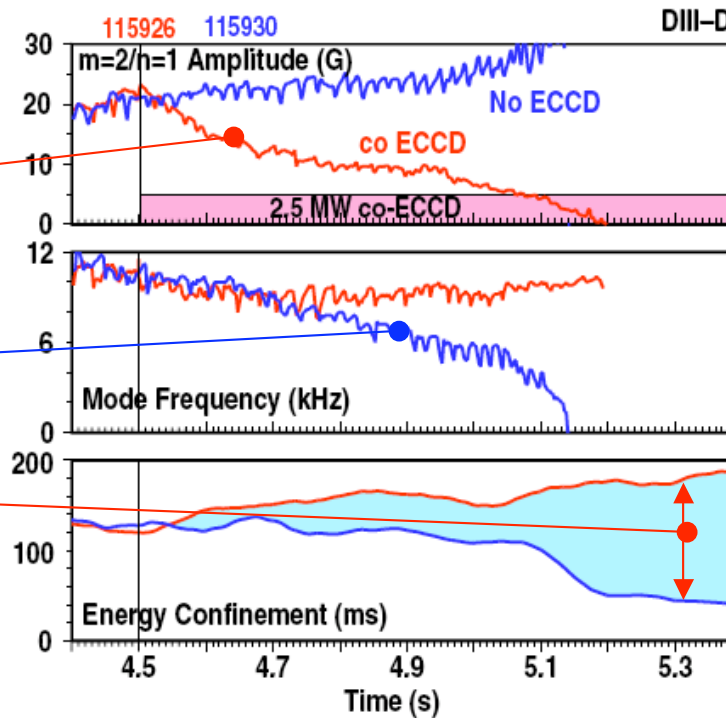
## NTM onset and confinement loss measured on ASDEX-U



- NTMs are slowly growing modes that break up the closed, nested flux surfaces needed for confinement
- NTMs cause growth of small, pre-existing magnetic islands – e.g. produced by sawteeth or ELMs
- Saturated modes can slow in rotation, *lock*, and lead to disruption

# It has been demonstrated experimentally that suppression of NTM by RF leads to improvement in confinement

- Electron cyclotron current drive drives down mode amplitude
- keeps mode rotating (no drop in frequency)
- improves energy confinement



R. Prater  
APS 2003

- Empirical scaling of NTM pressure limits in ITER leave no margin in performance
- “Understanding the physics of neoclassical island modes and finding means for their avoidance or for limiting their impact on plasma performance are therefore important issues for reactor tokamaks and ITER” – ITER Physics Basis (1999)

# The SWIM project is carried out in two physics campaigns distinguished by the time scale of unstable MHD motion

## Fast MHD phenomena – separation of time scales

- Response of plasma to RF much slower than fast MHD motion
- RF (mainly ICRH) drives slow plasma evolution, sets initial conditions for fast MHD event
- Example: sawtooth crash

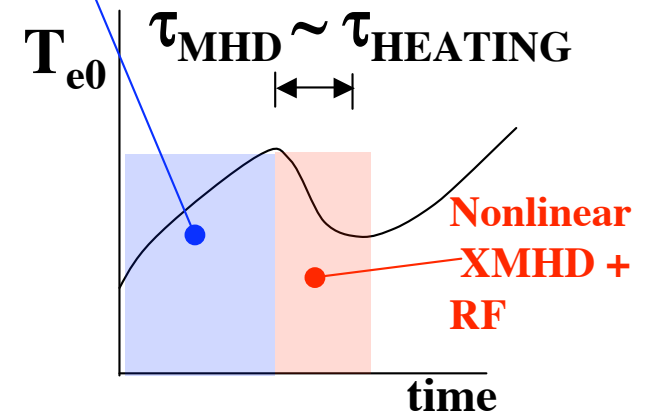
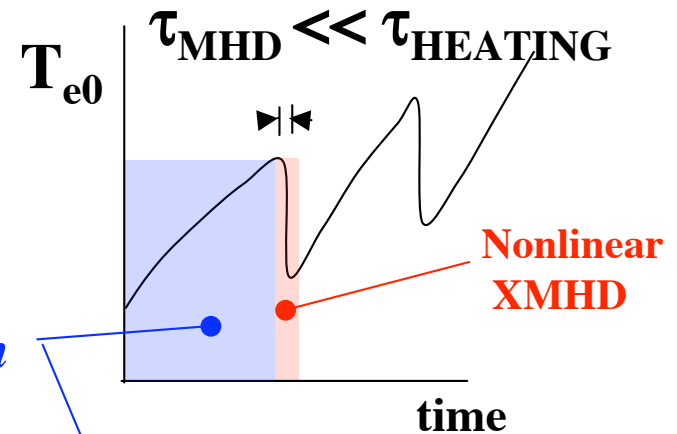
*Slow plasma evolution*

## Slow MHD phenomena – no separation of time scales

- RF affects dynamics of MHD events  $\Leftrightarrow$  MHD modifications affect RF drive plasma evolution
- Deals with multi-scale issue of parallel kinetic closure including RF (mainly ECRH)
- Example: Neoclassical Tearing Mode

## These two regimes are related

- Fast sawtooth crash can provide seed island for NTM growth
- Slow growth of NTM island can lead to fast disruption events
- Calculation of slow ramp of sawtooth, with incomplete reconnection or persistent islands, may actually require the same capabilities as NTM evolution



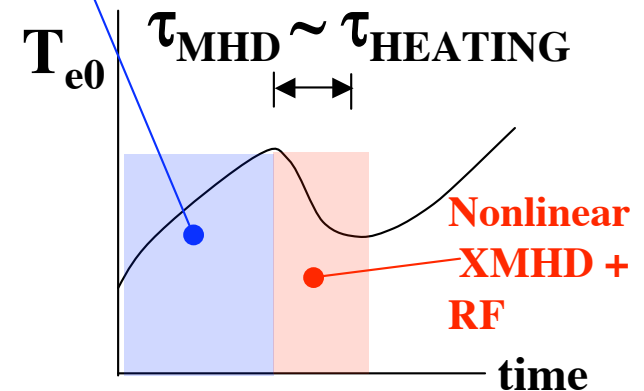
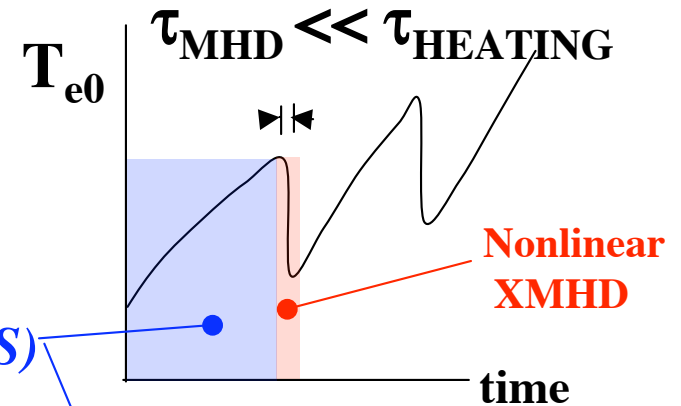
# A major element of the SWIM project is development of an Integrated Plasma Simulator (IPS)

## Objectives of Integrated Plasma Simulator

- Simulate slow time-scale plasma evolution for SWIM – Fast MHD campaign
- Provide advanced simulation capabilities for burning plasma research, beyond SWIM project

### *Integrated Plasma Simulator (IPS)*

- Serve as test-bed for tighter component coupling required in SWIM – Slow MHD campaign
- Gain experience in computer science and mathematics issues to be faced in a comprehensive fusion simulation
- *Develop a flexible, extensible computational framework capable of coupling in any fusion code and able to evolve to a complete simulation capability*





# Progress on Scientific Goals and Plans for following year

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- **Completion of design for first version of Integrated Plasma Simulator and its implementation**
- **Design and implementation of SWIM web portal**
- **Progress on physics studies**

# SWIM Software Goals & Requirements

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- **Develop an Integrated Plasma Simulator (IPS) supporting...**
  - Fusion simulation science needs (near term) → two SWIM physics campaigns, device modeling
  - Design study for future *full* integrated simulations (long term)
- **Explore interoperability and interchangeability of components in common infrastructure**
  - Looking towards a flexible “toolkit” for integrated modeling
  - Useful for V&V
- **Maximize (re)use of existing code**
- **Minimize changes to physics codes for non-physics driven reasons**
  - Avoid bifurcation of physics components – not different SWIM/stand alone versions
  - Ease of debugging
- **Capable of running on high-end systems from the start**

# IPS Design Approach

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- **Framework/component architecture**
  - Components initially existing codes wrapped up
  - Framework provides basic utility services
  - “Driver” component orchestrates simulation
  - “Plasma State” component is official data manager
- **Emphasize interfaces**
  - Carefully defined the mathematical functionality of the components
  - Components providing the **same functionality** should do so through the **same interface**
  - Project intentionally includes at least two distinct codes for most classes of functionality
- **Start simple, increase sophistication as science needs dictate**
  - File-based communication → in-memory data exchange
  - Whole codes wrapped with scripts → finer-grain native-language components
  - Project-specific framework → Common Component Architecture compliant framework

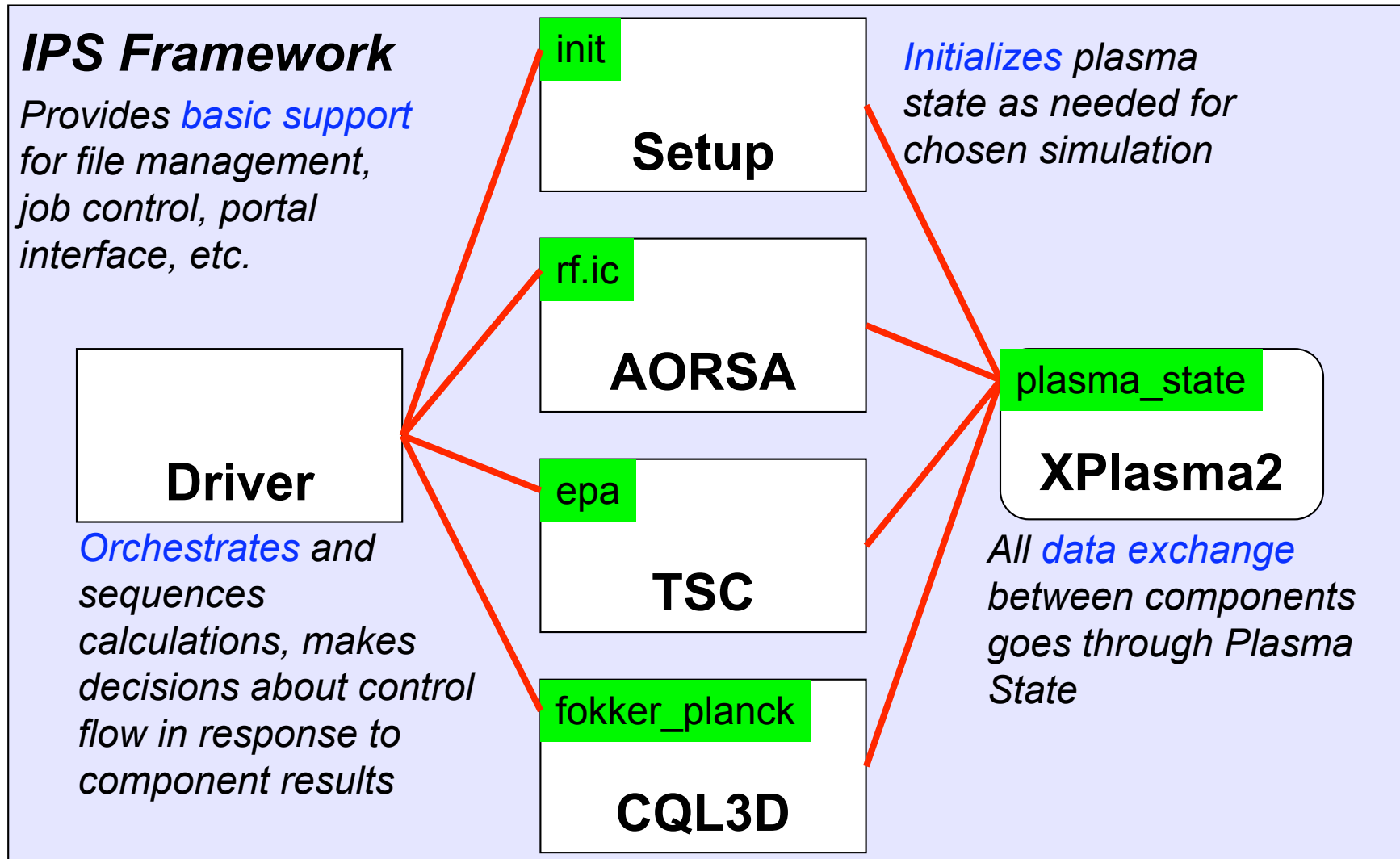
# IPS Framework Features

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- **Provides environment in which components are instantiated and executed**
  - **Manages association between interfaces and components implementing them**
- **Provides basic services to components**
  - **Configuration (input) management → simulation details specified in configuration file**
    - **Easily extensible to additional components w/o outside changes**
    - **Plan “Tokamak machine configuration file” to standardize machine specific**
  - **File management abstraction**
    - **Manages working directories**
    - **Temporary and permanent files, stored separately**
  - **Job management (parallel execution)**
  - **Interface with web portal**
    - **Without changes to underlying components**
    - **Framework can run without portal**
  - **Currently all part of a single `services` interface**
- **Framework implemented in Python**

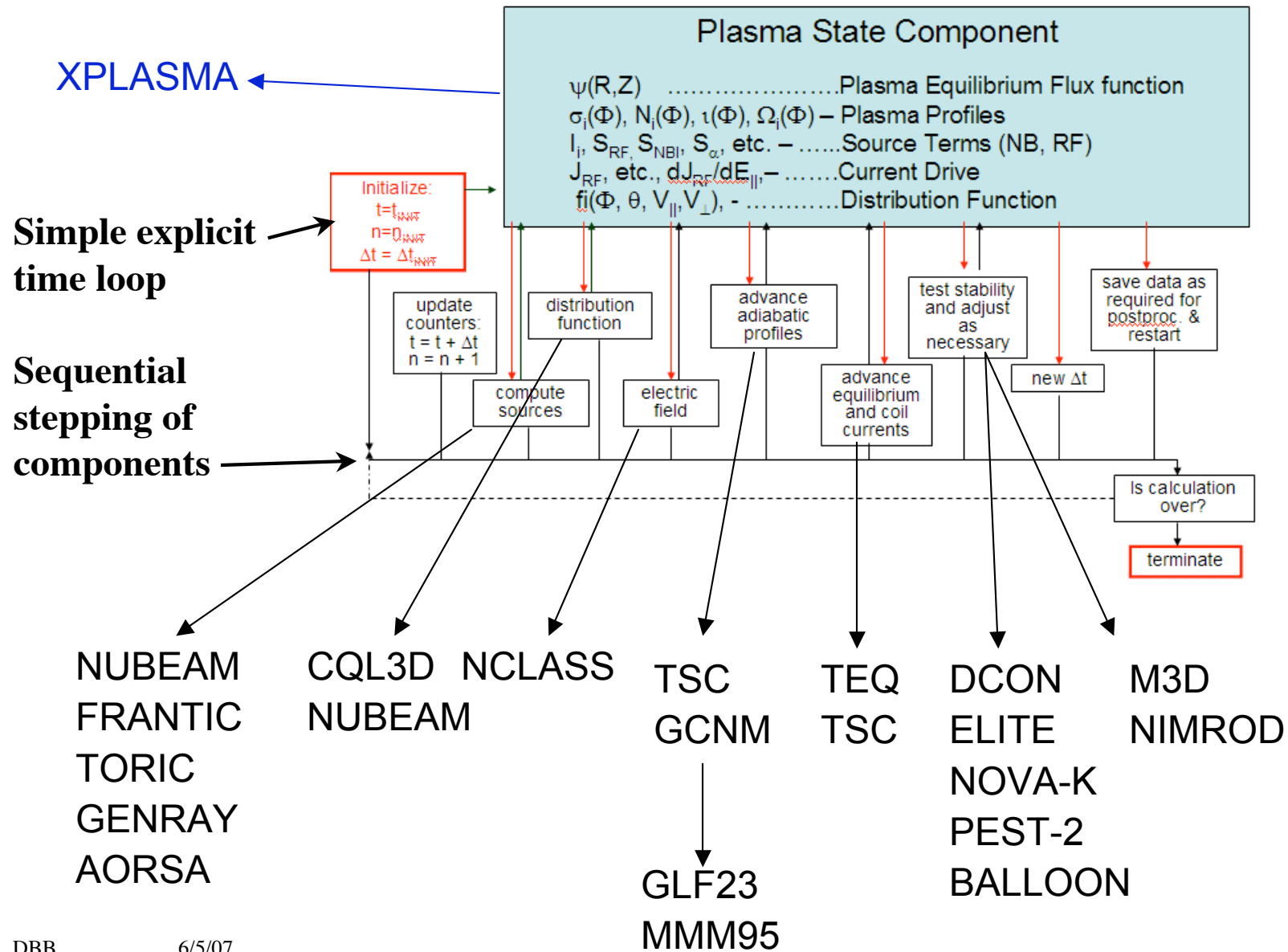
# The IPS is a system for composing fusion simulation applications

## → Schematic of an IPS Application



*Components implement (one or more) specific interfaces.  
A given interface may have multiple implementations.*

# Planned components and implementations (from 2006 PSACI)

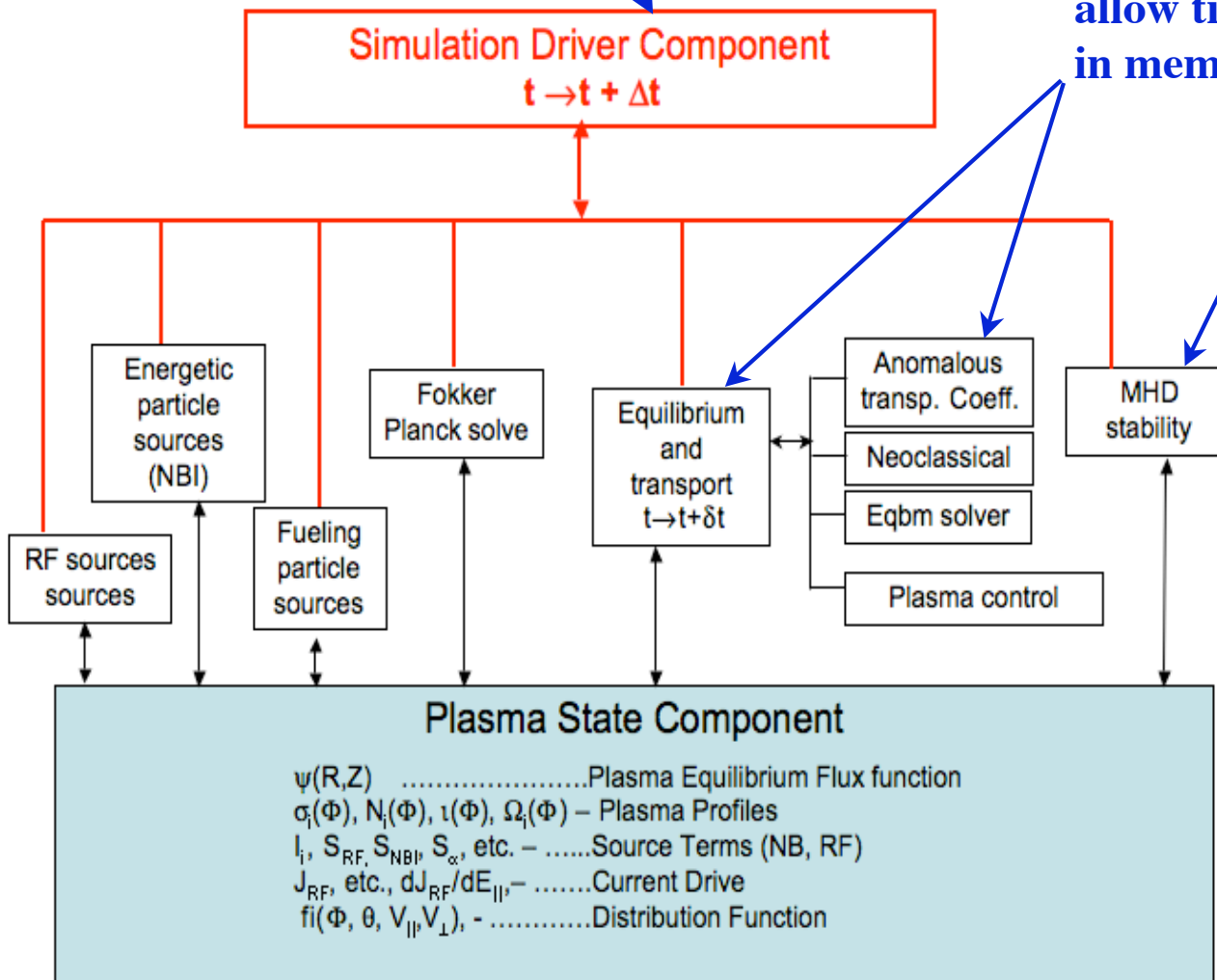


# New design allows for increased flexibility of simulation control and linkage

Driver physics layer allows extensibility, flexibility in controlling simulation

Composite components: allow tighter coupling, in memory communication

Same interface for linear/nonlinear MHD



# The Basic Component Interface

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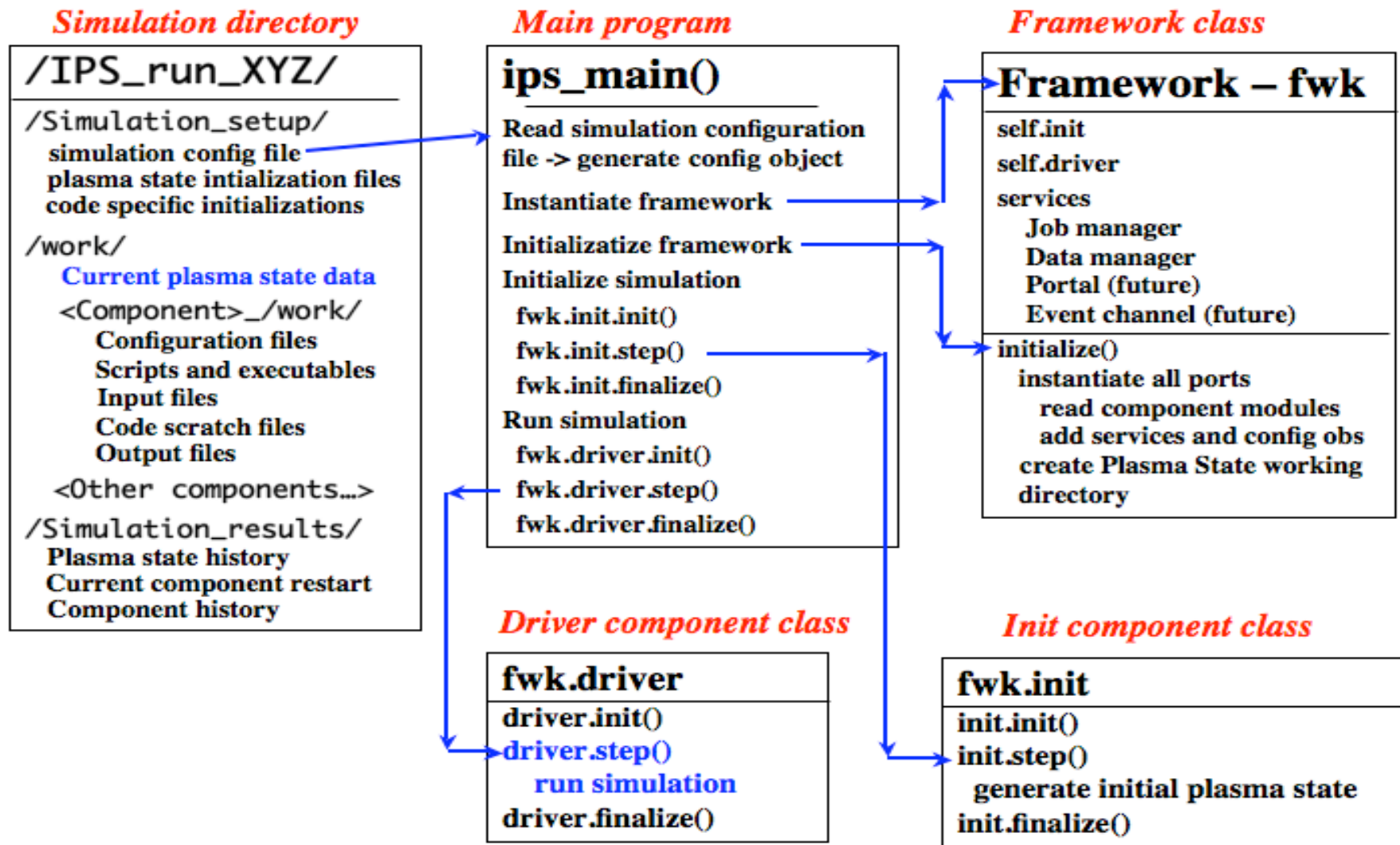
→ **Observation Most coarse-grain (application-level) components in a time-stepped simulation can be expressed with just a few basic operations**

- `Init(ialize)`
  - **Prepare to run component for a series of time steps**
- `Step`
  - **Do whatever computation is appropriate to the current time step**
- `Finalize`
  - **Clean up at end of run**

**In IPS almost everything (including the framework, simulation initialization and driver) is an instance of abstract class ‘Component’ and supports this interface.**



# IPS framework



Two distinguished components are called by ips\_main: init, driver

# Sketch of Basic IPS Driver

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**Read in simulation configuration**

**Setup initial plasma state**

**Foreach component  $c$  (*in appropriate order*)**

    Call `c.init`

**For  $t = t_i$  to  $t_f$**

**Foreach component  $c$  (*in appropriate order*)**

        Call `c.step(t)`

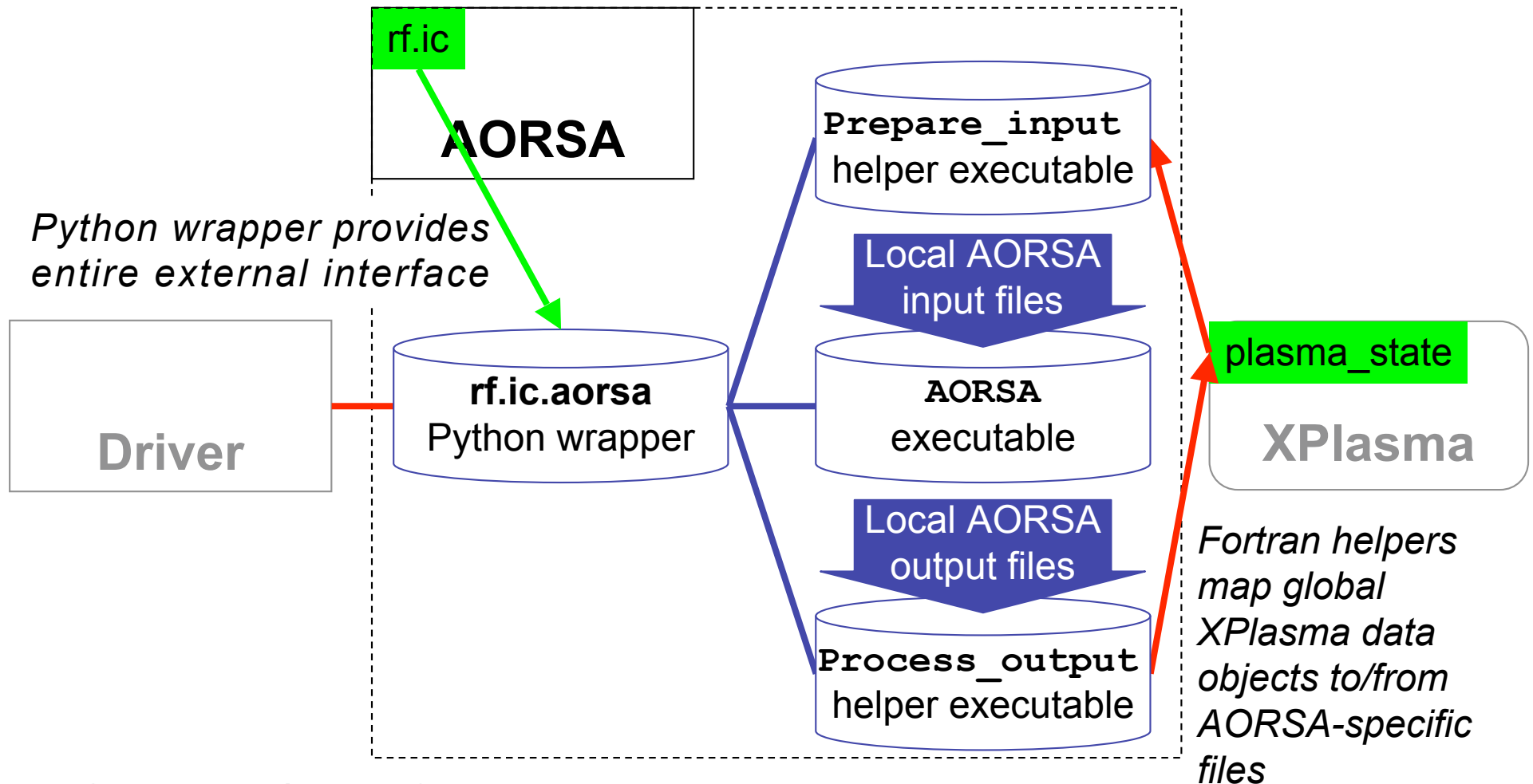
**Commit this time step to Plasma state**

**Stage output files**

**Foreach component  $c$  (*in appropriate order*)**

    Call `c.finalize`

# Schematic typical component internals – rf\_ic implemented by AORSA



IPS design/specifications say nothing about internal implementation of components.

# All Simulation data exchanged between components goes through Plasma State – components can produce other files

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- **Fortran 90 Module – built on PPPL’s XPLASMA2 library**
  - Distributed by NTCC, used in TRANSP
  - netCDF for backend storage
- **Formally a library at present, not a component**
- **Very simple user interface → functions: get, store, commit**
- **Other powerful XPLASMA functions available, but not required → e.g grid interpolation**
- **Supports multiple state instances (very important!) → e.g. current/prior state, pre-/post-sawtooth, etc**
- **PS data conventions (names, units, etc.) for IPS determined by (benevolent) dictator → extended as needed**
- **Data stored “as produced” → Consumer is responsible for adapting as needed**
- **Code is automatically generated from state specification text file → ease and accuracy of update**
- **Some types of data we don’t know how to deal with yet → distribution functions are just code dependent filenames**

## Our arsenal of developed components includes

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- **RF Solve – ion cyclotron two implementations**
  - **AORSA2D**
  - *TORIC – testing*
- **Fokker Planck Solve**
  - **CQL3D**
  - **NUBEAM not yet a wrapped component but can run as TSC/TRANSP coupling**
- **Equilibrium and profile advance (EPA)**
  - **TSC implementation**
  - **TSC replay implementation – reads state file from previously generated simulation directory tree – useful for testing and time-slice analysis by other components**

### Coming soon

- **Linear MHD component – multiple implementations: BALLOON, DCON, PEST-I and PEST-II, NOVA-K, Nonlinear MHD M3D/NIMROD**
- **MONITOR– accumulates state data into time series for plotting/monitoring with Elvis**
- **RF EC and LH components – implemented by GENRAY**
- **Fokker Planck solves – implemented by ORBIT-RF, NUBEAM**

## Plan for coming year – IPS

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- Continued implementation and testing of physics components
- Test harness for components and plasma state
- More extensive use of NLCF computers
- Implementation of more elaborate time stepping algorithms
  - Only the driver has the *big picture* of the simulation, not the components
  - Responding to un-planned events in the middle of a time step that require action by driver or other components – e.g. sawtooth events, plasma control actions, runtime faults
  - Development of an information rich data object returned to driver from components
  - Requires extending the basic interface used so far – interfaces no longer generic across components
- More use of in-memory data exchange → may require rethinking Plasma State
- Managing parallelism → some components serial, others highly parallel
- Analyze migration to standard component architecture (e.g. CCA)
  - Will facilitate leveraging outside components – I/O, math libraries, etc
  - Current design is intentionally close to CCA

# Progress on Scientific Goals and Plans for following year

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- **Completion of design for first release of Integrated Plasma Simulator and its implementation**
- **Design and implementation of SWIM web portal**
- **Progress on physics studies**

# **A web portal is being developed for IPS → to ease access security, submission, job monitoring, meta-data management**

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- **Security (transparent to the user)**
  - **Authentication** : User signs on securely with FusionGrid credentials- an id and password, operated by ESnet
  - **Authorization** : Component service provider checks to see if authenticated user is authorized to access its service
- **Component Submission and Monitoring**
  - Platform to securely initialize and instantiate simulation runs on remote systems at PPPL (mhd, viz) and ORNL (Jaguar) through the IPS Framework
  - User ability to monitor the run launched remotely via events notifying the user on the status of the component run
  - Browser visualizations / displays of run results
- **Meta-Data Management**
  - Automated generation and storage of metadata resulting from the runs to facilitate users to quickly retrieve information on runs made
  - Monitor run directories and store/extract information such as location, size, timestamp, owner as external meta-data and physics quantities of interest to users as internal meta-data



# Prototype is operational

The image displays four screenshots of a web portal interface, arranged in a 2x2 grid. Each screenshot is a Mozilla Firefox browser window.

- Top Left:** "pubcookie generic Login - Mozilla Firefox". URL: <https://star11.fusiongrid.org/login/>. Title: "Security Model". Content: "The resource you requested requires you to authenticate." Fields for "User ID" and "Password" with a "Log in" button. A warning message: "WARNING: Protect your privacy! Prevent unauthorized use! Completely exit your Web browser when you are finished." Copyright © 2007 Test Pubcookie Login Server hosted on star11.
- Top Right:** "SWIM Web Portal - Mozilla Firefox". URL: <https://star11.fusiongrid.org/restricted/index>. Title: "SWIM Web Portal". Content: "Launch and Monitor Current Simulation Runs:" with links for "Demo Code (PPPL)", "Event Monitor", and "Summary from Simulation Runs". A highlighted box contains the text "Portal Services".
- Bottom Left:** "pubcookie generic Login - Mozilla Firefox". URL: <https://star11.fusiongrid.org/restricted/TestCgiEventMonitor.py?Subscription=>. Title: "Monitor Current Simulation". Subscriptions: All | FSP\_Log | FSP\_Data | FSP\_Job | FSP\_Debug. A table with columns: TimeStamp, Subscription, Component, Run\_By, Event. A highlighted box contains the text "Monitor".
- Bottom Right:** "SWIM Web Portal - Mozilla Firefox". URL: <https://star11.fusiongrid.org/restricted/TestCgDataManager.py>. Title: "Summary Information on Simulation Runs". Search filters for Tokamak (D3D), Shot Number, User (abc), Component (AORSA), and E-Dot/W-Dot difference (3). A "Submit" button for an "SQL query" is shown. A highlighted box contains the text "MetaData Manager".

# Plan for coming year – Portal

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- **Proposed security model works on PPPL systems**
- **Meta-data management requires further organization**
  - **Scheme for generating unique run identifiers**
  - **Support internal meta-data queries as simulation components become available**
- **Provide browser-based graphical visualizations of run results with Elviz**
- **Release Portal as a production system that can accept new components as they become available**

# Progress on Scientific Goals and Plans for following year

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- **Completion of design for first release of Integrated Plasma Simulator and its implementation**
- **Design and implementation of SWIM web portal**
- **Progress on physics studies**

# The largest physics analysis task for SWIM is developing an MHD closure that includes RF effects → closures working group

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**RF effects produce additional contributions to the fluid equations and modify the fluid closure moments**

**Basic formulation starts from general kinetic equation**

$$\frac{df}{dt} = C(f) + Q(f),$$

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla + \frac{q_s}{m_s} (\vec{E} + \vec{v} \times \vec{B}) \cdot \frac{\partial}{\partial \vec{v}}$$

$$Q(f) = \frac{\partial}{\partial \vec{v}} \cdot \vec{D} \cdot \frac{\partial f}{\partial \vec{v}}$$

RF contributions enter via quasi-linear diffusion operators as functions in 5-D

**Taking moments yields**

$$\frac{\partial n_s}{\partial t} + \nabla \cdot (n_s \vec{v}_s) = 0,$$

$$m_s n_s \left( \frac{\partial \vec{v}_s}{\partial t} + \vec{v}_s \cdot \nabla \vec{v}_s \right) = n_s q_s (\vec{E} + \vec{v}_s \times \vec{B}) - \nabla p_s - \nabla \cdot \vec{\pi}_s + \vec{R}_s + \vec{F}_{s0}^{rf},$$

$$\frac{3}{2} n_s \left( \frac{\partial T_s}{\partial t} + \vec{v}_s \cdot \nabla T_s \right) + n_s T_s \nabla \cdot \vec{v}_s = -\nabla \cdot \vec{q}_s - \vec{\pi}_s : \nabla \vec{v}_s + Q_s + S_{s0}^{rf}$$

Additional terms due to RF

$$\vec{F}_{s0}^{rf} = \int d^3 \vec{v} m_s \vec{v} Q(f_s),$$

$$S_{s0}^{rf} = \int d^3 \vec{v} \frac{1}{2} m_s v^2 Q(f_s)$$

# While the fluid equations are exact, a treatment of the closure problem is needed

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A procedure to produce the needed closure information is under development - Hegna and Callen, Sherwood '07

- Assuming RF produces a small kinetic distortion

$$f_s = f_{Ms} + F_s, \quad F_s \ll f_{Ms}$$

- With  $f_s = f_{Ms} + F_s$ , the RF contributions to the fluid equations are determined

$$\vec{F}_{s0}^{rf} = \int d^3\vec{v} m_s \vec{v} Q(f_s) \cong \int d^3\vec{v} m_s \vec{v} Q(f_{Ms}) = \vec{F}_{s0}^{rf}(n_s, \vec{v}_s, T_s, \vec{E}_{rf}, \dots),$$

$$S_{s0}^{rf} = \int d^3\vec{v} \frac{1}{2} m_s v'^2 Q(f_s) \cong \int d^3\vec{v} \frac{1}{2} m_s v'^2 Q(f_{Ms}) = S_{s0}^{rf}(n_s, \vec{v}_s, T_s, \vec{E}_{rf}, \dots),$$

- However, we're not done yet --- the RF terms modify the closures

Using a Chapman-Enskog-like ansatz, an equation for the kinetic distortion can be derived

# Using a Chapman-Enskog-like approach, an equation for the kinetic distortion is derived with RF source terms

- The kinetic equation is given by

$$\frac{dF_s}{dt} - C(F_s) = Q(f_{Ms}) + \vec{v}' \cdot [\nabla \cdot \vec{\pi}_s - \vec{R}_s - \vec{F}_{s0}^{rf}] \frac{f_{Ms}}{n_s T_s} + \left( \frac{m_s v'^2}{3T_s} - 1 \right) [\vec{\pi}_s : \nabla \vec{v}_s + \nabla \cdot \vec{q}_s - Q_s - S_{s0}^{rf}] \frac{f_{Ms}}{n_s T_s} - \left( \frac{m_s v'^2}{2T_s} - \frac{5}{2} \right) \vec{v}' \cdot \nabla T_s \frac{f_{Ms}}{T_s} + \frac{m_s}{T_s} \left[ \vec{v}' \vec{v}' - \frac{v'^2}{3} \vec{I} \right] : \nabla \vec{v}_s \frac{f_{Ms}}{T_s}$$

Additional source terms for the kinetic distortion due to RF

- Simple applications have been worked out e. g., the Spitzer problem with RF

$$R_{\parallel} = \frac{m_e v_e}{n_e e^2 \Lambda_{00}} J_{\parallel} + \sum_{k=1} \frac{\Lambda_{0k}}{\Lambda_{00}} \frac{F_{ke}^{rf}}{n_e e}, \quad F_{je}^{rf} = \int d^3 \vec{v} \vec{v}' L_j^{3/2}(x) Q(f_{Me})$$

- For applications to magnetic islands, the kinetic equation takes on a form similar to that used by Held et al to calculate closures
  - Same operator on kinetic distortion  $F_s$ , the RF bits enter as additional sources

$$v_{\parallel} \nabla_{\parallel} F - C(F_s) \cong Q(f_{Ms}) - \vec{v}' \cdot [\vec{R}_s + \vec{F}_{s0}^{rf}] \frac{f_{Ms}}{n_s T_s} + \dots$$

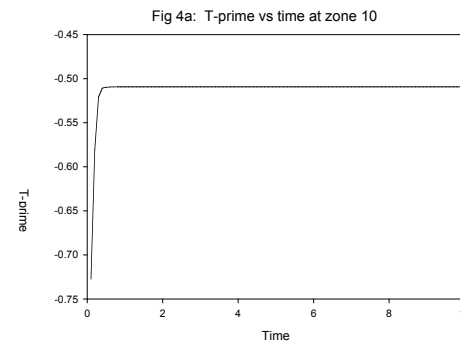
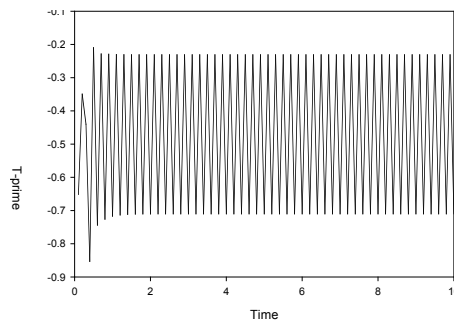
- Procedures for inverting this operator have been developed, Held *et al* '03

# Numerous improvements to SWIM physics models and codes in collaboration with other projects and base theory

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## PTRANSP project

- **New Newton method to deal with numerically stiff transport model such as GLF23 and MMM95**



- **Porcelli module for triggering sawtooth crashes**
- **Porcelli model for partial magnetic reconnection**

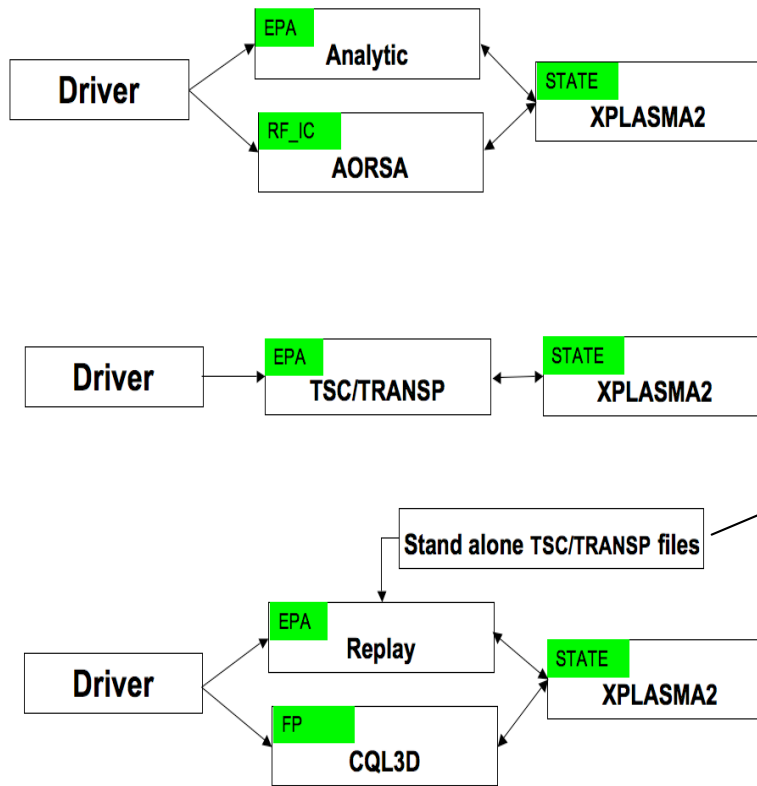
## SciDAC CEMM

- **Shared development of M3D and NIMROD as required for sawtooth and NTM calculations**

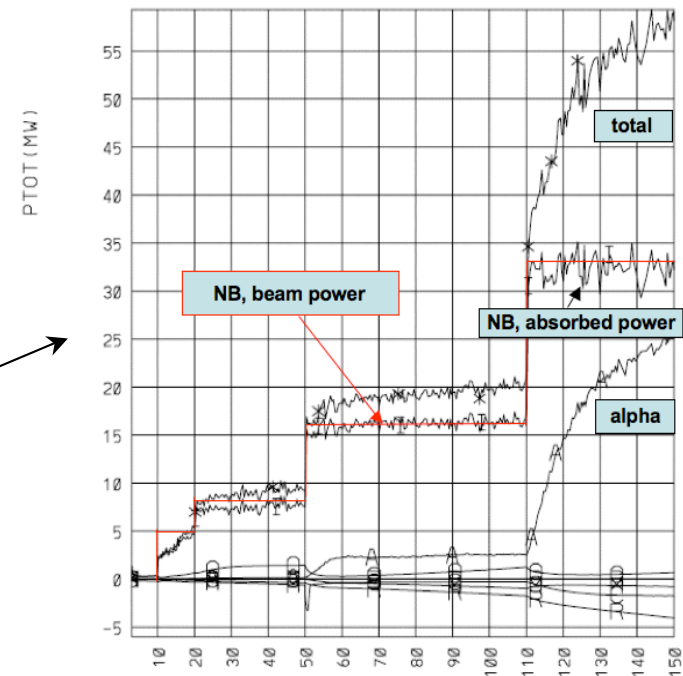
## SciDAC CSWPI

- **Improvements to AORSA, TORIC, CQL3D, ORBIT-RF driven by or supported by SWIM**

# Physics runs with IPS are beginning



Integrated power deposition in an off-axis, beam heated ITER discharge simulation of the first 150 s.



- Analysis of time slices using AORSA
- Time slice analysis of fast electron generation using CQL3D
- AORSA/TORIC benchmarking



# Plans for coming year – physics

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## Applications of IPS

- **Validation studies**
  - **AORSA/TORIC + CQL3D minority heating and rate of tail formation, C-mod comparisons**
- **Time slice simulations**
  - **AORSA comparisons for ITER scenario studies run with TORIC**
  - **Stability analysis of ITER scenario runs**
  - **Toroidal Alfvén Eigenmode studies on C-mod using M3D/NOVA-K**
- **Dynamic simulations**
  - **RF effects on sawtooth oscillations – DIII-D or JET**
  - **Runaway electron production in ITER startup/shutdown – have begun this study**

## Physics analysis and development

- **Slow MHD strategy (new post doc coming on board – U. Wisc.)**
  - **Restart computational tearing mode work and consider RF effects on classical tearing modes**
  - **Develop a phenomenological evolution equation for  $J_{rf}$  in MHD codes, using numerical RF sources**
  - **Derive a more rigorous closure model including RF**

# Role of collaborations

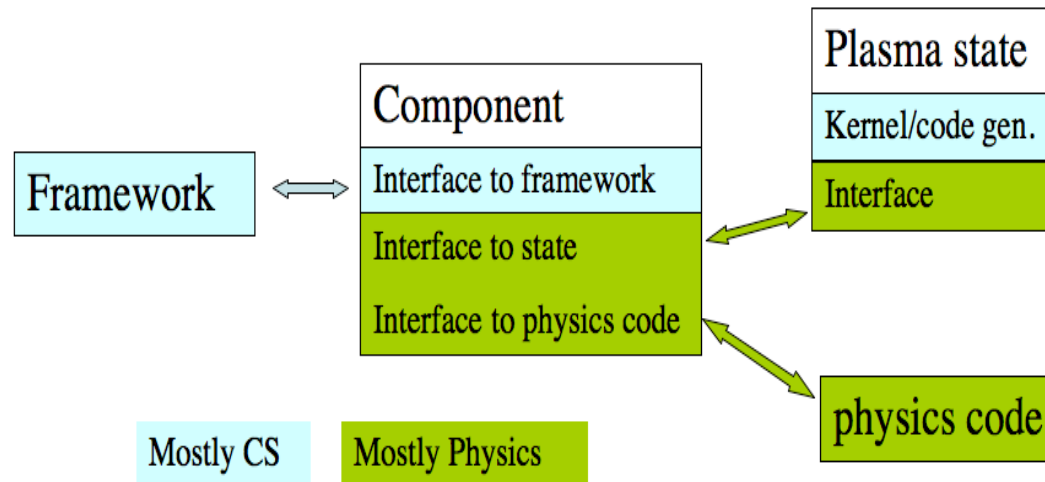
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- **SciDAC – SWIM is built on collaborations with other projects**
  - **Center for Extended MHD modeling (CEMM) ↔ Linear and non-linear MHD**
  - **Center for Simulation of Wave-Plasma Interaction (CSWPI) ↔ RF and Fokker Planck**
  - **Predictive TRANSP (PTRANSF) ↔ Plasma State, TRANSP**
  - **Look forward to working with new SciDAC projects ↔ energetic particle, turbulent transport**
- **OASCR Centers for Enabling Technology (CET)**
  - **Toward Optimal Petascale Simulations (TOPS) ↔ advanced solvers, application of PETc to NIMROD**
  - **Center for Technology for Advanced Scientific Component Software (TASCS) ↔ component architecture, CCA**
  - **Center for Interoperable Technologies for Advanced Petascale Simulations (ITAPS) ↔ mesh transfer**
  - **Visualization and Analytics Center for Enabling Technologies (VACET) ↔ visualization, analysis of magnetic islands**
- **Students – Columbia, Princeton Univ, IU, U. Wisc ↔ ORNL, TechX, LLNL, PPPL**
- **International collaborations**
  - **International Tokamak Physics Activity (ITPA) ↔ SWIM physics/ CS at Integrated Modeling a Global Effort (IMAGE, ITPA subgroup)**
  - **US Japan Workshop on Integrated Modeling of Fusion Plasmas ↔ SWIM and US CS/Math participation**

# Internal Collaborations

We spent a lot of time defining functionality and specifying interfaces

We have 4 groups of developers – framework, component, plasma state, physics code



Allows people to focus on what they do best

- **Project user/advisory committee – M. Greenwald (MIT), C. Kessel (PPPL), M. Murakami (ORNL/DIII-D), A. Siegel (ANL), A. Sussman (U. MD)**
- **Communication – Project meetings, web site, conference calls, SVN repository**

# Role of leadership class computing

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## **INCITE project Simulation of Wave Interactions and MHD**

- **Early years mostly CEMM and CSWPI → SWIM later years**
- **Renewed in 2007**
- **On track to use our 2007 allocation**

## **Major codes ported to Jaguar**

- **M3D, NIMROD, AORSA, CQL3D, ORBIT-RF, Plasma State/  
XPLASMA2**
- **Have had issues with availability, stability, utilities (like the compiler)**

## **Porting to PPPL SGI cluster**

- **A gateway for development and testing SWIM invested in 16 SGI processors on PPPL cluster**
- **All major codes also ported to PPPL cluster**

## Directed deliverables for next year

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- **Public release of Integrated Plasma Simulator**
- **Transition of IPS to Jaguar**
- **Slow MHD – effect of RF on classical tearing mode studied with NIMROD**
- **Initial sawtooth simulation with IPS – Demonstrate transition from 2D (axisymmetric) equilibrium to 3D nonlinear MHD code (NIMROD and/or MHD), compute sawtooth event, and transition back to axisymmetric equilibrium when mode re-symmetrizes**