

# AToM: Advanced Tokamak Modeling

## Introduction and first physics results

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O. Meneghini, D. Orlov, E. D'Azevedo, J.M. Park, S. Smith,  
P. Snyder, M. Umansky

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# AToM: Advanced Tokamak Modeling

FES/ASCR SciDAC Project: 09-2014 through 08-2017

**Multi-institutional project: GA, UCSD, ORNL, LLNL**

- The goal of AToM is to **enhance and extend** predictive modeling capabilities that currently exist within the US magnetic fusion program.
- The approach is to **support** rather than **subvert** current workflows, build new essential infrastructure, and guide integration.
- The central philosophy is pragmatic: take a **bottom-up** approach that leverages **existing research activities** and **collected wisdom** embodied in legacy tools.
- Move **smoothly and surely** toward a whole device modeling (WDM) capability that has the most important feature: **users**.

# The AToM Team

## Institutional Breakdown

### General Atomics

J. Candy, O. Meneghini (poster), D. Schissel, S. Smith, P. Snyder

### UCSD

C. Holland, V. Izzo, D. Orlov

### ORNL

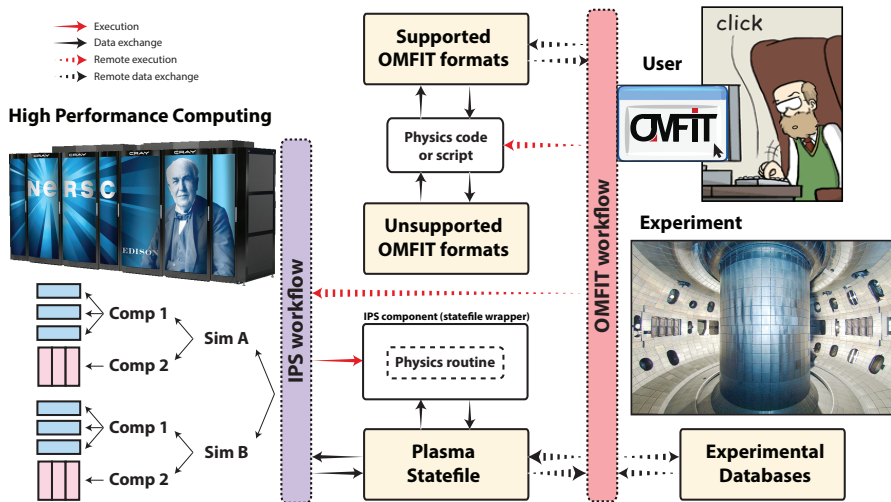
D. Bernholdt, D. Green (poster), D. Batchelor, J-M. Park, S. Diem,  
E. D'Azevedo

### LLNL

M. Dorf, M. Dorr, M. Umansky

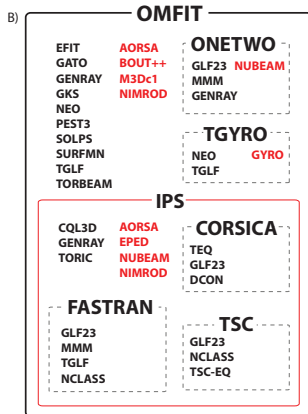
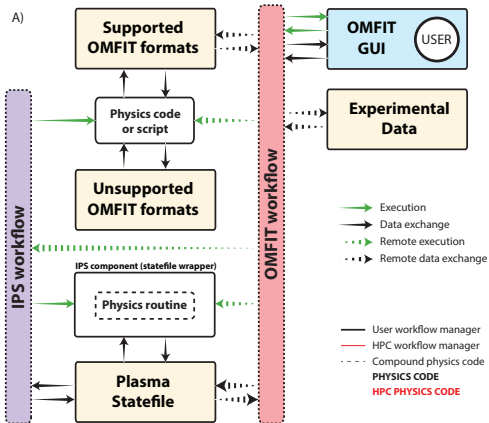
# AToM couples IPS and OMFIT frameworks

AToM = OMFIT (user interface) + IPS (HPC scheduling)



# AToM: Advanced Tokamak Modeling

## Multiple levels of component and framework integration



# AToM: Advanced Tokamak Modeling

## Available components

C2	CGYRO	COGENT	CURRAY
DAKOTA	EFIT	EPED	ESC
FASTRAN	GATO	GENRAY	GLF23
GYRO	IPS	NEO	TSC
NIMROD	NUBEAM	ntcc library	OMFIT
pstool	TGLF	TGYRO	TORAY
TORIC	M3D-C1	TSC	PRGEN
LE3	NEO3D	ONETWO	TRANSP
BOUT++	AORSA	TORBEAM	SOLPS
SURFMN	CORSICA		

# The OMFIT-tree Data Structure

## The centerpiece of OMFIT

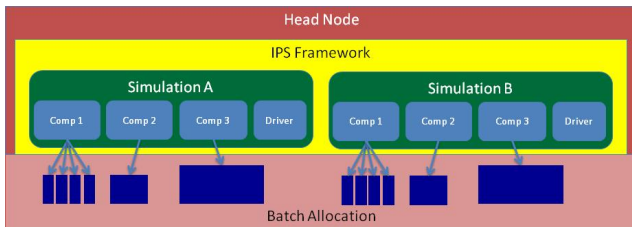
The **OMFIT-tree** is a hierarchical, self-descriptive data structure that enables data exchange between different codes

- Collect data **independent of origin/type**.
- Component content stored in a **subtree**
- **No *a priori* decision** of what is stored and how
- Codes communicate by referring to **tree data**
- **Free-form** equivalent of elusive fusion *statefile*

Like *MDS+* or the file system on your own laptop, the data is stored in the **most natural form** to accomplish a given task

# AToM: Advanced Tokamak Modeling

## Integrated Plasma Simulator (IPS)



- Enables integration of MPP component codes.
- Wraps (unmodified) codes in a **standard component interface**.
- 4 levels of parallelism.
- Supports advanced algorithms like **Parareal**.

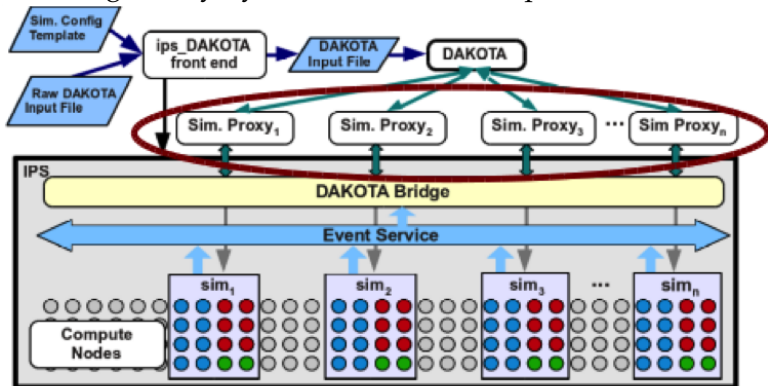


# Integrated DAKOTA-IPS Use Cases

## IPS-DAKOTA integration

Single IPS framework instance

Manage many dynamic DAKOTA coupled simulations



# New AToM OMFIT-IPS Interface

Take advantage of predefined structure of IPS simulation

New OMFIT modules:

**IPScore:**

manage IPS configuration and execution

**IPSworkflow:**

extract workflow from existing IPS simulation

The screenshot displays the OMFIT GUI with the 'IPSworkflow GUI' window open. The left sidebar shows a tree view of OMFIT modules, including 'IPScore', 'INPUTS', 'OUTPUTS', 'SCRIPTS', 'PLOTS', 'GUI', and 'COMPONENTS'. The main window is titled 'IPSworkflow GUI' and contains a 'Inputs' tab with a table for beam parameters (Beam #1 to #14) and a 'Execution' tab with various configuration fields. The 'Execution' tab includes options for 'Co-current beam', ion species (A and Z), beam voltages, powers, and current fractions. It also defines source grid dimensions, aperture shape and dimensions, tangency radius, and focal lengths. At the bottom, it specifies the server ('edison'), walltime ('1:00:00'), queue ('regular'), and mppwidth ('auto'). A button at the bottom right reads 'Execute IPS workflow and fetch results'.

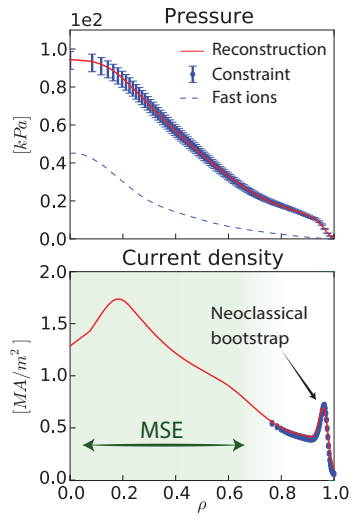
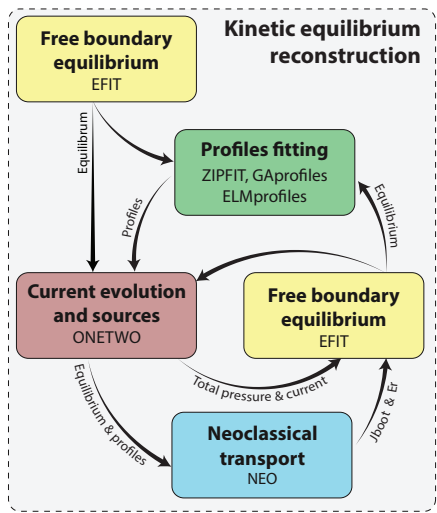
# AToM: Advanced Tokamak Modeling

## Seven Research Thrusts

- ① Maintain OMFIT+IPS **frameworks**, provide wrappers and streamlining
- ② Create simulation **workflows** for the core, pedestal and scrape-off-layer
- ③ Develop workflows for experimental **validation**
- ④ Accelerate **COGENT** integration into AToM with **FASTMath**
- ⑤ Carry out **SUPER** performance engineering of **xGYRO/NEO**
- ⑥ Establish a **data management** scheme, provenance and portal services
- ⑦ Provide user **support** and community outreach

# DIII-D kinetic EFIT reconstruction

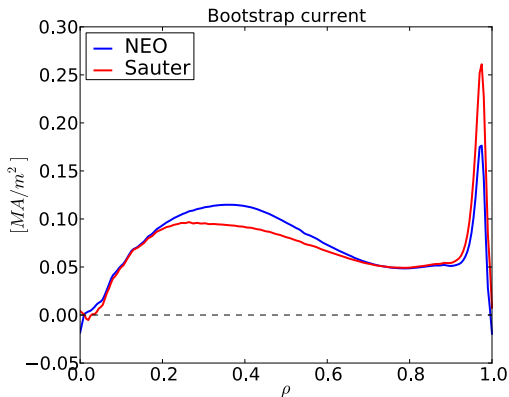
The foundation of most DIII-D physics studies



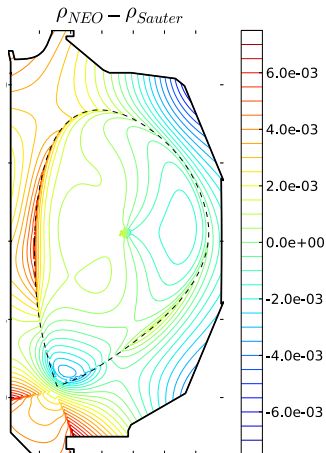
#145419 2600ms

# First-principles NEO bootstrap current

Now integrated into kinetic-EFIT workflow



- Sauter model usually good but inaccurate in some plasma regimes



- NEO calculation gives lower magnetic  $\chi^2$  than Sauter

# Core Transport Theory in a Nutshell

Sophisticated multiple space/timescale ordering

## Equilibrium

$$\vec{k} = 0$$
$$\exp\left(-\frac{m_a v^2}{2T_a}\right)$$
$$\frac{\partial}{\partial \tau_0}$$

## Fluctuations

$$\vec{k} = (k_x, k_y)$$
$$\text{NEO: } \vec{k} = 0$$
$$\text{GYRO: } \vec{k} > 0$$
$$\frac{\partial}{\partial \tau_1}$$

## Transport

$$\vec{k} + \vec{k}' = 0$$
$$\frac{\partial}{\partial \tau_2}$$

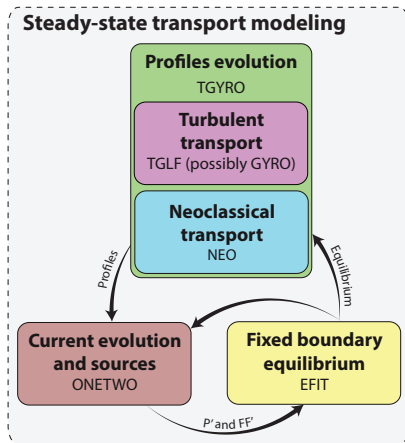
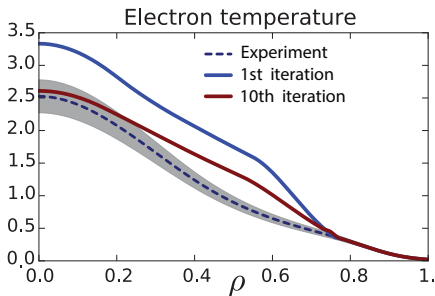
$$F_0 + \lambda F_1 + \lambda^2 F_2 = 0$$

$$\lambda \doteq \frac{\text{ion gyroradius}}{\text{device size}} \sim \frac{1}{500}$$

# Steady-state profile prediction

TGYRO+TGLF+NEO+ONETWO+EFIT

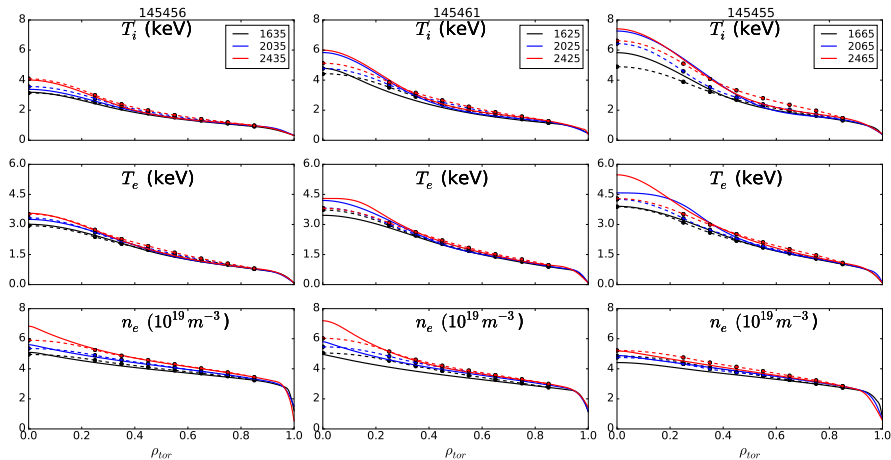
- Efficient steady state solution by decoupling timescales
- Important interplay between transport and EFIT equilibria
- Workflow is the basis of recent FNSF scenario development



# TGYRO+TGLF predictions for 3,5,7 MW of NBI

Experimental profiles (solid) versus TGYRO+TGLF (dashed)

The **global trends** are well-captured,  
but significant **local gradient errors** can occur.

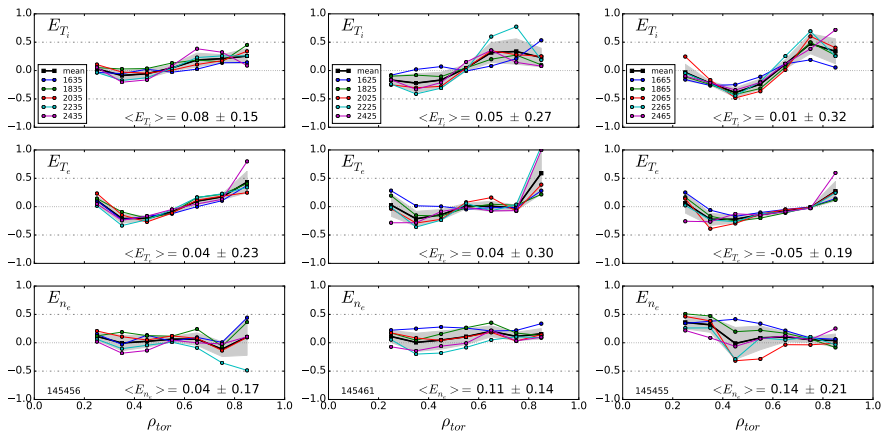




# Local gradient error metrics

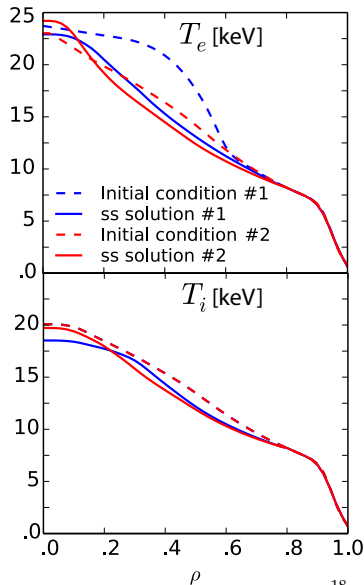
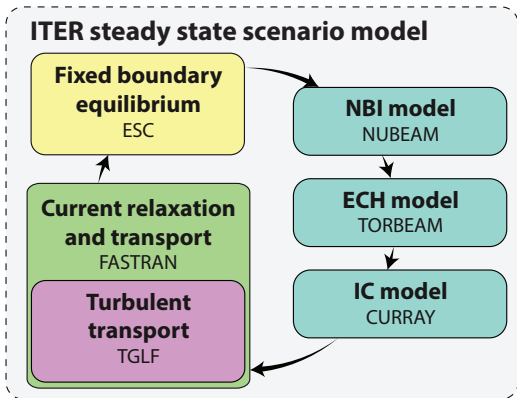
$$E_Y(\rho) = [\nabla Y_{sim}(\rho) - \nabla Y_{exp}(\rho)] / \nabla Y_{exp}(\rho)$$

Trend toward modest **under-prediction** of  $\nabla T$  closer to magnetic axis, and **over-prediction** toward the edge



# IPS workflow for ITER steady-state scenario

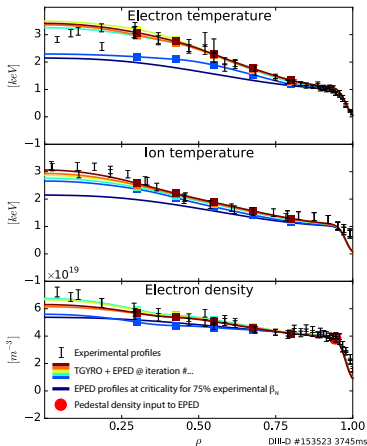
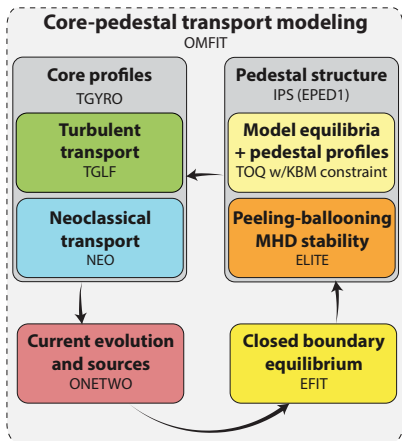
Steady-state  $T_e, T_i$  versus initial condition



# Self-consistent equilibrium-core-pedestal modeling

*Dynamic Pedestal demonstrated by AToM (see Meneghini poster)*

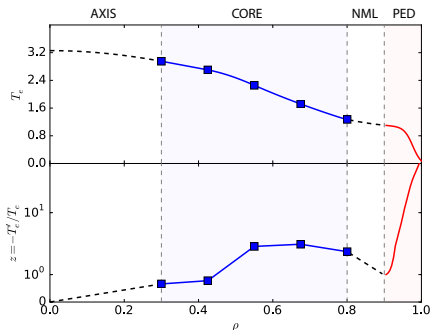
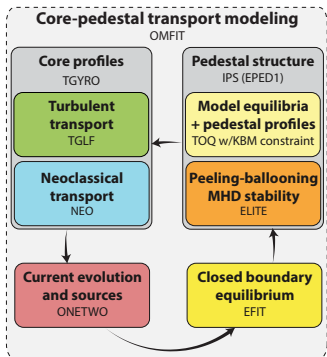
**New capability:** Self-consistent prediction of pressure, confinement and fusion power using only pedestal density  $n_e$ .



# Self-consistent equilibrium-core-pedestal modeling

## Separation of MHD, transport and current diffusion timescales

Method of solution looks like **finding roots of a nonlinear system**, not **time-dependent advection-diffusion**

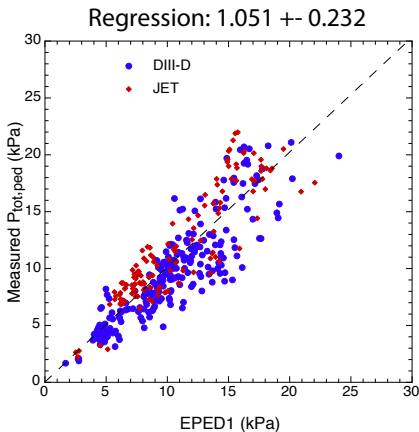
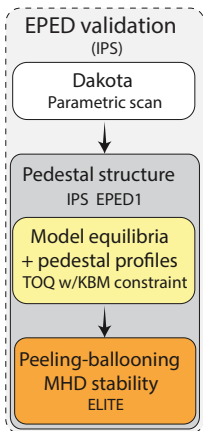


Compact, elegant description in terms of **local gradient profile**

# Self-consistent equilibrium-core-pedestal modeling

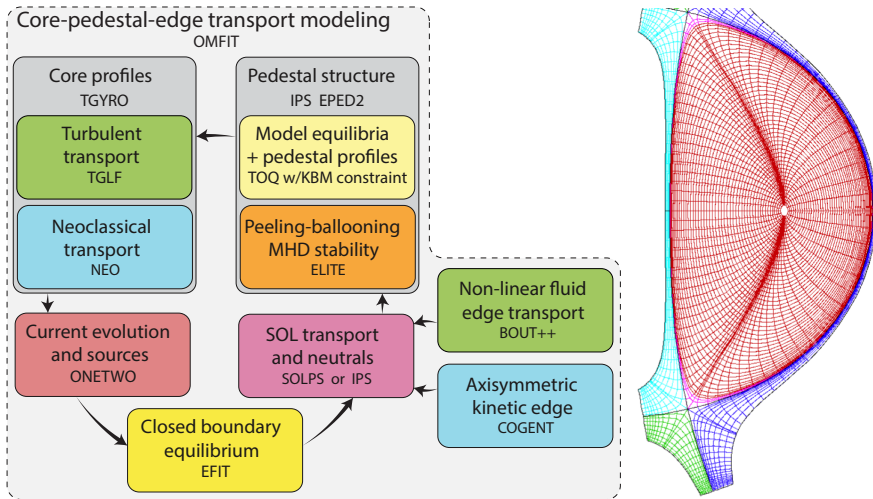
## IPS-EPED1 workflow (FASTRAN DIII-D hybrid scaling-law)

IPS-EPED1 reproduces [Snyder 2009] validation results, **1.5 hours at NERSC on 3600 cores** versus **1 week on GA workstation**



# Upcoming core-pedestal-SOL workflow

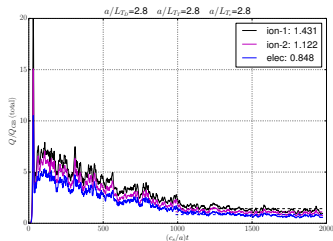
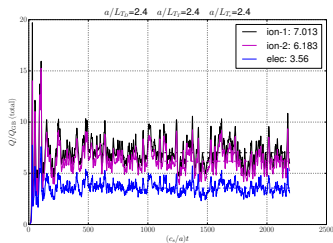
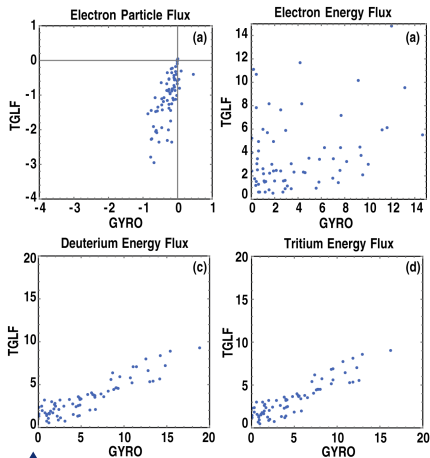
Coupling SOLPS (via IPS), BOUT++, COGENT



# Using AToM infrastructure to recalibrate TGLF

Reduced model based on calibration to HPC simulations

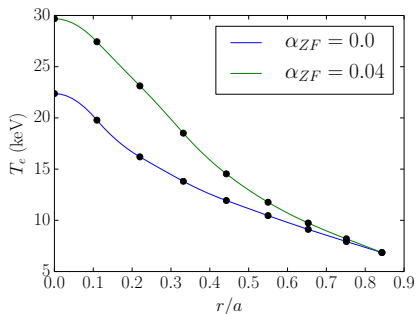
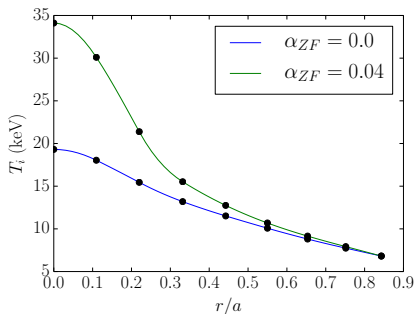
ITER simulation ensemble using **IPS-GYRO** and **TGYRO-GYRO** to capture subtle **zonal-flow stabilization** mechanism



# Using AToM infrastructure to recalibrate TGLF

## State-of-the-art ITER hybrid performance prediction

GYRO-TGYRO recalibration specifically for ITER **doubles** the predicted fusion power (to approximately 1GW).





# AToM NIMROD module

## Remove barrier to entry for new users

The screenshot displays the NIMROD GUI interface. On the left is a file browser showing the project structure, with 'GAprofiles' highlighted by a red box (6). The central panel contains the following fields and buttons:

- Run / Regression cases: Run a scan (4)
- Server: edison (1)
- Nimrod install root (on server): /global/project/projectdirs/atom/atom-instal-edison/nimrod (2)
- Nimrod executable name (on server): 'nimrod-ser'
- Storage directory (on server): '/scratch1/scratchdirs/lzsu/OMFIT/NIMRODruns/'
- Run ID: 'wdm15n6'
- Additional input files: # = 1
- auxiliary input 1: 'density\_profile'
- deploy auxiliary input 1 as: 'density\_profile'
- Use auxiliary input 1 to run: 'jimsset'
- Restart step: '0021'
- Run job: with batch script using qsub (3)
- batch script: 'run.nimrod'
- Buttons: Run NIMSET, Submit NIMROD job + monitor + fetch

On the right, Figure 2 shows a 2D cross-section of a plasma configuration with a color-coded density profile. Figure 3 shows a log-linear plot of Magnetic Energy (J) versus Time (ms) for current values of 0.0, 1.0, 2.0, 3.0, 4.0, and 5.0. Red arrows point to the x-axis labels 'x=0.83699' and 'y=-0.75102' on the right side of the interface.

# AToM NIMROD module

## Recent developments and highlights

- Local or remote execution
- Points to NIMROD installation in **NERSC AToM project directory** by default
- Run in serial or parallel
- Automatically run scans over input parameters and **organize output** for easy comparison
- Store results of **multiple runs** within a project
- Extract density profile from **GProfiles** module and write to NIMROD accepted file format
- **Automatic parsing** and plotting of NIMROD input and output file formats

# AToM COGENT module: Nonlinear Kinetic Edge Code

## Data preparation and execution within AToM

The screenshot displays the OMFIT - COGENT application interface. The main window is titled "COGENT Main GUI" and contains several sections:

- Help** and **EDIT subGUI** buttons.
- EFIT grid size = 85x85** and **Operation = Generate g-file from SNAP file**.
- OMFIT[EFIT][GUIS][SNAP]gui** section with a **Load SNAP file from =** field.
- Run Hypnotoad** button.
- OUT: coefficients1 - Coefficient file, at [COGENT\_Coefficients]** and **OUT: hypnotoad.id - hypnotoad state file, at [hypnotoad\_state]**.
- Run grid post-processing** button.
- OUT: DCT\_coefficients.txt - Nodal coefficient file, at [nodal\_COGENT\_Coefficients]** and **OUT: COGENT\_mapping.txt - Nodal Grid file, at [nodal\_grid]**.
- Run Fix\_X** button.
- OUT: fixed\_nodal\_grid.txt - Fixed Nodal Grid file, at [fixed\_nodal\_grid]**.
- Job Server = jedson**.
- Submit COGENT Job** and **Monitor Job** buttons.
- OUT: COGENT\_PLOTS - Plot files directory, at [plot\_files\_dir]** and **IN: COGENT\_PLOTS - Plot files directory, at [plot\_files\_dir]**.
- Run VISIT** button.

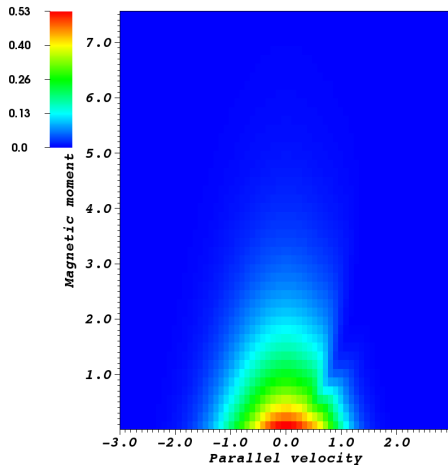
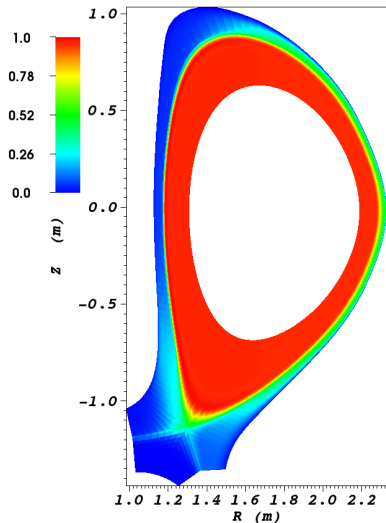
The background shows a terminal window with the following output:

```
[[MainSettings]] [[SERVER]] [*d3d3d3*] [[*teu
[[MainSettings]] [[SERVER]] [*d3d3d3*] [*RDD
[[MainSettings]] [[SERVER]] [*id*]
[[MainSettings]] [[SERVER]] [*matlab*]
[[SERVER]] [*return*] [*teu
[[SERVER]] [*return*] [*teu
[[SERVER]] [*return*] [*teu
[[SERVER]] [*xmasprid*]
directory: /global/...
```



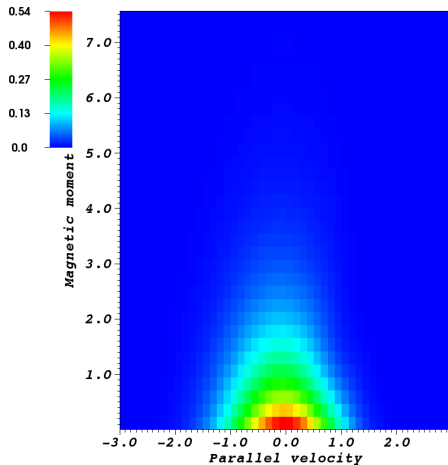
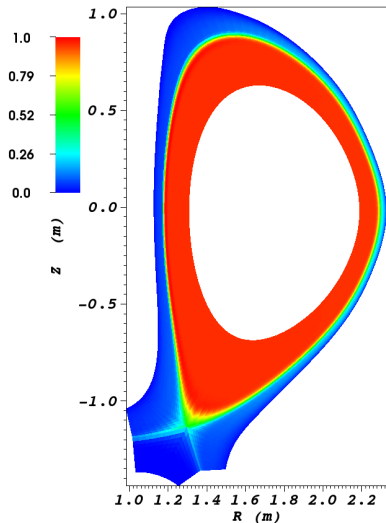
# COGENT Ion-Orbit Loss in DIII-D Geometry

## Collisionless loss cone



# COGENT Ion-Orbit Loss in DIII-D Geometry

Refilling of loss cone with nonlinear FP collisions



# AToM accelerates US integrated modeling capability

Poised to make a significant contribution to ITER

ITER-IMAS mimics EU-ITM framework: **Kepler** workflow manager and **Consistent Physical Objects** (CPOs) as data structures

ITER is committed to its data structure but **not to framework**

- ITER will likely allow use of frameworks from different institutions

**Natural selection** will favour the best predictive modeling solution

- AToM interface planned for ITER-IMAS data structure
- **User adoption** and scientific impact will define success

