AToM: Advanced Tokamak Modeling
Introduction and first physics results

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P. Snyder, M. Umansky

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General Atomics, UCSD, Oak Ridge National Laboratory, Lawrence Livermore National Laboratory, FASTMath, SUPER, SciDAC Scientific Discovery through Advanced Computing

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

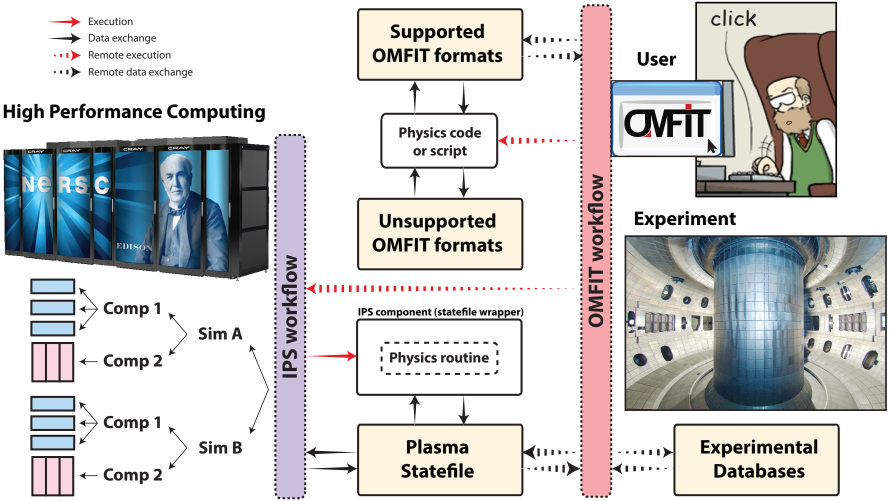
D. Bernholdt, D. Green (poster), D. Batchelor, J-M. Park, S. Diem, E. D'Azevedo

LLNL

M. Dorf, M. Dorr, M. Umansky

AToM couples IPS and OMFIT frameworks

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



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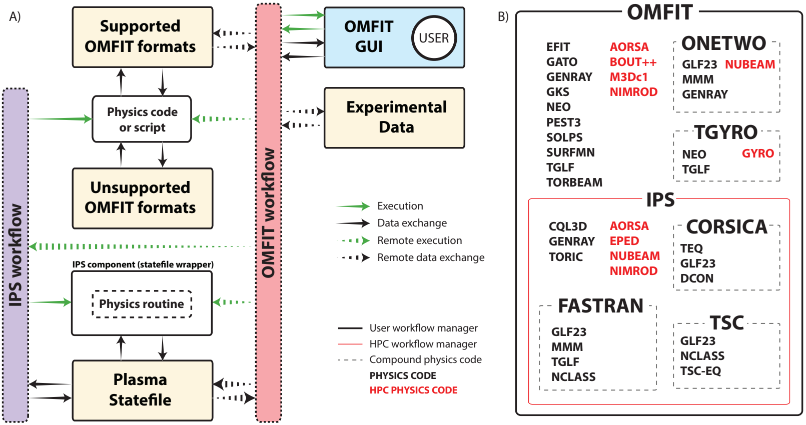
Multiple levels of component and framework integration



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

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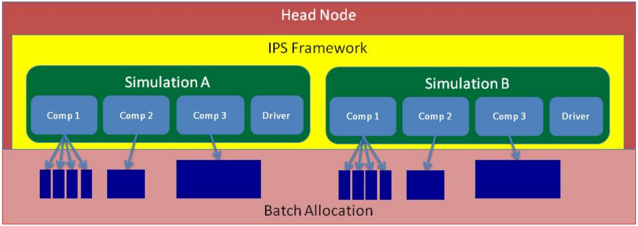
Integrated Plasma Simulator (IPS)

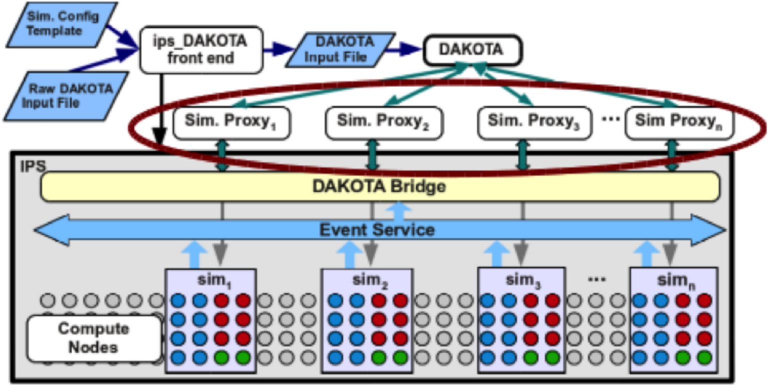


- Enables integration of MPP component codes.
- Wraps (unmodified) codes in a **standard component interface**.
- 4 levels of parallelism.
- Supports advanced algorithms like **Parareal**.

Integrated DAKOTA-IPS Use Cases

IPS-DAKOTA integration

Single IPS framework instance
Manage many dynamic DAKOTA coupled simulations



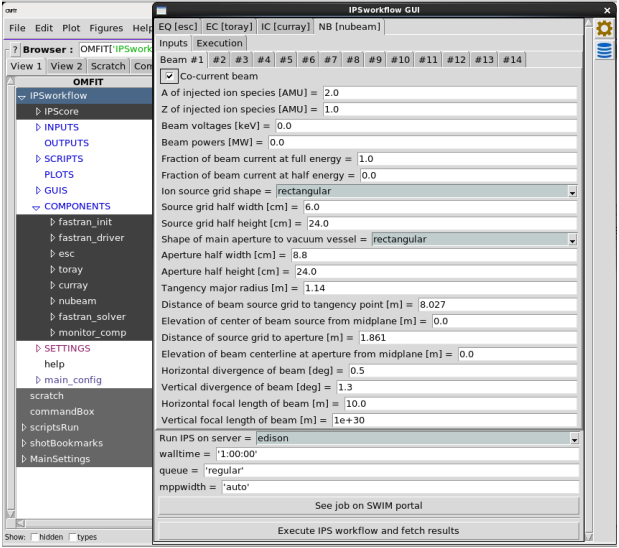
New AToM OMFIT-IPS Interface

Take advantage of predefined structure of IPS simulation

New OMFIT modules:

IPScore:
manage IPS configuration and execution

IPSworkflow:
extract workflow from existing IPS simulation



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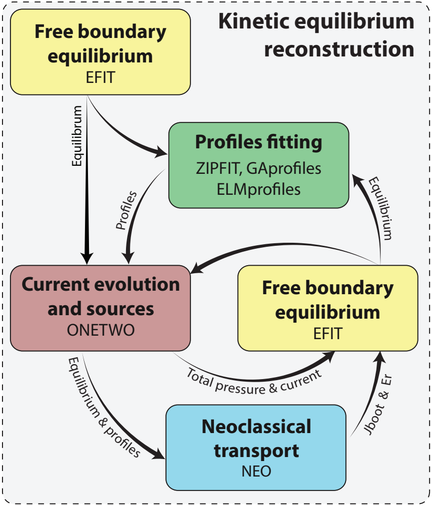
AToM: Advanced Tokamak Modeling

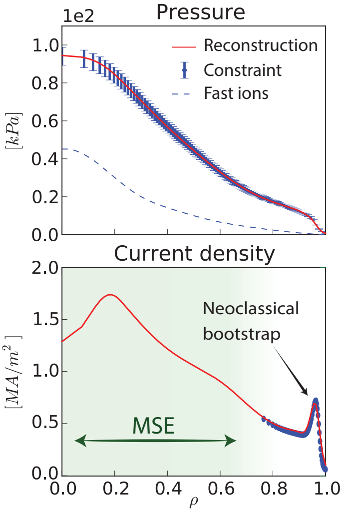
Seven Research Thrusts

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

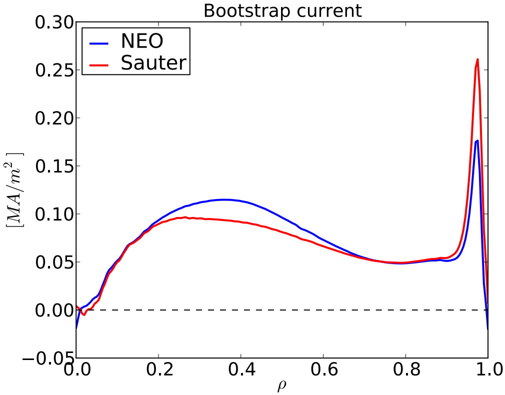


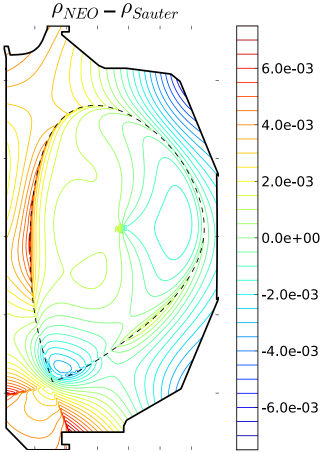


#145419 2600ms

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 χ^2 than Sauter

Core Transport Theory in a Nutshell

Sophisticated multiple space/timescale ordering

Equilibrium

$$\vec{k} = 0$$

$$\exp\left(-\frac{m_a v^2}{2\,T_a}\right)$$

$$\frac{\partial}{\partial \tau_0}$$

Fluctuations

$$\vec{k} = (k_x, k_y)$$

$$\text{NEO: } \vec{k} = 0$$

$$\text{GYRO: } \vec{k} > 0$$

$$\frac{\partial}{\partial \tau_1}$$

Transport

$$\vec{k} + \vec{k}' = 0$$

$$\frac{\partial}{\partial \tau_2}$$

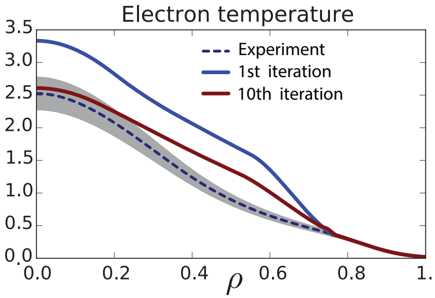
$$F_0 + \lambda F_1 + \lambda^2 F_2 = 0$$

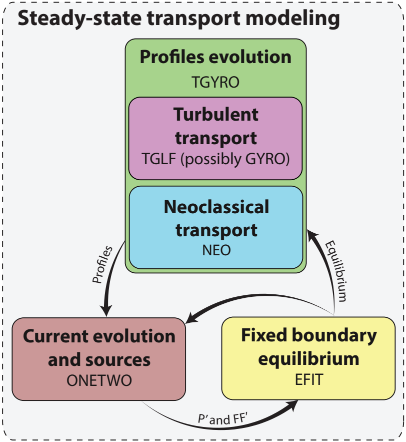
$$\lambda \doteq \frac{\text{ion gyroradius}}{\text{device size}} \sim \frac{1}{500}$$

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

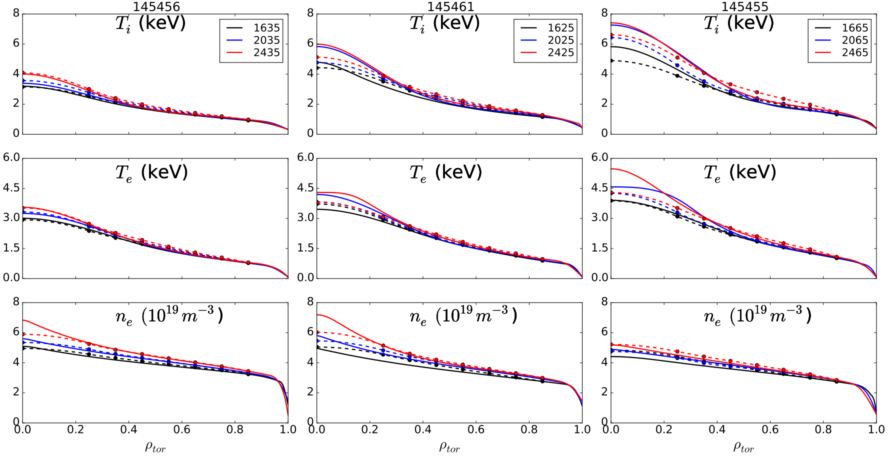




TGYRO+TGLF predictions for 3,5,7 MW of NBI

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

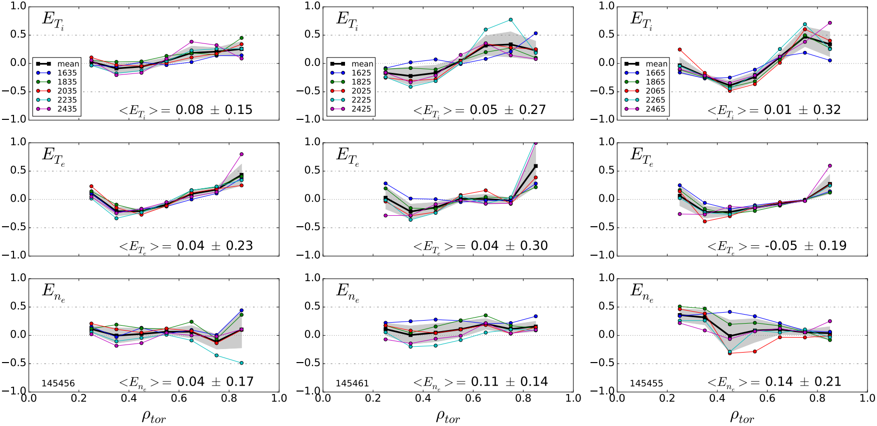
The **global trends** are well-captured,
but significant **local gradient errors** can occur.



Local gradient error metrics

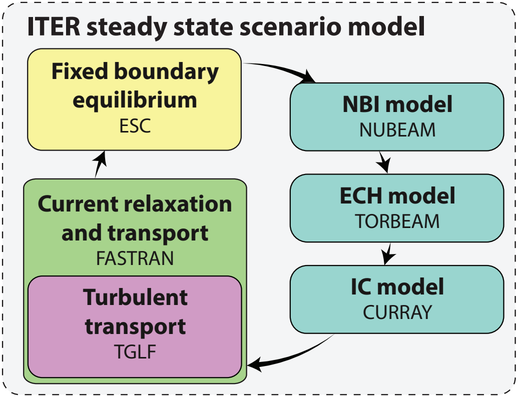
$$E_Y(\rho) = \left[\nabla Y_{sim}(\rho) - \nabla Y_{exp}(\rho)\right] / \nabla Y_{exp}(\rho)$$

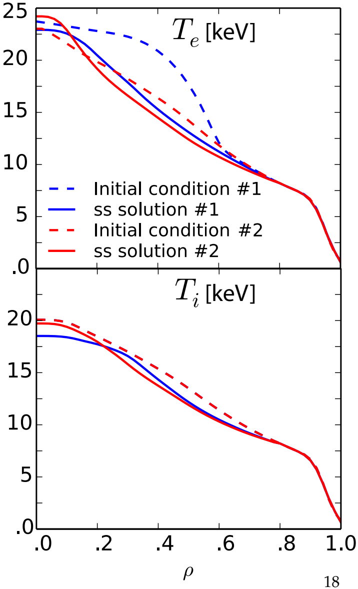
Trend toward modest **under-prediction** of ∇T closer to magnetic axis, and **over-prediction** toward the edge



IPS workflow for ITER steady-state scenario

Steady-state T_e, T_i versus initial condition

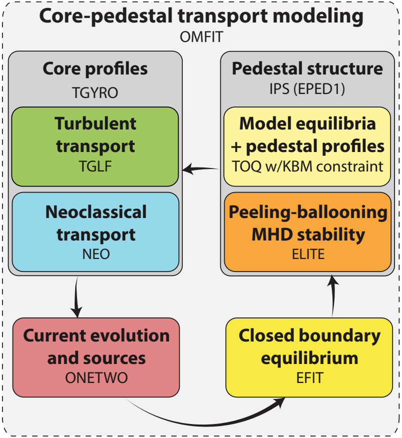


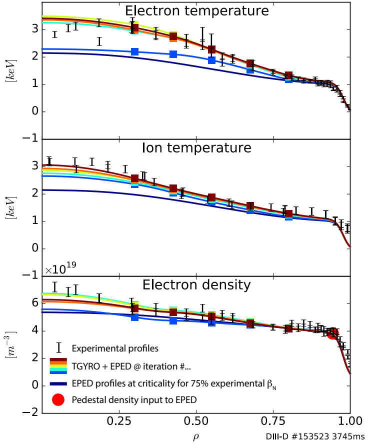


Self-consistent equilibrium-core-pedestal modeling

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.

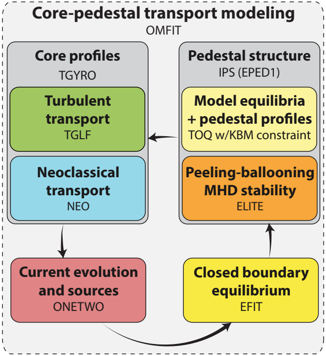


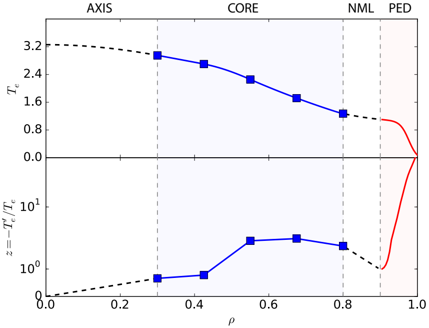


Self-consistent equilibrium-core-pedestal modeling

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**

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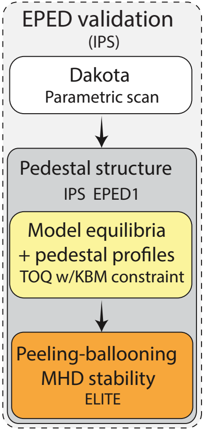
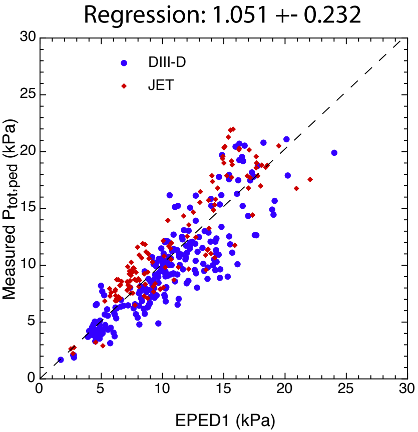
Self-consistent equilibrium-core-pedestal modeling

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





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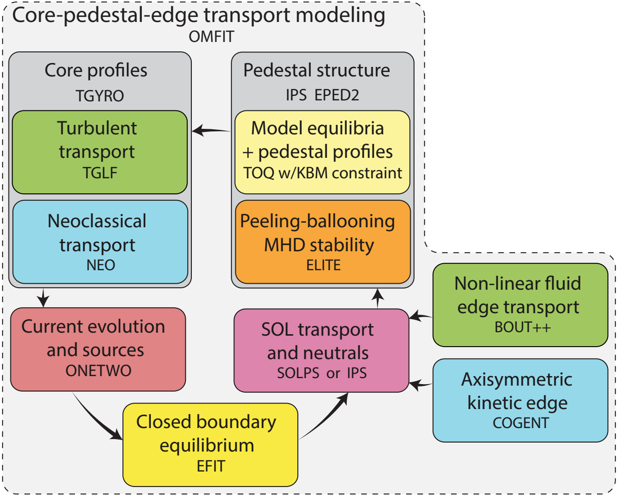
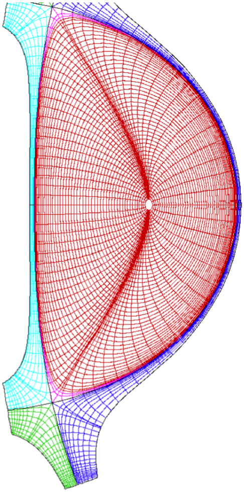
Upcoming core-pedestal-SOL workflow

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

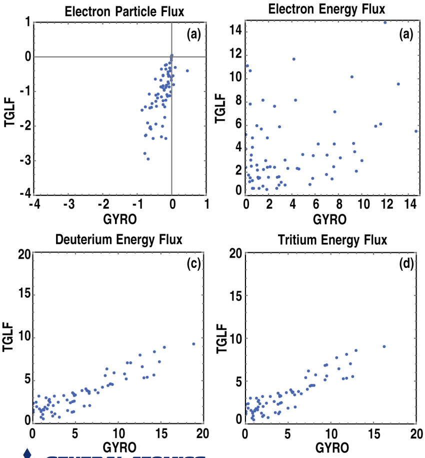


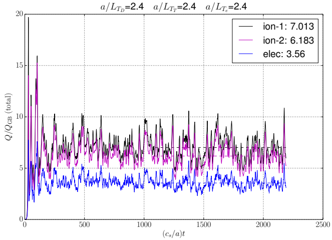


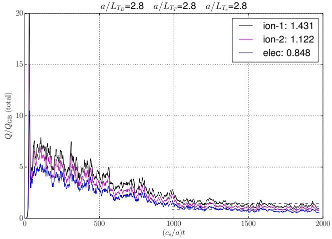
Using AToM infrastructure to recalibrate TGLF

Reduced model based on calibration to HPC simulations

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



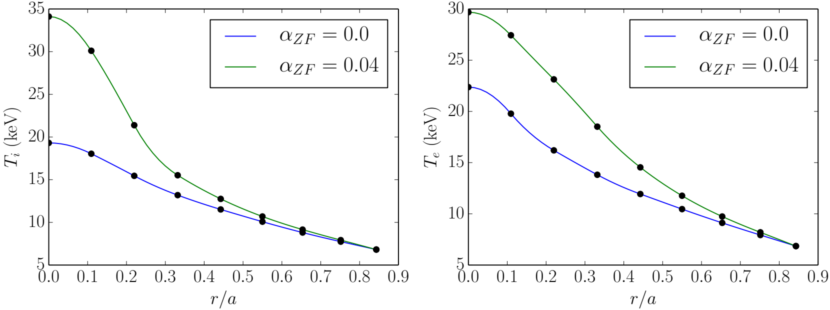




Using AToM infrastructure to recalibrate TGLF

State-of-the-art ITER hybrid performance prediction

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



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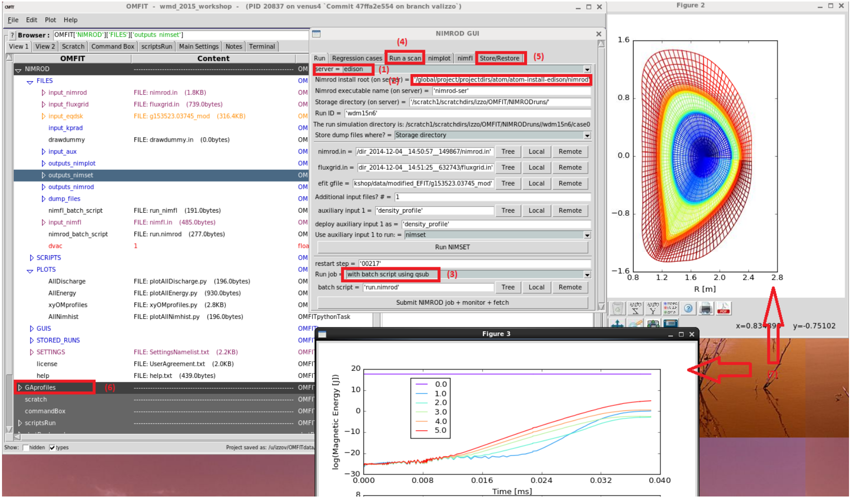
AToM NIMROD module

Remove barrier to entry for new users



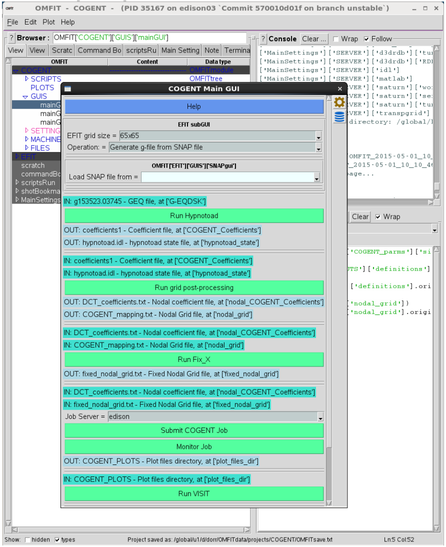
AToM NIMROD module

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 **GAprofiles** 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



Lawrence Livermore National Laboratory

FASTMATH

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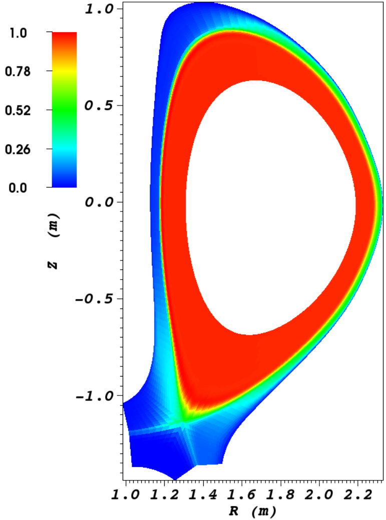
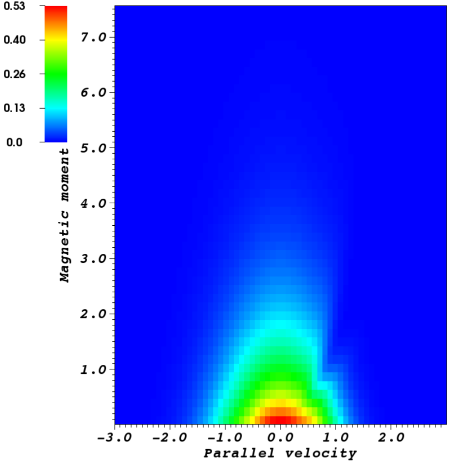
COGENT Ion-Orbit Loss in DIII-D Geometry

Collisionless loss cone





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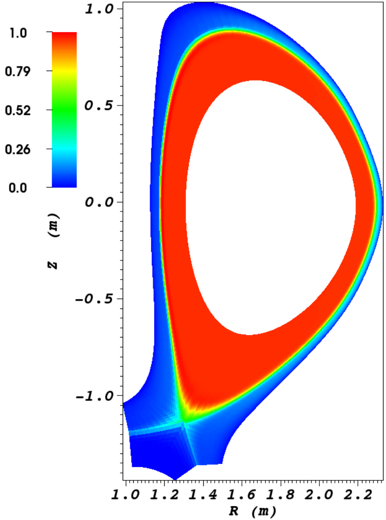
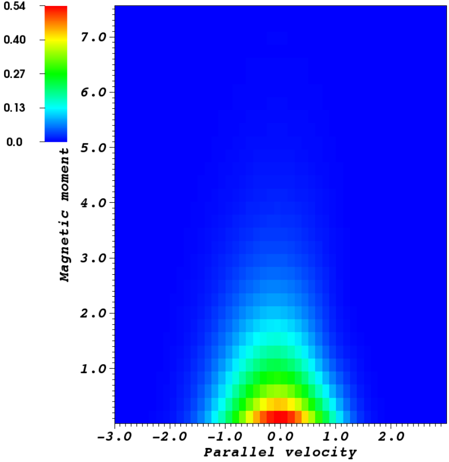
COGENT Ion-Orbit Loss in DIII-D Geometry

Refilling of loss cone with nonlinear FP collisions





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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