Advanced Tokamak Modeling Environment for Fusion Plasmas: Physics
J.M. Park\textsuperscript{1}, D.L. Green\textsuperscript{1}, J. Candy\textsuperscript{2}, O. Meneghini\textsuperscript{3}, C. Holland\textsuperscript{3} and ATOM Team
\textsuperscript{1}ORNL, \textsuperscript{2}GA, \textsuperscript{3}UCSD

**Introduction**

ATOM core-edge integrated workflows

Guiding philosophy of ATOM - take a bottoms-up, collaborative approach that focuses on supporting, leveraging, and integrating the wide spectrum of existing research activities throughout the US fusion community, to grow and improve a Whole Device Modeling (WDM) capability that has broad community support and buy-in. In practice, this means developing flexible software environment and workflows to couple existing and in-development physics component.

ATOM provides two core-edge integrated workflows:

1. OMFIT-based fast Whole Device Modeling
2. IPS-based High Performance Computing Whole Device Modeling, enabling a wide range of physics studies, even totally new

OMFIT-based fast WDM

IPS-based HPC WDM

- Use machine learning accelerated models for EPED, NED, and TGLF
- Transfer data between components using ORAS

One step closer toward a WDM capability

Self-consistent profile prediction from magnetic axis to wall

- Iterative solution procedure to match boundary conditions between the core, edge pedestal, and SOL
- Self-consistent profile across the regions, especially separatrix values
- Enable study of strong interaction between the regions

**First-principle model, performance, connect to ATOM workflows**

Future recalibration of TGLF with CGYRO

TGLF: the heart of ATOM profile-prediction capability

- Linear gyro-Landau-fluid eigenvalue solver
- Saturated potential intensity derived from a database of nonlinear GYRO simulations
- Database resolves only long-wavelength turbulence: $k_T < 1$

CGYRO: generate future database for TGLF calibration

- New nonlocal spectral solver for collisional edge
- Arbitrary-wavelength spectral formulation
- Designed from scratch for multiscale

CGYRO simulation: low rotation DIII-D ITER baseline discharge

- Nearly all electron flux arises from multiscale regime
- Experimental value $Q_{\text{rms}} = 8$ accurately recovered

**Physics and scenario exploration**

From present-day experiments to ITER and beyond

**Ex.**

- **Present-day experiments**
  - CGYRO simulation: low rotation DIII-D ITER baseline discharge
  - Experimental value $Q_{\text{rms}} = 8$ accurately recovered

**Future reactor design**

- **Support ITER**
  - Validate WDM, identify modeling gaps
  - Drive new development

- **Future reactor design**
  - Design next step U.S. reactor
  - Develop advanced tokamak path to a future reactor

**Optimize, find new regimes**

Enabled by efficient utilization of HPC resources

- Multi-dimensional parametric scan
  - $B_n$, $l_n$, density, $P_w$, $P_e$
  - Monte Carlo sampling
  - Each point: fully theory-based integrated modeling

- Parameterize key performance
  - $Q_{\text{rms}} = Q_{\text{rms}}^\text{ideal}
  - $(S_w - S_w^\text{ideal})^2 = B_n 0.5 P_e 0.5 0.5 0.5$

- Search optimum design/operation point

**Validation and uncertainty quantification**

Tightly coupled to ATOM workflows and physics studies

- Initial focus: in-depth core transport model studies
  - Ex. TGLF captures core plasma response to heating changes in low-mode mode plasmas

- Next step: extend to multi-component modeling
  - Ex. Core-edge-impurity coupling – Can we predict response of impurities in core and pedestal to changes in RF heating?

**ATOM Use Cases**

Entry point for collaboration with ATOM

- ATOM validation and scenario modeling will be organized about benchmark use cases
  - Well-documented datasets describing plasma discharges of interest for component and workflow validation
  - Use cases provide clear way of benchmarking competing models, tracking improvements, assessing real-world performance

Each use case will include

- Magnetic equilibria and profile data in accessible format
- Relevant supporting data and analysis (power balance data, fluctuation measurements, MHD mode amplitudes)
- Provenance documentation (publications/models)

**Candidate use cases**

1. DIII-D L-mode shortfall, ITER baseline, steady-state discharges
2. Alcator C-Mod LOC/SOC plasmas, EDA H-mode toroidal field scan
3. ITER inductive, hybrid, and steady-state scenarios
4. ARIES ACT-1/ACT-2 reactor scenarios
5. ...