The Advanced Tokamak Modeling Environment (AToM) for Fusion Plasmas

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on behalf of the **AToM team**
http://scidac.github.io/atom/index.html

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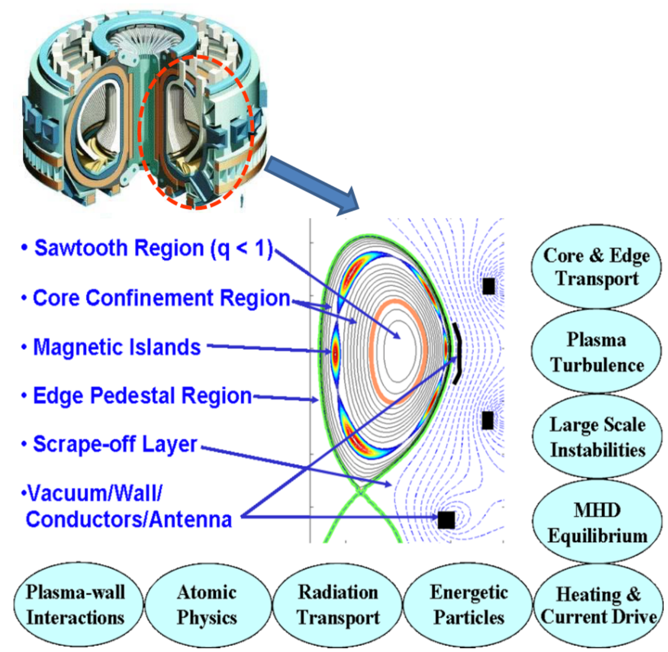
SciDAC
Scientific Discovery through Advanced Computing

UC San Diego

AToM is 1 of 9 SciDAC-4 partnerships working to address modeling needs of US MFE program

- AToM focus is **whole-device modeling (WDM):** assemblies of physics components that provide a sufficiently comprehensive integrated simulation of the plasma

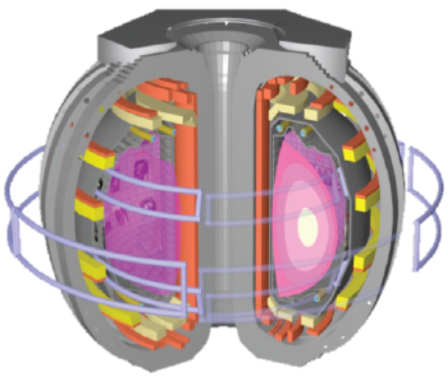
- **AToM guiding philosophy**
  - take a *bottoms-up*, *collaborative* approach that focuses on
  - supporting, leveraging, and integrating the wide spectrum of *existing* research activities throughout the US fusion community,
  - to grow and improve a WDM capability that has *broad community support and buy-in*.

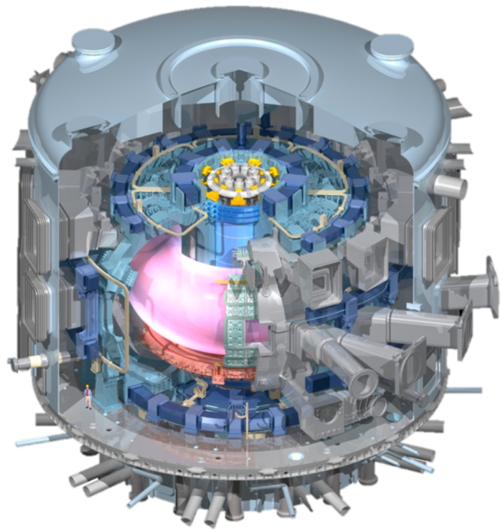


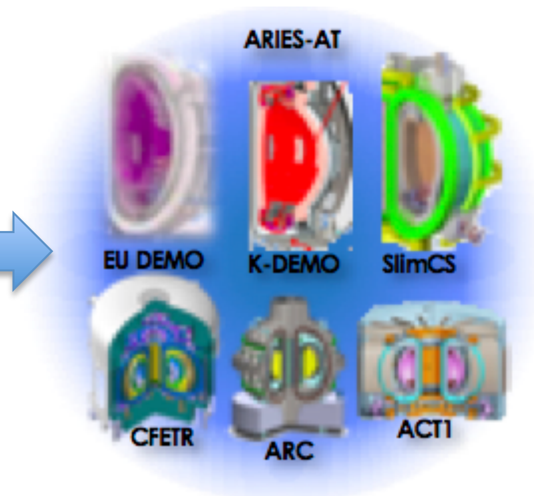
  - In practice, this means developing flexible software environment and workflows to couple existing and in-development physics components

AToM's scope and vision extends from current-day devices to future reactor facilities

Present-day experiments	Support ITER	Future reactor design





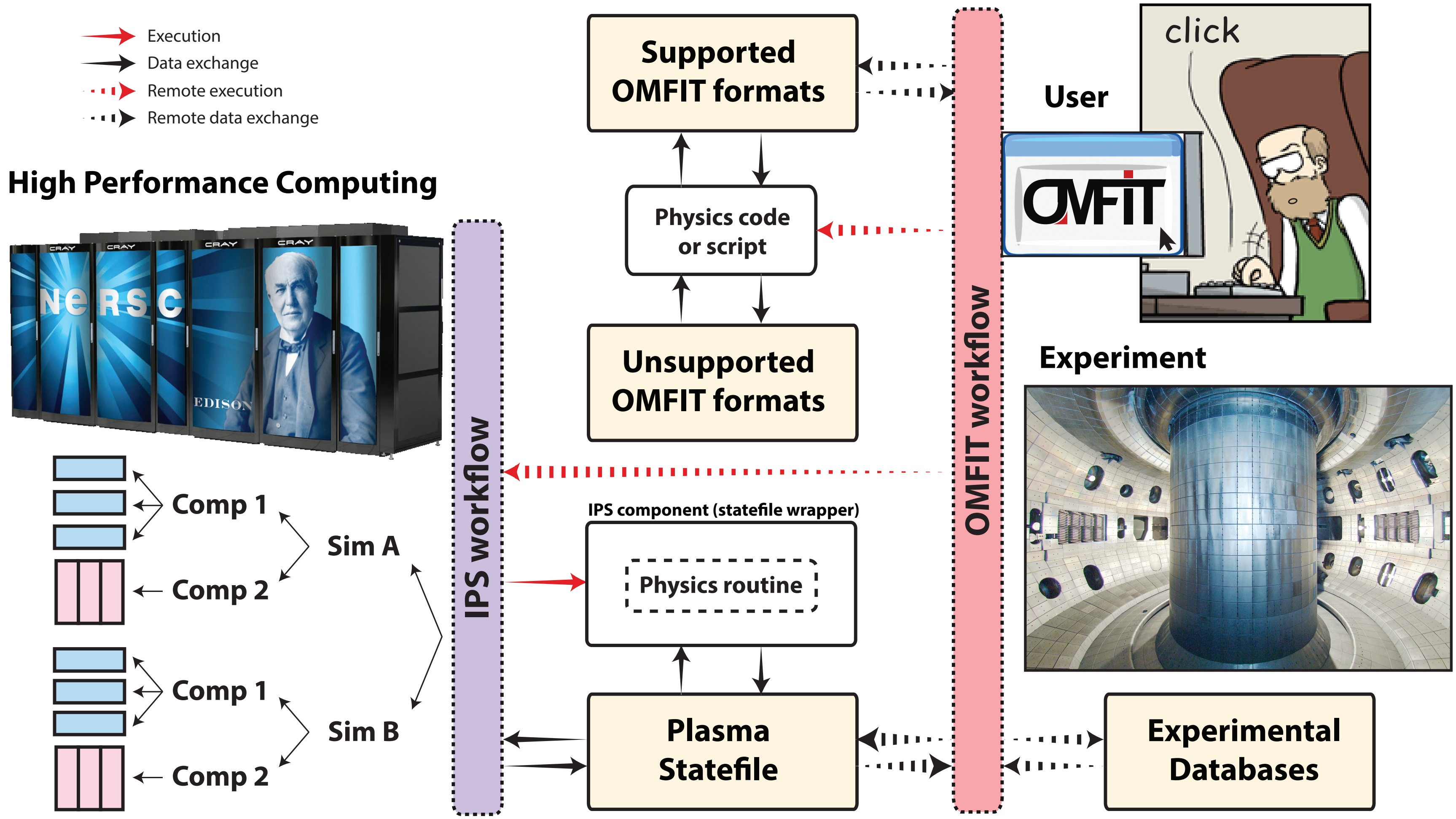


Present-day experiments
- Validate existing WDM capabilities
- Identify modeling gaps
- Drive new development

Support ITER
- Test WDM capabilities in burning plasma conditions
- Optimize ITER operation scenarios

Future reactor design
- Examine how to best optimize devices with varying goals and missions

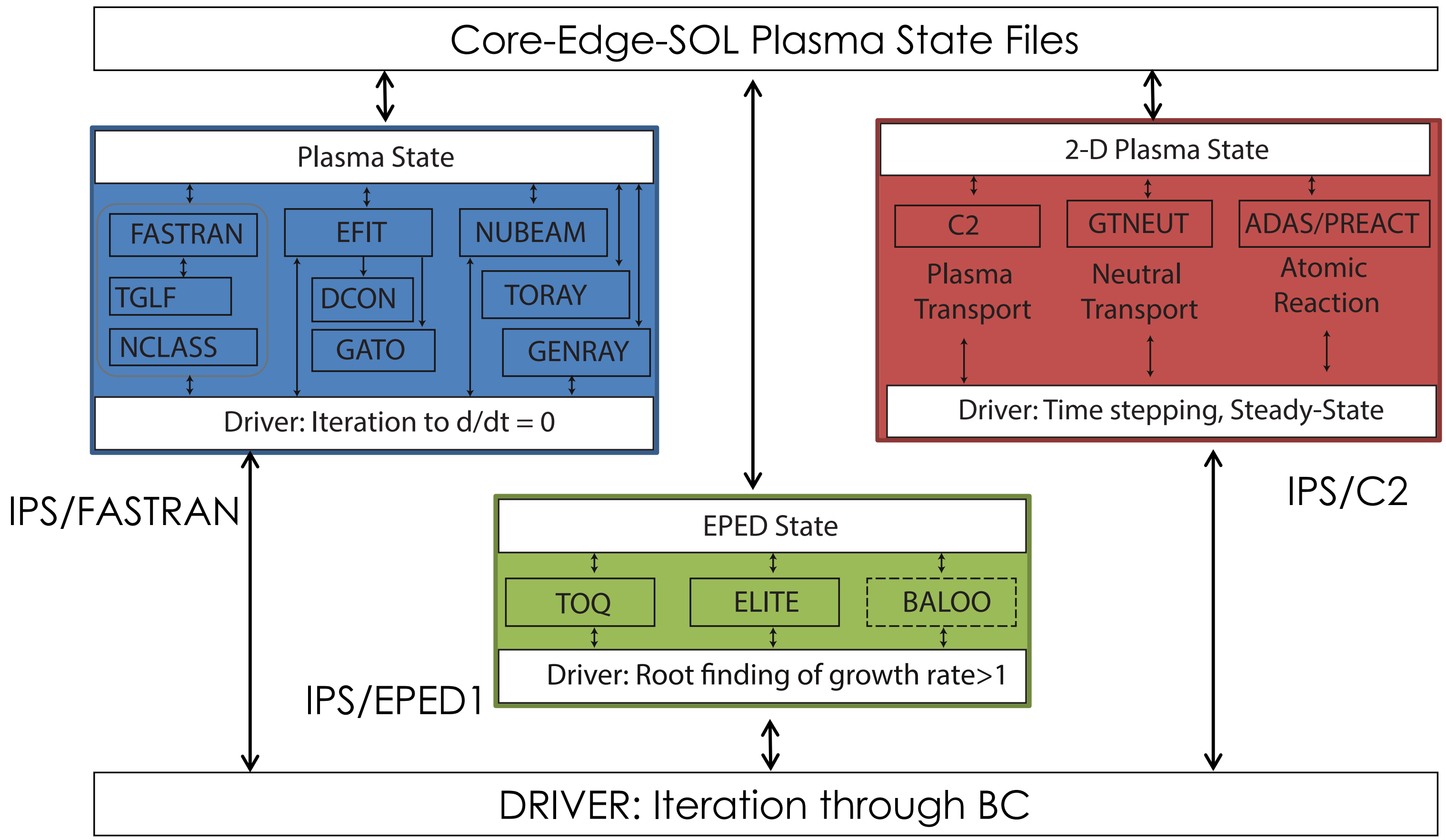
AToM couples IPS and OMFIT computing frameworks and effectively exploits their synergy



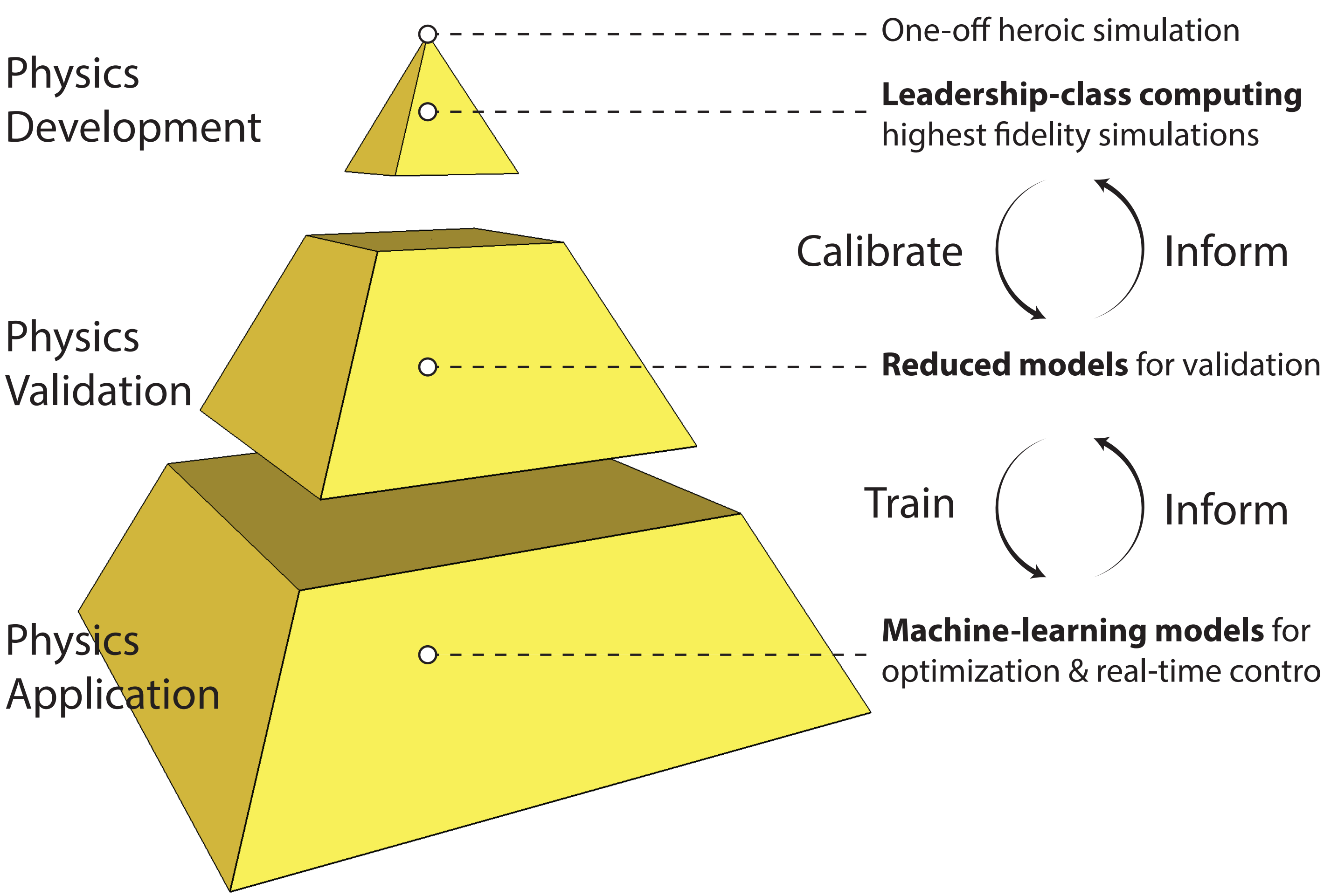
PhD comics © J. Cham

AToM supports flexible workflows based on coupling of multiple physics components

- Core-Edge-Scrape Off Layer prediction requires coupling 15 physics components, executed on NERSC Edison Cray XC30 machine



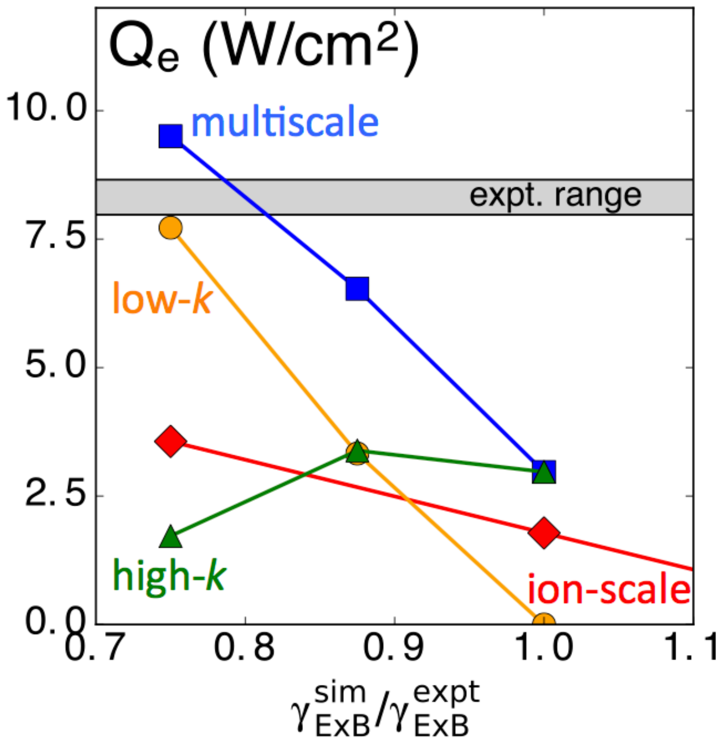
Practical integrated studies require hierarchy of fast, efficient, and accurate physics components



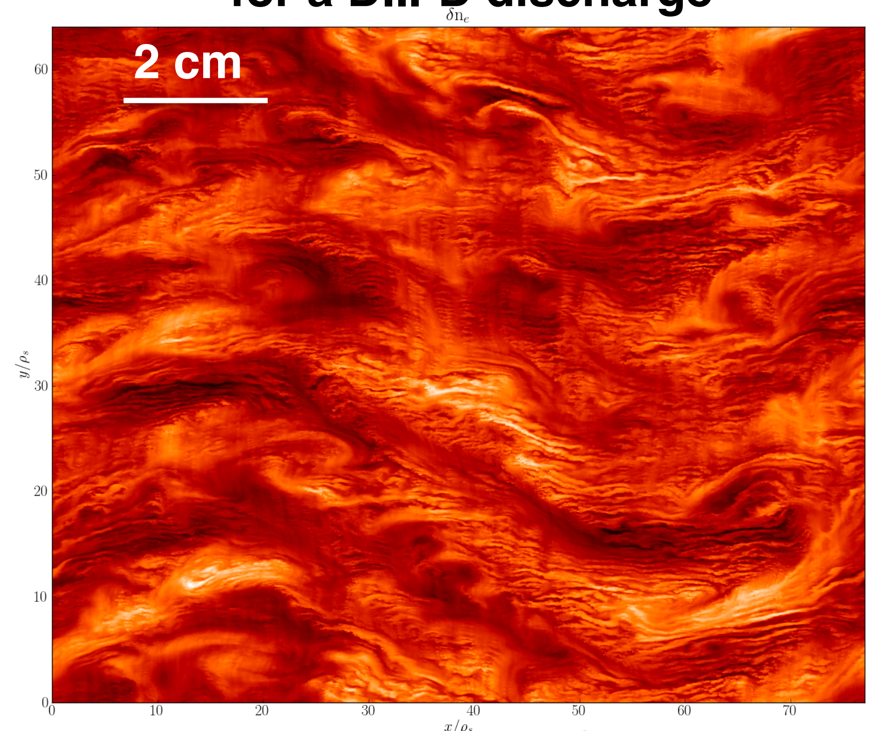
Direct simulation on LCF allows us to better understand complex multiscale dynamics

- Nonlinear gyrokinetic simulations yield highest fidelity transport predictions but require $10^3 – 10^7$ core-hours to simulate small fraction of plasma volume & duration

Holland *et al* 2017 Nucl. Fusion



Simulated turbulent fluctuations for a DIII-D discharge



New results from 2019 INCITE award

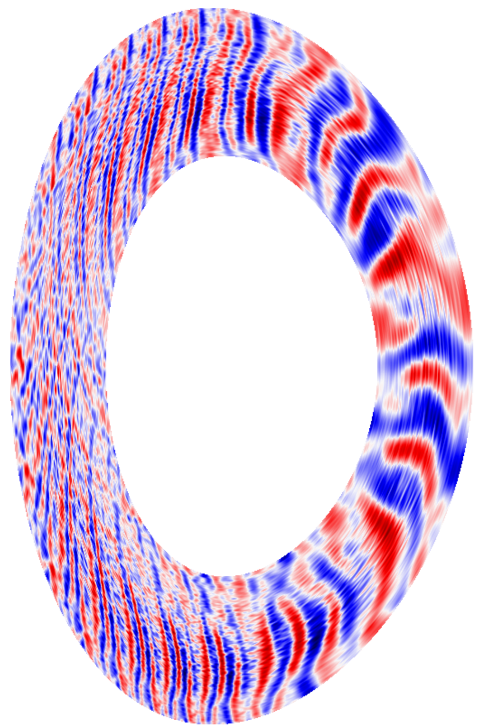
4986 nodes on Titan (80k compute cores)

HPC resources need to explore plasma dynamics in new parameter regimes

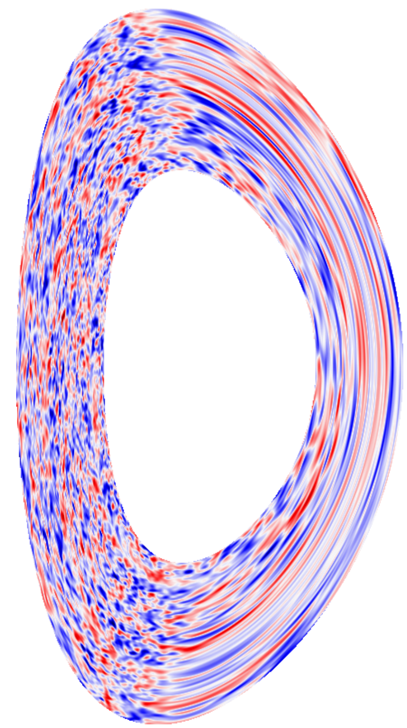
- New CGYRO simulations predict microtearing modes (MTMs) drive significant transport in steady-state plasma core region

- MTMs can be qualitatively different than more commonly studied instabilities like ITG (ion temperature gradient)

ITG in low bootstrap fraction DIII-D H-mode



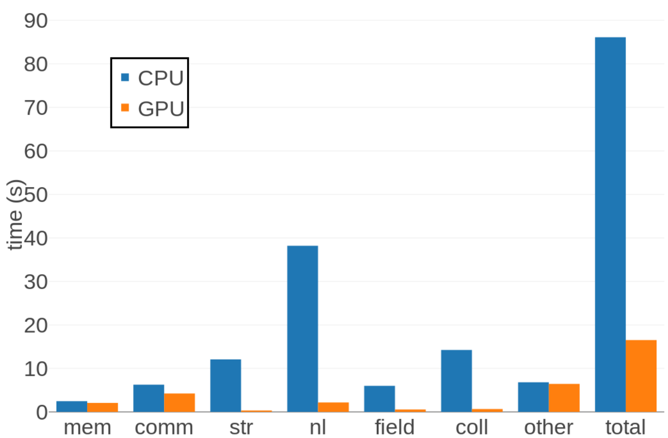
MTM in high bootstrap fraction DIII-D H-mode



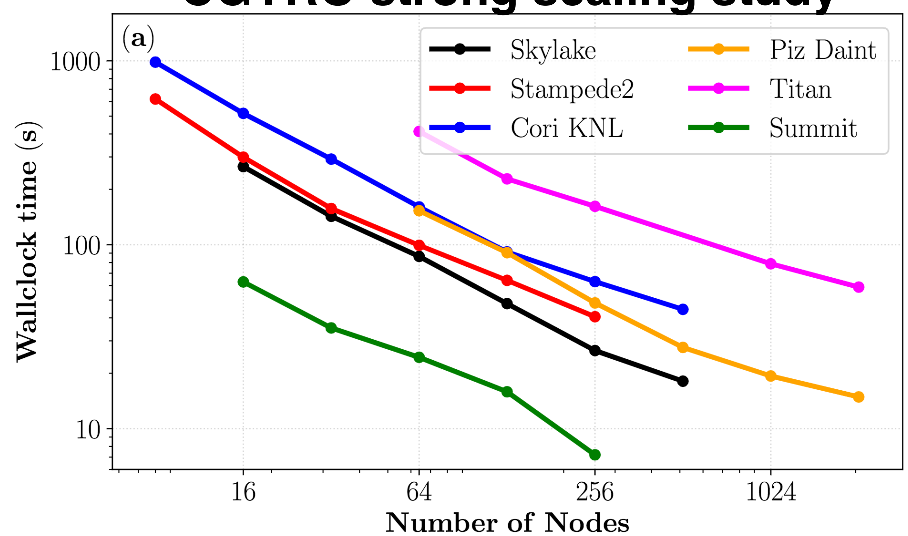
Optimization of CGYRO for Summit yielding 10x increase in code-performance from Titan

- Enables scope and scale of new high-fidelity simulations to **improve our reduced models and thereby our practical predictive modeling capabilities**

CGYRO CPU-only vs. CPU-GPU on Power9 node

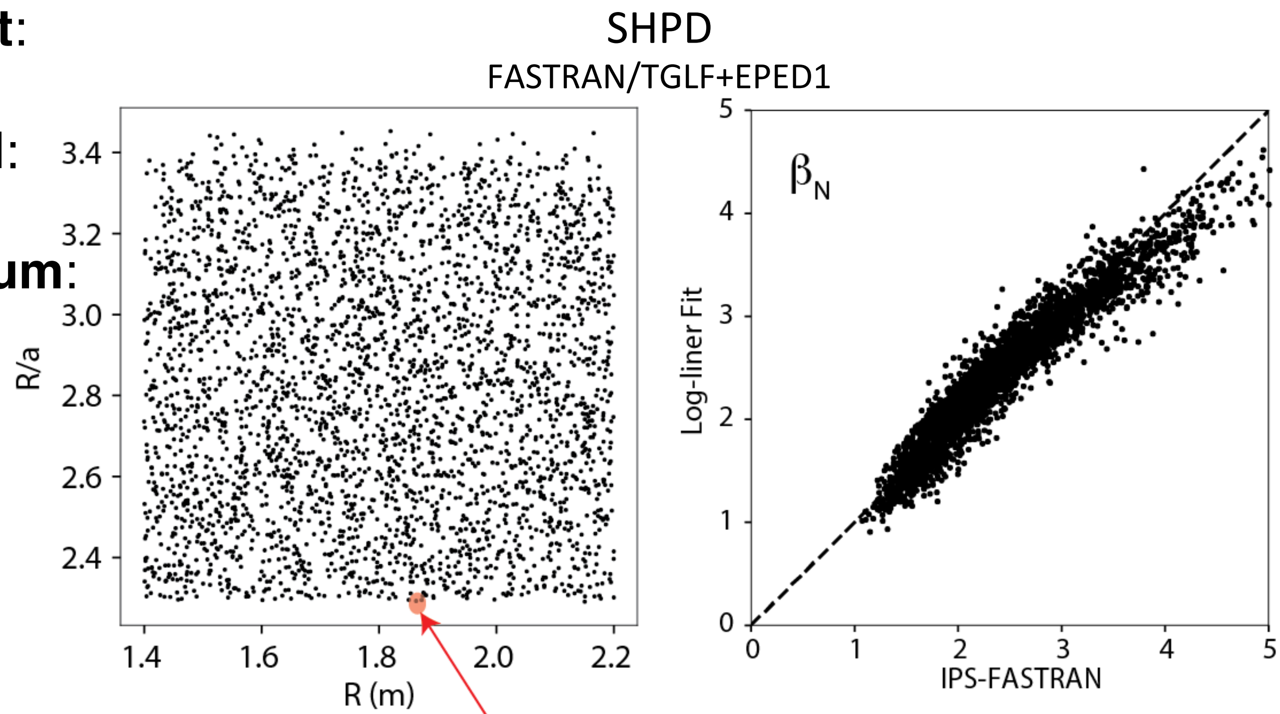


CGYRO strong scaling study



HPC + Capacity: Reactor design study using full physics models with IPS-FASTRAN

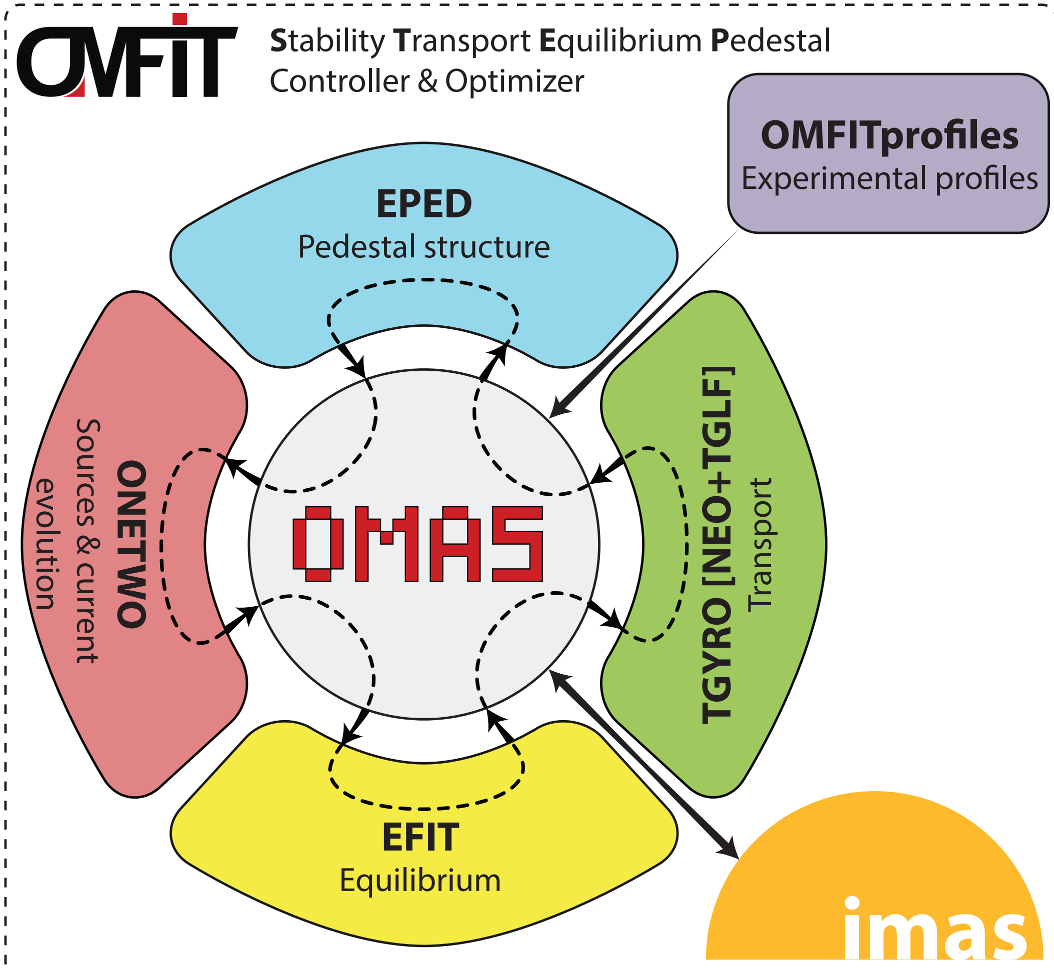
- Multi-dimensional parametric scan with random sampling
  - **Core transport**: TGLF
  - **Edge pedestal**: EPED1
  - **MHD equilibrium**: EFIT
  - **H/CD**: NFREYA, TORAY-GA
  - **MHD stability**: DCON

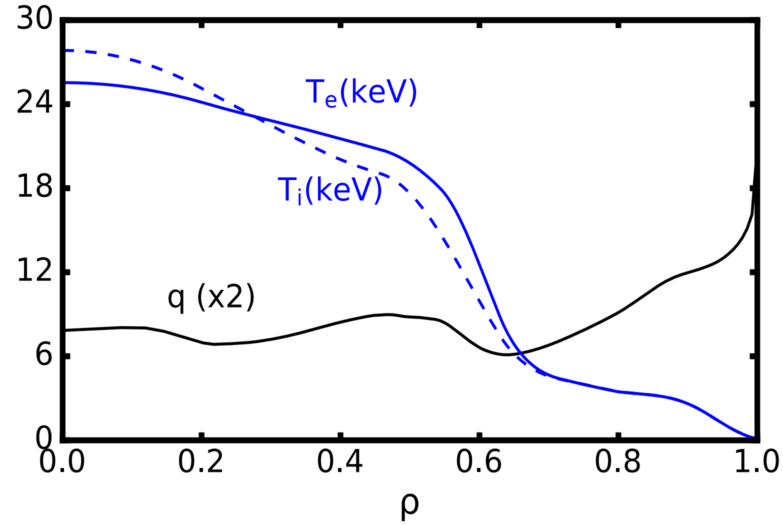


Each data point
= IPS-FASTRAN modeling with fully physics models

- Efficient utilization of HPC
  - IPS + DAKOTA
  - Massive serial

OMFIT STEP module supports discharge design and optimization for current and future machines



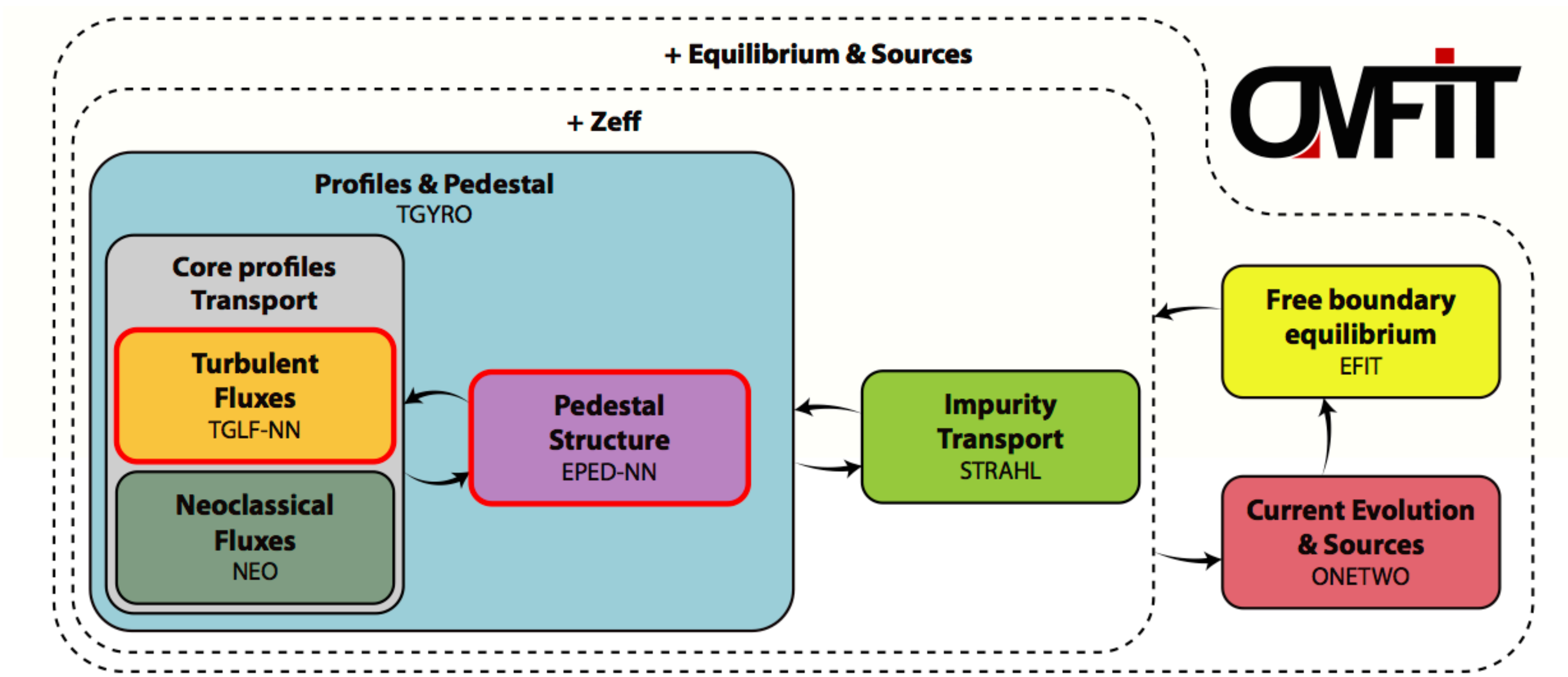


Predicted ITER steady-state Q ≥ 5 scenario with day-1 heating

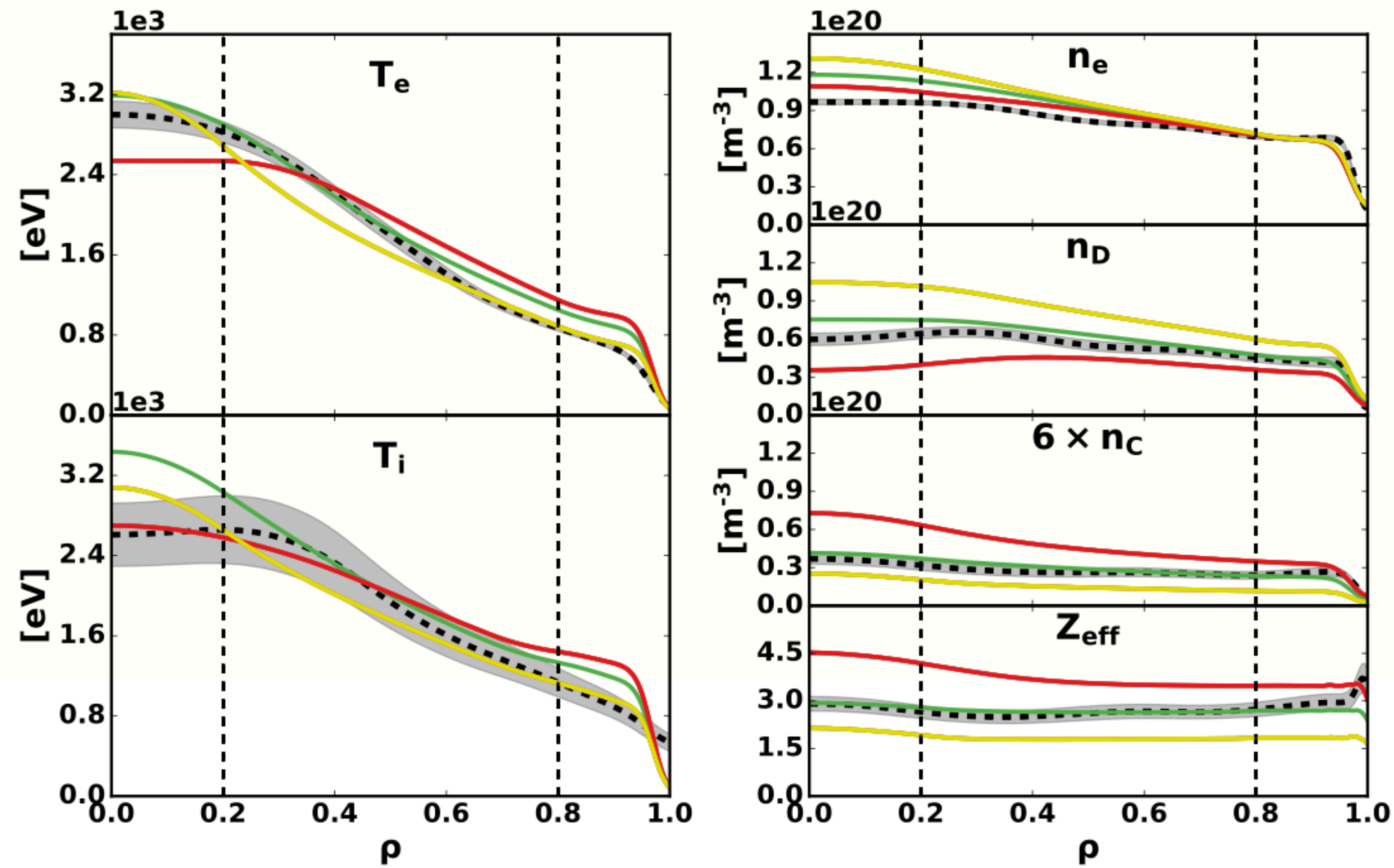
(J. McClenaghan *et al*, 2018 IAEA FEC)

Developed workflow for coupled core-pedestal simulations with self-consistent impurity transport

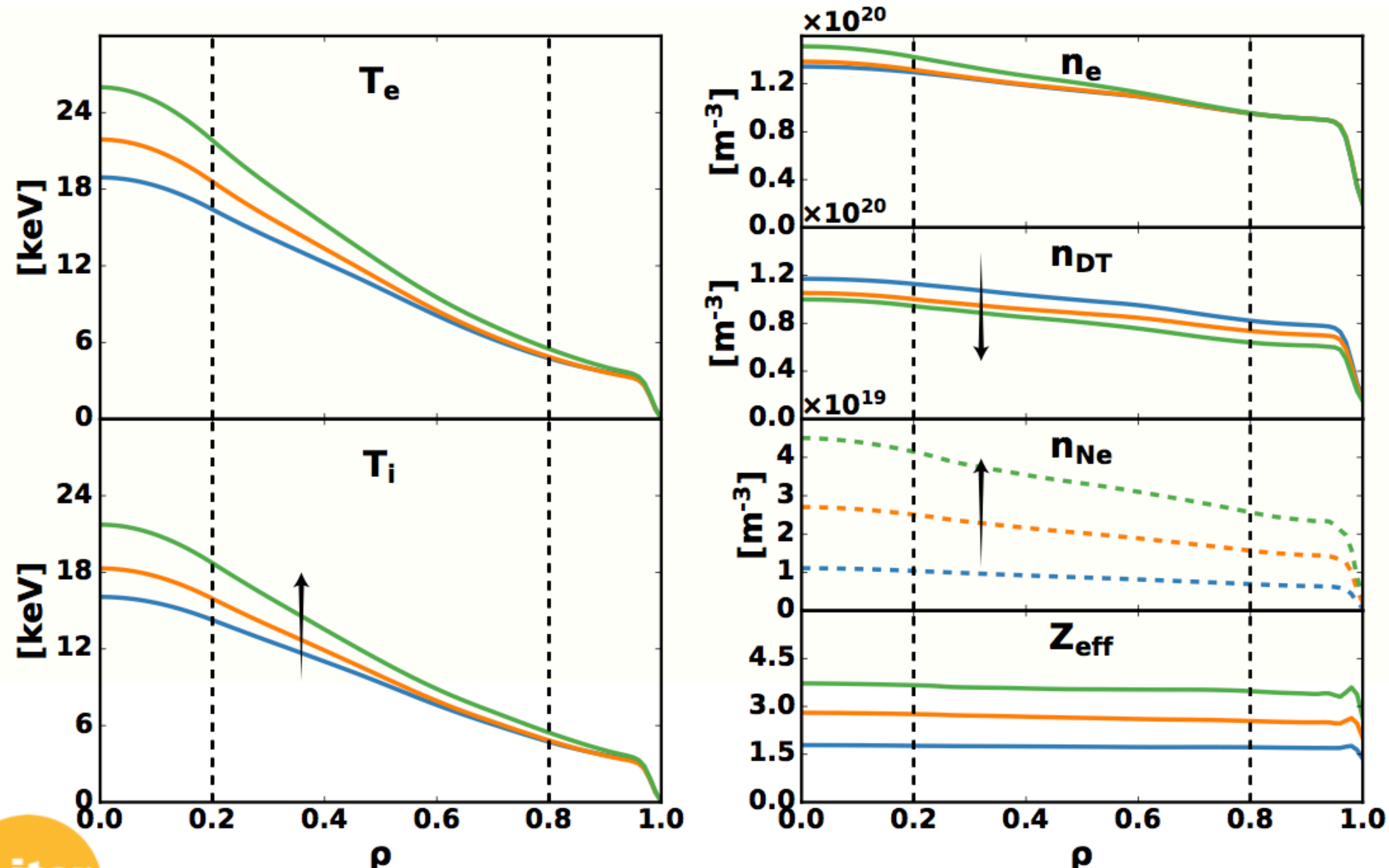
- Three nested self-consistency loops
  - Core profiles + pedestal + impurities + equilibrium & sources
  - Used neural net models to speedup critical bottlenecks
  - Compatible with ITER IMAS data structures (leveraging OMAS)



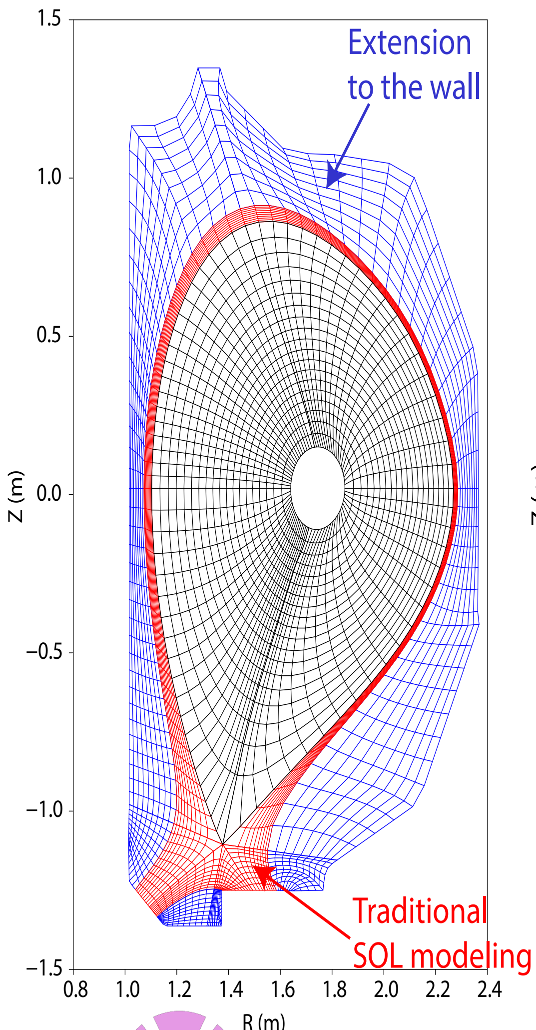
Predictions for varying carbon content (0.5, 1.0, 1.5) in DIII-D shows how impurity seeding can improve pedestal

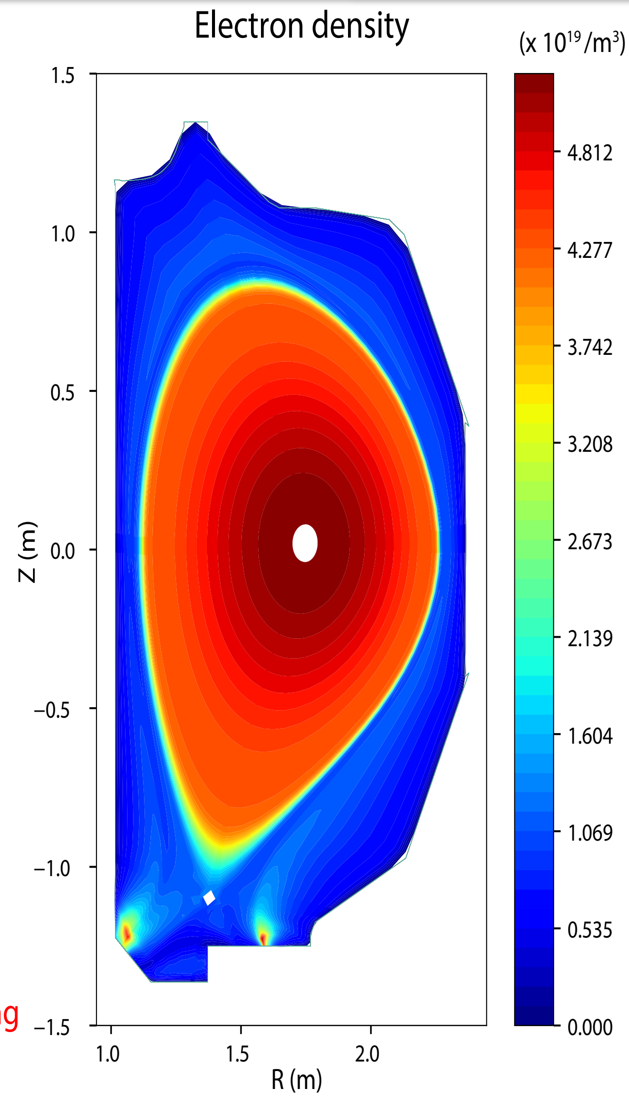


Initial ITER simulations show small dependency of Q_{fusion} on Z_{eff}: tradeoff pedestal height for core dilution



IPS-CESOL is Being Extended to Wall





- Non-orthogonal/non-field aligned grid in **far-SOL region**
  - High-order FVM for accurate calculation of anisotropic transport
  - Fully unstructured grid supporting triangular grid
- 2-D impurity transport in the entire region of tokamak
  - Plug&Play of FASTRAN(1-D) and C2(2-D) for transport in core region
  - Poloidal anisotropy of radial transport

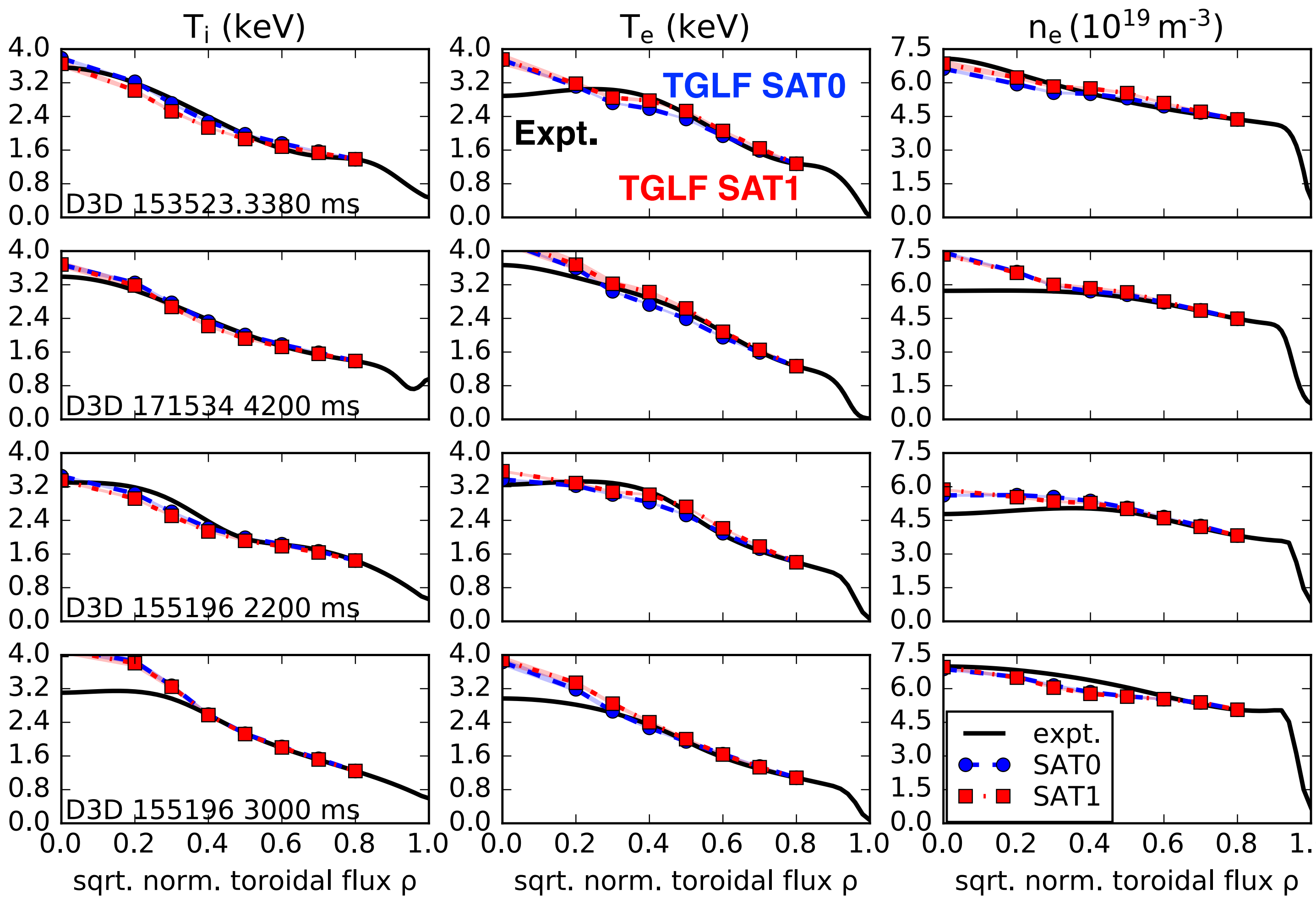
AToM Validation and Physics Studies Coordinated Through Use Cases

- Observe that most every modeling effort eventually settles on certain sets of input parameters which provide benchmark points for regression testing and/or physics studies
  - Can be, but not necessarily, drawn from actual experiments

- Plan to organize AToM validation and scenario modeling work about **uses cases**- well-documented datasets describing discharges of interest for component and workflow validation

- Envision **development of use cases as iterative process**- start simple and grow as needed by maturity of physics and validation workflows

Example Use Case Application: Benchmarking Model Fidelity on Scaled ITER H-mode Discharges from DIII-D



P_{ECH} = 3.4 MW
P_{NBI} = 2.8 MW
T_{inj} = 0.6 N-m

P_{ECH} = 3.5 MW
P_{NBI} = 2.8 MW
T_{inj} = 1.5 N-m

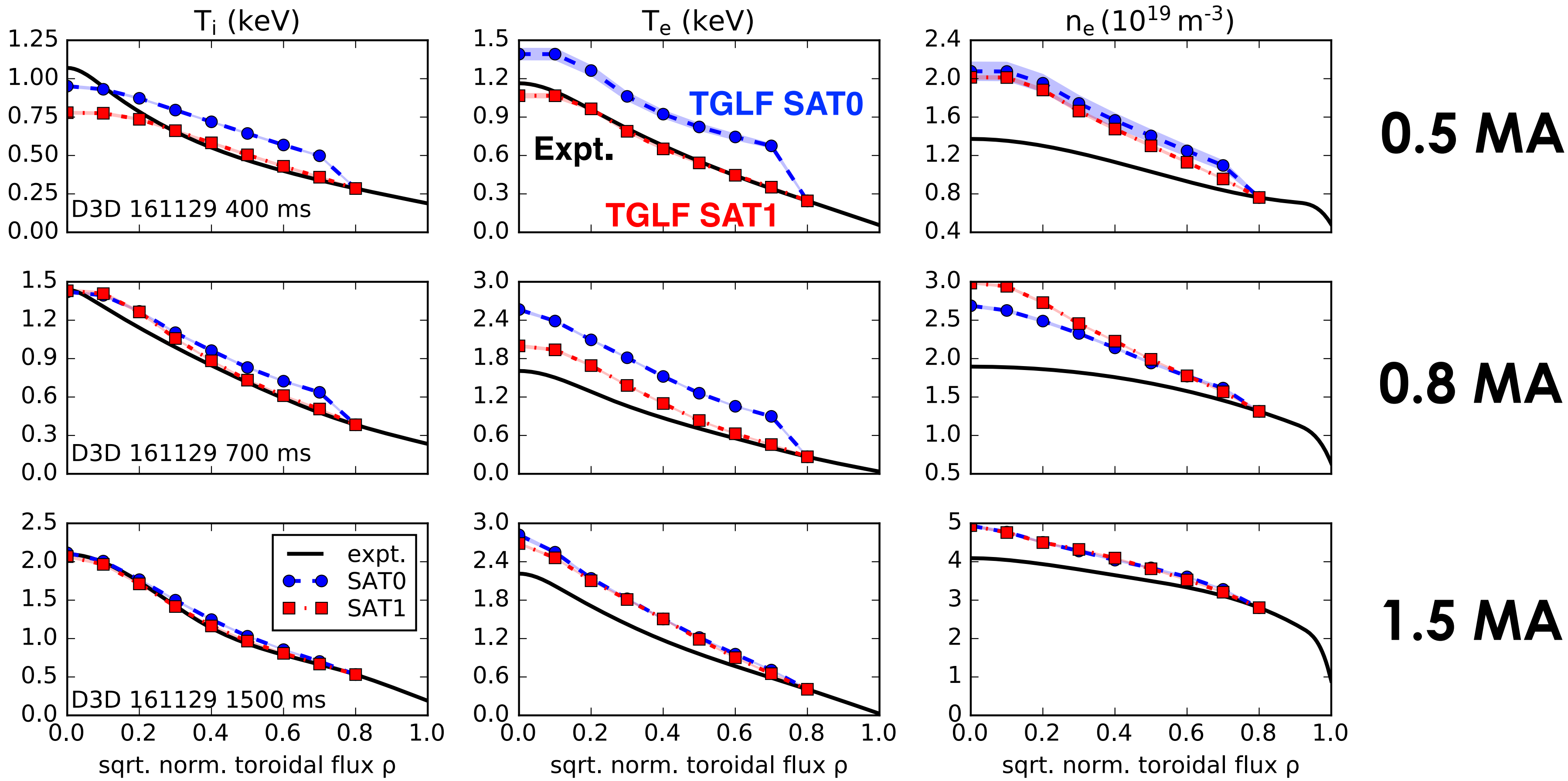
P_{ECH} = 3.3 MW
P_{NBI} = 2.7 MW
T_{inj} = 2.3 N-m

P_{ECH} = 0 MW
P_{NBI} = 2.8 MW
T_{inj} = 1.5N-m

C. Holland et al, Nucl. Fusion **57** 066043 (2017)
B. A. Grierson et al, Phys. Plasmas **25** 022509 (2018)

Use Case Application #2: Testing Model Fidelity for Scaled ITER Startup Phase

- Newer model (SAT1) performs much better at low current, but still errors in density prediction



G. R. McKee et al, Nucl. Fusion **57** 086032 (2017)

New Project: Developing a Multi-SciDAC Use Case Physics Study

- **Key physics question for fusion reactor design**: how to control accumulation of metal impurities from wall in plasma core through use of RF heating actuators

- Coordinated effort between **AToM**, **RF-SciDAC**, and **PSI-2** to develop **practical, validated core-to-wall predictive capability of impurity response to radio-frequency (RF) heating**

- Project has two components:
  - **Validation** of workflows like STEP, CESOL using data from Alcator C-Mod
  - **Predictions** for response in ITER baseline scenario

AToM working to deliver practical, high-fidelity whole-device modeling capabilities

- **Longer term goal**: partnering with other SciDAC centers to integrate and improve both high-fidelity and reduced model components for:
  - RF heating & current drive (PI: P. Bonoli)
  - energetic particle transport (PI: Z. Lin)
  - plasma edge & scrape-off layer physics (PI: C. S. Chang) (PI: D. Hatch)
  - plasma-material interactions (PI: B. Wirth)
  - disruptions (PI: S. Jardin) (PI: X. Tang)
  - runaway electrons (PI: D. Brennan)