AToM
Tokamak Profile Prediction with Dynamic Pedestal

Orso Meneghini
J. Candy, D. L. Green, M. Dorf, C.Holland, D.E. Bernholdt, M. Dorr,
D. Shissel, S. P. Smith, P.B. Snyder, W. Elwasif, E.DAzevedo, J.M. Park,
D. Batchelor, V.Izzo, D. Orlov, M. Umansky

2015 SciDAC-3 Principal Investigator Meeting

Jul 22nd-24th 2015 - Bethesda MD

AToM
GENERAL ATOMICS
OAK RIDGE National Laboratory
UCSD
Lawrence Livermore National Laboratory
FASTMATH
SUPER
SciDAC
Scientific Discovery through Advanced Computing

Outline - Initial physics applications of the AToM project

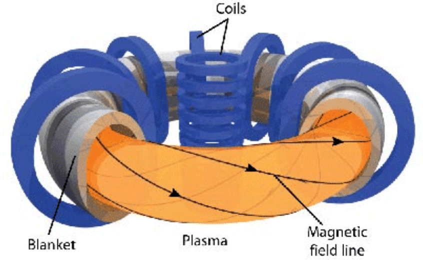
1. Introduction
2. Overview of the AToM project
3. Milestone results
    - Integrated OMFIT and IPS frameworks
    - Performance engineered EPED1 workflow with IPS
    - Coupled core-pedestal predictive modeling
4. Ongoing and future work

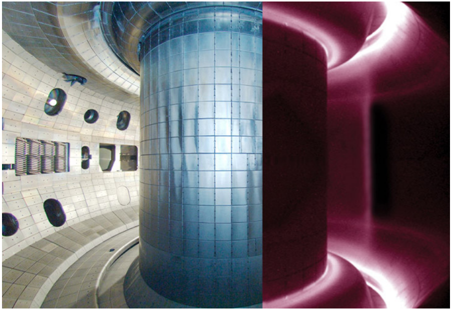
Plasma confinement in a Tokamak

In a tokamak, plasma confinement is maintained, in part, by a poloidal magnetic field sustained by a toroidal current flowing into the plasma

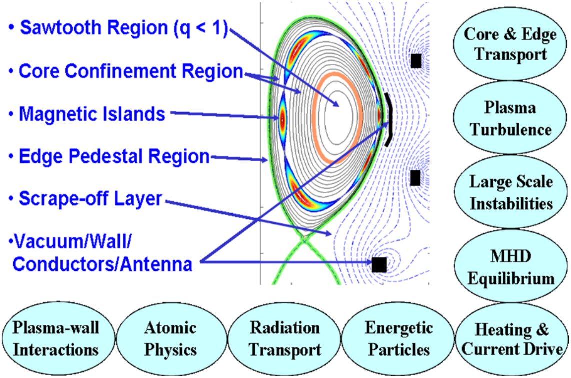
Usually driven by an inductively produced DC electric field, so that the Tokamak operates only in a pulsed mode

Steady-state tokamak operation, require ways to sustain continuous plasma current





The magnetic fusion integrated modeling challenge



- Sawtooth Region ($q < 1$)
- Core Confinement Region
- Magnetic Islands
- Edge Pedestal Region
- Scrape-off Layer
- Vacuum/Wall/ Conductors/Antenna

Core & Edge Transport

Plasma Turbulence

Large Scale Instabilities

MHD Equilibrium

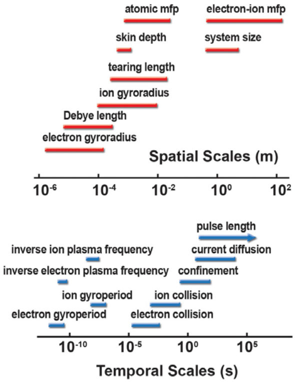
Heating & Current Drive

Plasma-wall Interactions

Atomic Physics

Radiation Transport

Energetic Particles



AToM: multi-institution FES/ASCR SciDAC project (sept. 2014)

Not a new physics code, but rather a concept:

"To enhance and extend present modeling capabilities,
by supporting, leveraging, and integrating existing research"

ATOM

GENERAL ATOMICS
OAK RIDGE National Laboratory
UCSD
Lawrence Livermore National Laboratory
FASTMATH
SUPER

- **Pragmatic bottom-up** philosophy leverages **existing research activities** and **collected wisdom** embodied in legacy tools
- Approach is to **support rather than subvert** current workflows, build new essential infrastructure, and guide integration
- Move **smoothly and surely** toward a whole device modeling (WDM) capability that has the most important feature: **users**

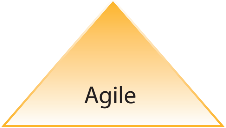
AToM embraces the agile software development methodology

Assume design requirements are
well known and immutable

Structured development process

- Methodology:
  - Big design up-front
  - Delivered in full
  - Users test at the end
- Hard to change
- High investment risk

Adaptive development process



Assume design requirements are
not well known or evolving

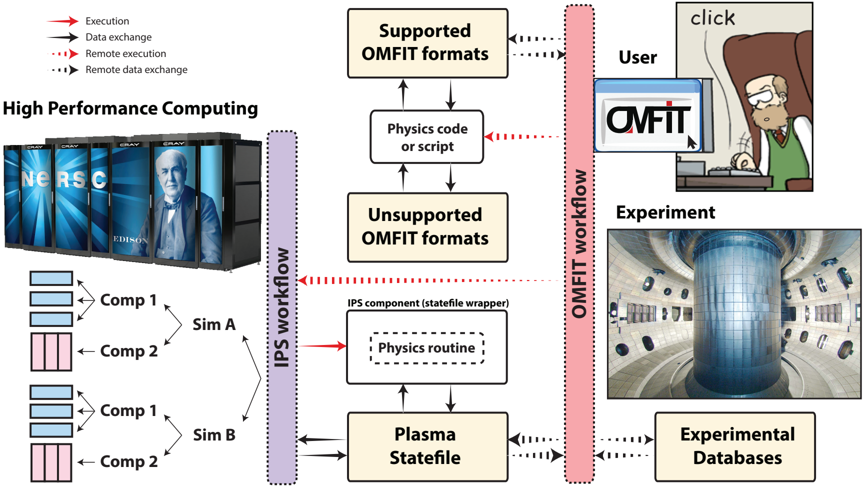
- Methodology:
  - Start simple
  - Incremental deliveries
  - Embed users feedback
- Easy to change
- Lower investment risk

AToM: Seven research thrusts

1. Couple OMFIT+IPS frameworks, provide wrappers and workflows
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 (c)GYRO/NEO
6. Establish a data management scheme, tracking provenance and establish portal services
7. Provide user support and community outreach

AToM enabled coupling of IPS and OMFIT framework and is effectively exploiting their synergy

- **IPS**: provides powerful HPC scheduling capabilities
- **OMFIT**: provides interface to users, experiments and codes



Execution
Data exchange
Remote execution
Remote data exchange

High Performance Computing

Comp 1
Comp 2
Sim A
Comp 1
Comp 2
Sim B

IPS workflow

Supported OMFIT formats

Physics code or script

Unsupported OMFIT formats

IPS component (statefile wrapper)

Physics routine

Plasma Statefile

OMFIT workflow

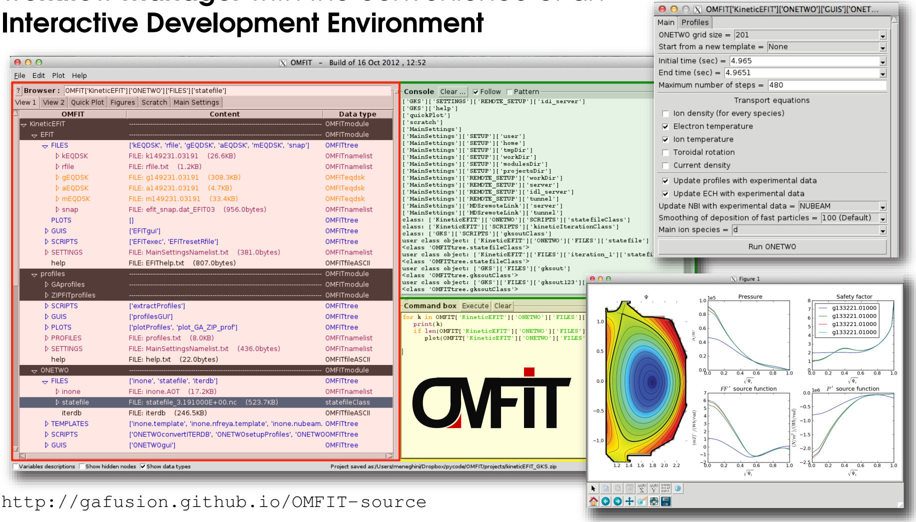
User

Experiment

Experimental Databases

One **M**odeling **F**ramework for **I**ntegrated **T**asks

A versatile framework that combines the capabilities of a **workflow manager** with the convenience of an **Interactive Development Environment**



OMFIT – Build of 16 Oct 2012 , 12:52

OMFIT	Content	Data type
KineticEFIT	--	OMFITmodule
EFIT	--	OMFITmodule
FILES	['kEQDSK', 'rfile', 'gEQDSK', 'aEQDSK', 'mEQDSK', 'snap']	OMFITtree
kEQDSK	FILE: k149231.03191 (26.6KB)	OMFITnamelist
rfile	FILE: rfile.txt (1.2KB)	OMFITnamelist
gEQDSK	FILE: g149231.03191 (308.3KB)	OMFITeqdsk
aEQDSK	FILE: a149231.03191 (4.7KB)	OMFITeqdsk
mEQDSK	FILE: m149231.03191 (33.4KB)	OMFITeqdsk
snap	FILE: efit_snap.dat_EFIT03 (956.0bytes)	OMFITnamelist
PLOTS	[]	OMFITtree
GUIS	['EFITgui']	OMFITtree
SCRIPTS	['EFITexec', 'EFITresetRfile']	OMFITtree
SETTINGS	FILE: MainSettingsNamelist.txt (381.0bytes)	OMFITnamelist
help	FILE: EFIThelp.txt (807.0bytes)	OMFITfileASCII
profiles	--	OMFITmodule
GAprofiles	--	OMFITmodule
ZIPFITprofiles	--	OMFITmodule
SCRIPTS	['extractProfiles']	OMFITtree
GUIS	['profilesGUI']	OMFITtree
PLOTS	['plotProfiles', 'plot_GA_ZIP_prof']	OMFITtree
PROFILES	FILE: profiles.txt (8.0KB)	OMFITnamelist
SETTINGS	FILE: MainSettingsNamelist.txt (436.0bytes)	OMFITnamelist
help	FILE: help.txt (22.0bytes)	OMFITfileASCII
ONETWO	--	OMFITmodule
FILES	['inone', 'statefile', 'iterdb']	OMFITtree
inone	FILE: inone.AOT (17.2KB)	OMFITnamelist
statefile	FILE: statefile_3.191000E+00.nc (523.7KB)	statefileClass
iterdb	FILE: iterdb (246.5KB)	OMFITfileASCII
TEMPLATES	['inone.template', 'inone.nfreya.template', 'inone.nubeam.	OMFITtree
SCRIPTS	['ONETWOconvertITERDB', 'ONETWOsetupProfiles', 'ONETWO	OMFITtree
GUIS	['ONETWOgui']	OMFITtree

☐ Variables descriptions ☐ Show hidden nodes ☑ Show data types

Project saved as:/Users/meneghini/Dropbox/pycode/OMFIT/projects/kineticEFIT_GKS.zip

```
['GKS']['SETTINGS']['REMOTE_SETUP']['idl_server']
['GKS']['help']
['quickPlot']
['scratch']
['MainSettings']
['MainSettings']['SETUP']['user']
['MainSettings']['SETUP']['home']
['MainSettings']['SETUP']['tmpDir']
['MainSettings']['SETUP']['workDir']
['MainSettings']['SETUP']['modulesDir']
['MainSettings']['SETUP']['projectsDir']
['MainSettings']['REMOTE_SETUP']['workDir']
['MainSettings']['REMOTE_SETUP']['server']
['MainSettings']['REMOTE_SETUP']['idl_server']
['MainSettings']['REMOTE_SETUP']['tunnel']
['MainSettings']['MDSremoteLink']['server']
['MainSettings']['MDSremoteLink']['tunnel']
class: ['KineticEFIT']['ONETWO']['SCRIPTS']['statefileClass']
class: ['KineticEFIT']['SCRIPTS']['kineticIterationClass']
class: ['GKS']['SCRIPTS']['gksoutClass']
user class object: ['KineticEFIT']['ONETWO']['FILES']['statefile']
<class 'OMFITtree.statefileClass'>
user class object: ['KineticEFIT']['FILES']['iteration_1']['statefi
<class 'OMFITtree.statefileClass'>
user class object: ['GKS']['FILES']['gksout']
<class 'OMFITtree.gksoutClass'>
user class object: ['GKS']['FILES']['gksout123'][
<class 'OMFITtree.gksoutClass'>
```

```
for k in OMFIT['KineticEFIT']['ONETWO']['FILES'][
   print(k)
   if len(OMFIT['KineticEFIT']['ONETWO']['FILES']
      plot(OMFIT['KineticEFIT']['ONETWO']['FILES'
```

OMFIT['KineticEFIT']['ONETWO']['GUIS']['ONET...

ONETWO grid size = 201
Start from a new template = None
Initial time (sec) = 4.965
End time (sec) = 4.9651
Maximum number of steps = 480

Transport equations

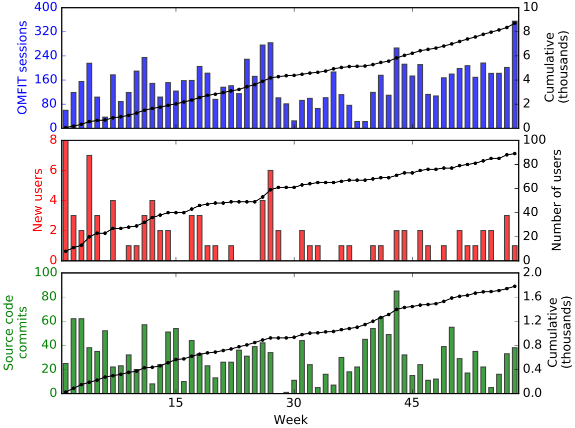
☐ Ion density (for every species)
☑ Electron temperature
☑ Ion temperature
☐ Toroidal rotation
☐ Current density

☑ Update profiles with experimental data
☑ Update ECH with experimental data
Update NBI with experimental data = NUBEAM
Smoothing of deposition of fast particles = 100 (Default)
Main ion species = d

http://gafusion.github.io/OMFIT-source

OMFIT is a vibrant project, actively used by many researchers, for a broad range of applications

We judge our success based on **user adoption** and **scientific impact**



After 3 years, used in support of some of the work that lead to:

- 16 journal publications
- 32 conference proceedings

`gafusion.github.io/OMFIT-source/publications.html`

Integral part of the **AToM** SciDAC project

The centerpiece of OMFIT is its flexible data structure

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

- Collect data independently of its origin and type
- Objects' content appear in their subtree
- No a-priori decision of what is stored and how
- Codes exchange data by referring to quantities in the tree

Same functionality as the "statefile" structures of other frameworks...

...but **free-form !**

Like *MDS+* or *file-system* on your own laptop: the data is stored however it is deemed more logical to accomplish a certain task

With N codes, it's an N^2 problem! How is it possible to make all these codes talk to one another?

- By reading/writing a few (10+) standard scientific data formats OMFIT can interact with many different codes
- Often codes need to exchange only small amount of data
- Exploit existing integration efforts:
  - Many codes already accept each others′ files
  - Conversion utilities that are already available
- Real-world applications do not require coupling N^2 codes!

Several advantages:

- No need to modify codes and their I/O
  - No burden on developers of individual codes
  - Effort done by users interested in integrating
  - Compatible with distributed community developments
- Does not exclude use of data structures from other frameworks
  - Skips all-together arguments about which data structure to use
  - Survival of the framework does not depend on widespread adoption of its own data structure by the community

Other important characteristics of the OMFIT framework

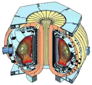
Lightweight, pure-Python framework is easy to install, maintain, and expand

Code execution is natively **remote**, and can be **parallel**

Python scripting and **component based approach** allow building of powerful and complex workflows

Graphical user interfaces ease execution of each component and their interaction

Power users retain full control of their codes I/O and execution

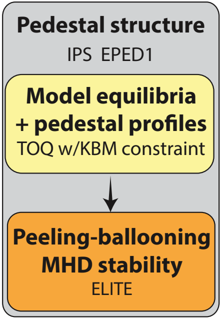


Integrated with experimental databases for data analysis, generation of code inputs, and validation

Collaborative environment encourages users contributions, and community revision

Adapting EPED1 workflow for HPC with IPS enabled new possibilities

- Parametric variations of β_N to find achievable stable pedestal
- 93 TOQ equilibria, 651 ELITE runs: ~ 20 min on 651 cores at NERSC



Pedestal structure

IPS EPED1

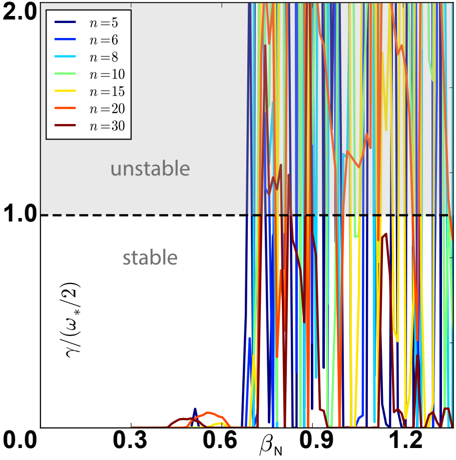
Model equilibria + pedestal profiles

TOQ w/KBM constraint

Peeling-ballooning MHD stability

ELITE

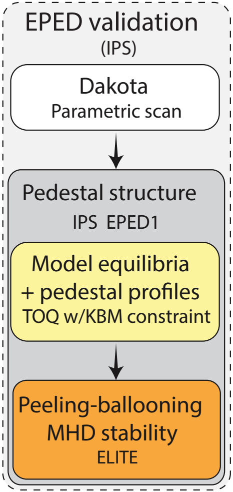
EPED1 pedestal stability analysis



J.M. Park
P. Snyder
W. Elwasif
D.E. Bernholdt
& IPS team

Adapting EPED1 workflow for HPC with IPS enabled new possibilities

- IPS-EPED1 reproduces (Snyder 2009) validation results
- ~1.5 hour at NERSC with 3600 cores instead of ~1 week



EPED validation (IPS)

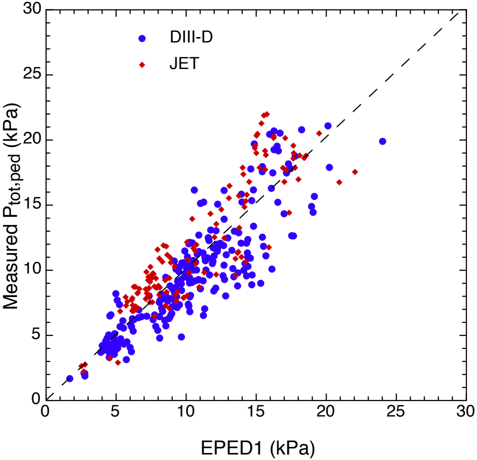
Dakota
Parametric scan

Pedestal structure
IPS EPED1

Model equilibria
+ pedestal profiles
TOQ w/KBM constraint

Peeling-ballooning
MHD stability
ELITE

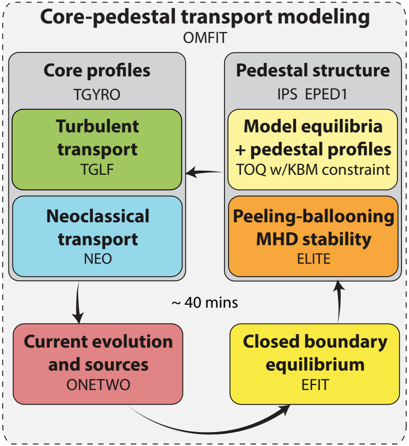
Regression: 1.051 +- 0.232



J.M. Park
P. Snyder
W. Elwasif
D.E. Bernholdt
& IPS team

OMFIT workflow enabled first-principles self-consistent equilibrium, core transport, and edge stability predictions

Separation of MHD, transport, and current diffusion timescales



Core-pedestal transport modeling

OMFIT

Core profiles

TGYRO

Turbulent transport

TGLF

Neoclassical transport

NEO

Pedestal structure

IPS EPED1

Model equilibria + pedestal profiles

TOQ w/KBM constraint

Peeling-ballooning MHD stability

ELITE

~ 40 mins

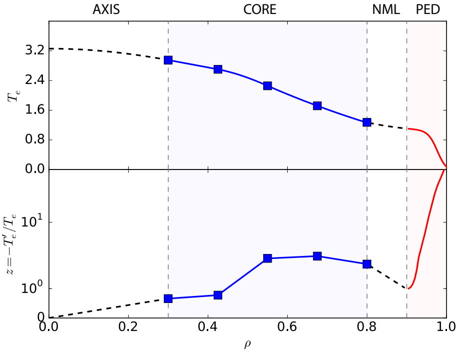
Current evolution and sources

ONETWO

Closed boundary equilibrium

EFIT

+ setup and postprocessing

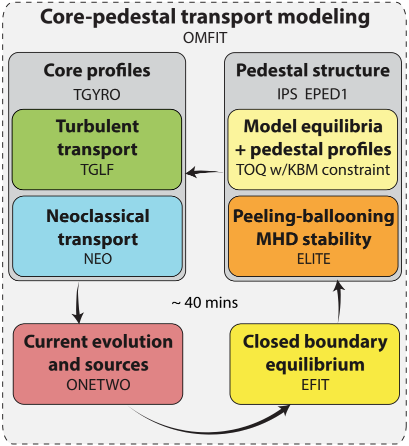


Four radial zones:

PED	Pedestal structure model (PB+KBM)
NML	Linear scale-length interpolation
CORE	Reduced gyrokinetic model
AXIS	Linear scale-length to zero

OMFIT workflow enabled first-principles self-consistent equilibrium, core transport, and edge stability predictions

Separation of MHD, transport, and current diffusion timescales



Core-pedestal transport modeling
OMFIT

Core profiles
TGYRO

Turbulent transport
TGLF

Neoclassical transport
NEO

Pedestal structure
IPS EPED1

Model equilibria + pedestal profiles
TOQ w/KBM constraint

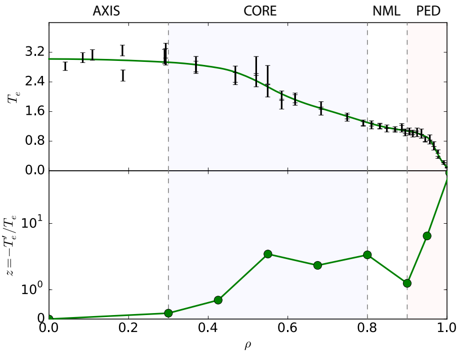
Peeling-ballooning MHD stability
ELITE

~ 40 mins

Current evolution and sources
ONETWO

Closed boundary equilibrium
EFIT

+ setup and postprocessing

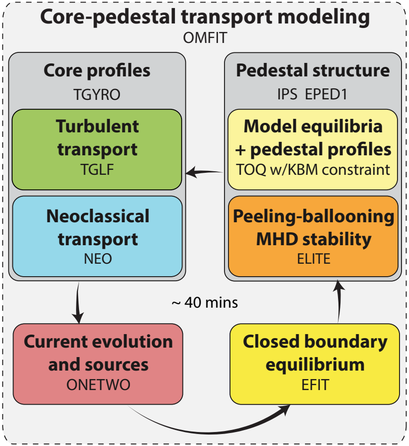


Approach inspired by linear scale-length fitting of experimental data:

- Using few TGLF calculation points
- Radial zone locations

OMFIT workflow enabled first-principles self-consistent equilibrium, core transport, and edge stability predictions

Separation of MHD, transport, and current diffusion timescales



Core-pedestal transport modeling
OMFIT

Core profiles
TGYRO

Turbulent transport
TGLF

Neoclassical transport
NEO

Pedestal structure
IPS EPED1

Model equilibria + pedestal profiles
TOQ w/KBM constraint

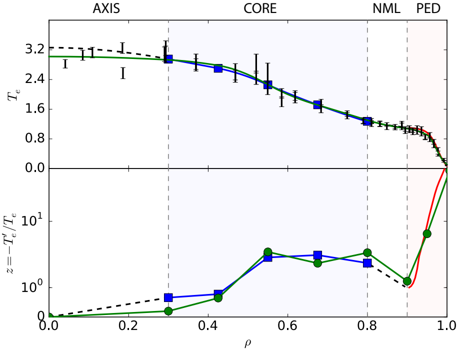
Peeling-ballooning MHD stability
ELITE

~ 40 mins

Current evolution and sources
ONETWO

Closed boundary equilibrium
EFIT

+ setup and postprocessing

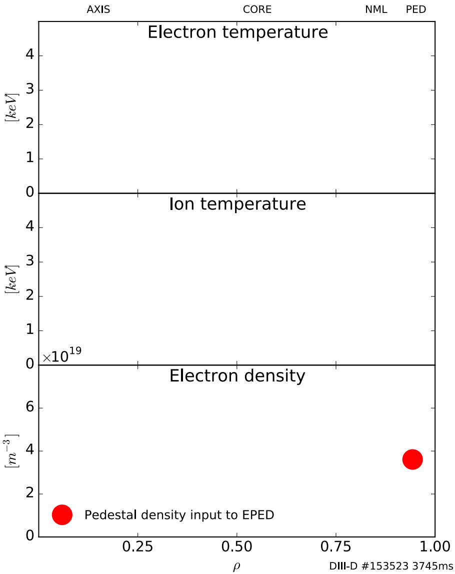


Approach inspired by linear scale-length fitting of experimental data:

- Using few TGLF calculation points
- Radial zone locations

First applied this workflow to DIII-D ITER baseline scenario with low torque and electron heating

- Inputs are *shape*, B_t, fixed $J(r)$ and $\omega(r)$, $n_{e,\mathrm{ped}}$, Z_{eff}, sources, and guess for β_N

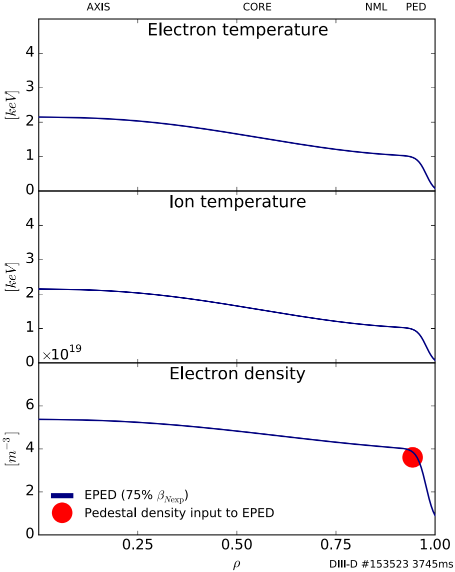


DIII-D #153523 3745ms

First applied this workflow to DIII-D ITER baseline scenario with low torque and electron heating

- Inputs are *shape*, B_t, fixed $J(r)$ and $\omega(r)$, $n_{e,\mathrm{ped}}$, Z_{eff}, sources, and guess for β_N

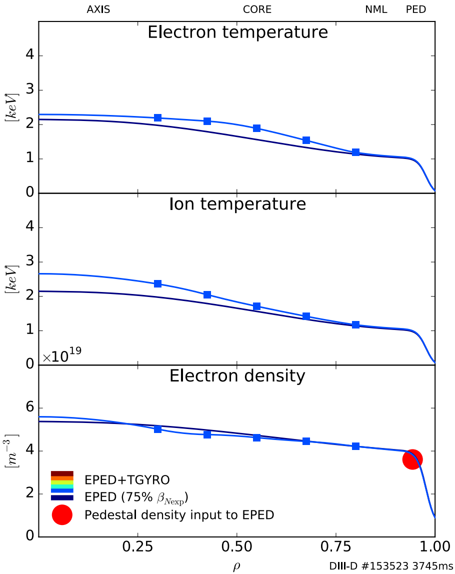
- Start with EPED. First run uses (poor) initial guess for β_N $\beta_\mathrm{N} = 75\%\ \beta_{\mathrm{N,exp}}$



DIII-D #153523 3745ms

First applied this workflow to DIII-D ITER baseline scenario with low torque and electron heating

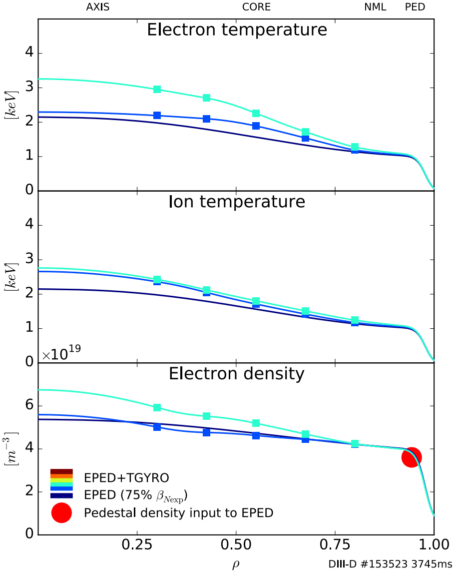
- Inputs are *shape*, B_t, fixed $J(r)$ and $\omega(r)$, $n_{e,\mathrm{ped}}$, Z_{eff}, sources, and guess for β_N
- Start with EPED. First run uses (poor) initial guess for β_N $\beta_\mathrm{N} = 75\%\,\beta_{\mathrm{N,exp}}$
- TGYRO to predict profiles and β_N. Then iterate...



DIII-D #153523 3745ms

First applied this workflow to DIII-D ITER baseline scenario with low torque and electron heating

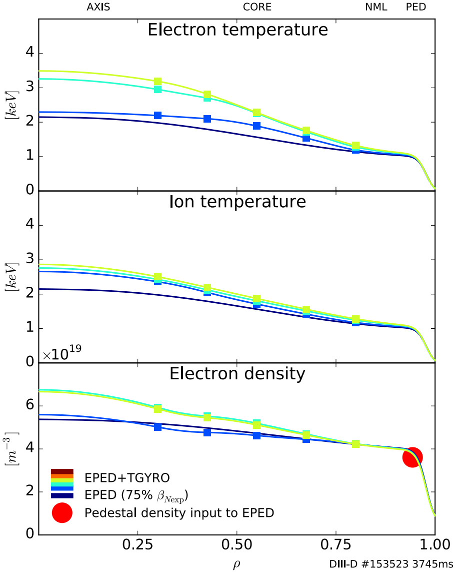
- Inputs are *shape*, B_t, fixed $J(r)$ and $\omega(r)$, $n_{e,\mathrm{ped}}$, Z_{eff}, sources, and guess for β_{N}
- Start with EPED. First run uses (poor) initial guess for β_{N} $\beta_{\mathrm{N}} = 75\%\ \beta_{\mathrm{N,exp}}$
- TGYRO to predict profiles and β_{N}. Then iterate...



DIII-D #153523 3745ms

First applied this workflow to DIII-D ITER baseline scenario with low torque and electron heating

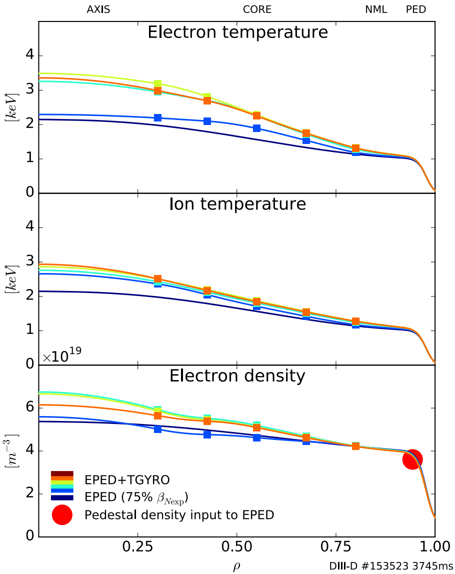
- Inputs are *shape*, B_t, fixed $J(r)$ and $\omega(r)$, $n_{e,\mathrm{ped}}$, Z_{eff}, sources, and guess for β_{N}
- Start with EPED. First run uses (poor) initial guess for β_{N} $\beta_{\mathrm{N}} = 75\%\ \beta_{\mathrm{N,exp}}$
- TGYRO to predict profiles and β_{N}. Then iterate...



DIII-D #153523 3745ms

First applied this workflow to DIII-D ITER baseline scenario with low torque and electron heating

- Inputs are *shape*, B_t, fixed $J(r)$ and $\omega(r)$, $n_{e,\mathrm{ped}}$, Z_{eff}, sources, and guess for β_{N}
- Start with EPED. First run uses (poor) initial guess for β_{N} $\beta_{\mathrm{N}} = 75\%\, \beta_{\mathrm{N,exp}}$
- TGYRO to predict profiles and β_{N}. Then iterate...



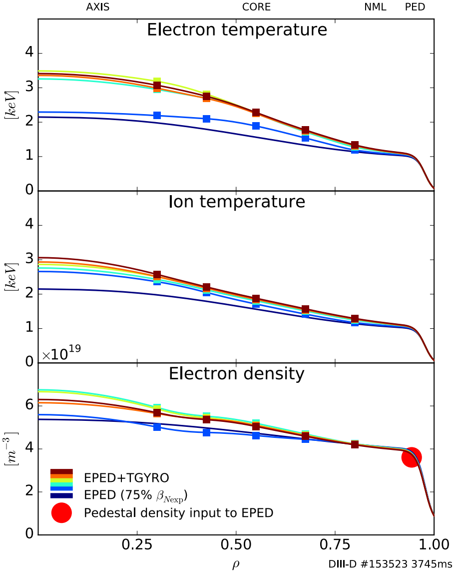
DIII-D #153523 3745ms

First applied this workflow to DIII-D ITER baseline scenario with low torque and electron heating

- Inputs are *shape*, B_t, fixed $J(r)$ and $\omega(r)$, $n_{e,\mathrm{ped}}$, Z_{eff}, sources, and guess for β_{N}

- Start with EPED. First run uses (poor) initial guess for β_{N} $\beta_{\mathrm{N}} = 75\%\ \beta_{\mathrm{N,exp}}$

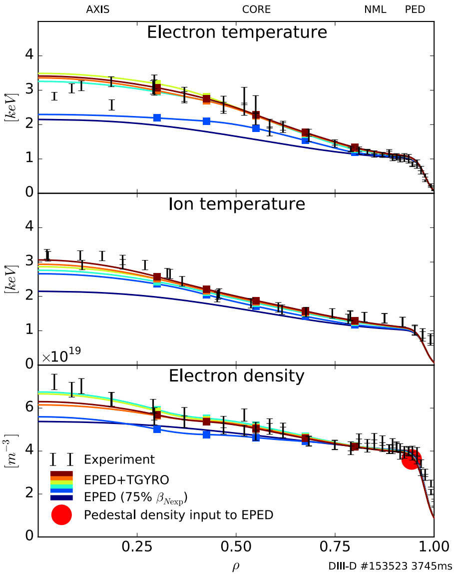
- TGYRO to predict profiles and β_{N}. Then iterate...



DIII-D #153523 3745ms

First applied this workflow to DIII-D ITER baseline scenario with low torque and electron heating

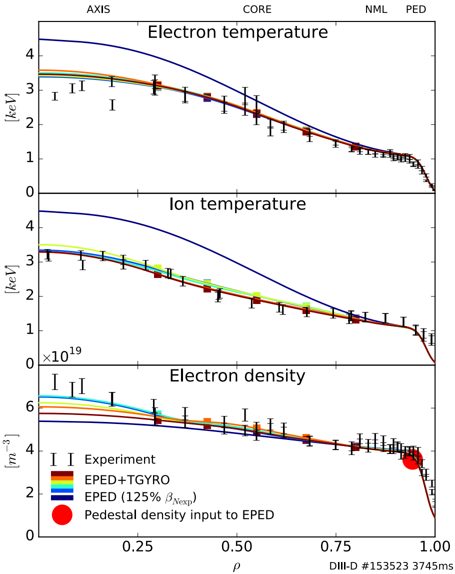
- Inputs are *shape*, B_t, fixed $J(r)$ and $\omega(r)$, $n_{e,\mathrm{ped}}$, Z_{eff}, sources, and guess for β_N
- Start with EPED. First run uses (poor) initial guess for β_N $\beta_\mathrm{N} = 75\%\,\beta_{\mathrm{N,exp}}$
- TGYRO to predict profiles and β_N. Then iterate...
- Matched measurements very well across the plasma



DIII-D #153523 3745ms

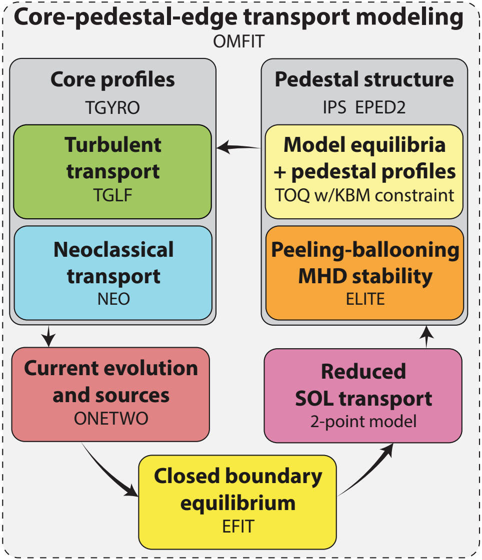
First applied this workflow to DIII-D ITER baseline scenario with low torque and electron heating

- Inputs are *shape*, B_t, fixed $J(r)$ and $\omega(r)$, $n_{e,\mathrm{ped}}$, Z_{eff}, sources, and guess for β_{N}
- Start with EPED. First run uses (poor) initial guess for β_{N} $\beta_{\mathrm{N}} = 125\%\,\beta_{\mathrm{N,exp}}$
- TGYRO to predict profiles and β_{N}. Then iterate...
- Matched measurements very well across the plasma
- Similar result for initial over/under-guess of β_{N}



DIII-D #153523 3745ms

Extend model beyond separatrix by developing a coupled core-pedestal-SOL workflow



Core-pedestal-edge transport modeling
OMFIT

Core profiles
TGYRO

Turbulent transport
TGLF

Neoclassical transport
NEO

Pedestal structure
IPS EPED2

Model equilibria + pedestal profiles
TOQ w/KBM constraint

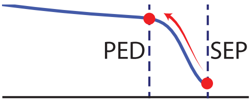
Peeling-ballooning MHD stability
ELITE

Current evolution and sources
ONETWO

Reduced SOL transport
2-point model

Closed boundary equilibrium
EFIT

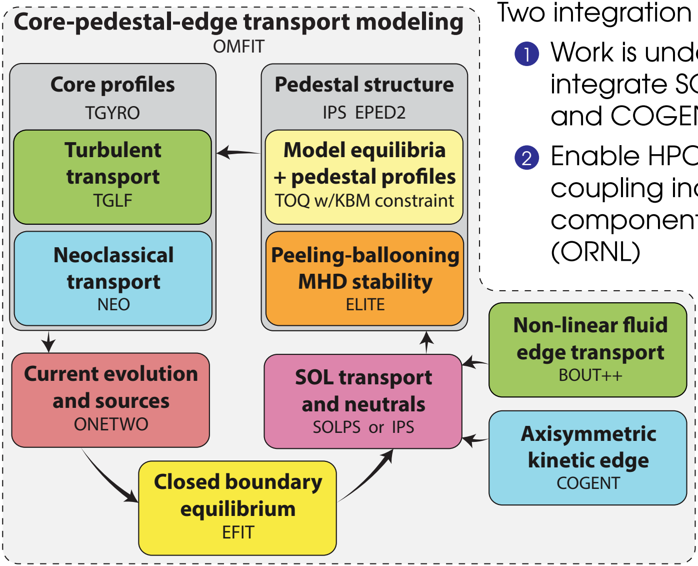
Extend EPED1 to predict pedestal structure based on $n_{e,\rm sep}$ and $T_{e,\rm sep}$ (P. Snyder EPED2)



- Ratio of pedestal to separatrix density can be calculated based on ETG or other physics models (e.g. with TGLF)

To start, estimate $n_{e,\rm sep}$ and $T_{e,\rm sep}$ with a reduced 2-point SOL model

Extend model beyond separatrix by developing a first-principles coupled core-pedestal-SOL workflow



Core-pedestal-edge transport modeling
OMFIT

Core profiles
TGYRO

Turbulent transport
TGLF

Neoclassical transport
NEO

Pedestal structure
IPS EPED2

Model equilibria + pedestal profiles
TOQ w/KBM constraint

Peeling-ballooning MHD stability
ELITE

Current evolution and sources
ONETWO

SOL transport and neutrals
SOLPS or IPS

Non-linear fluid edge transport
BOUT++

Axisymmetric kinetic edge
COGENT

Closed boundary equilibrium
EFIT

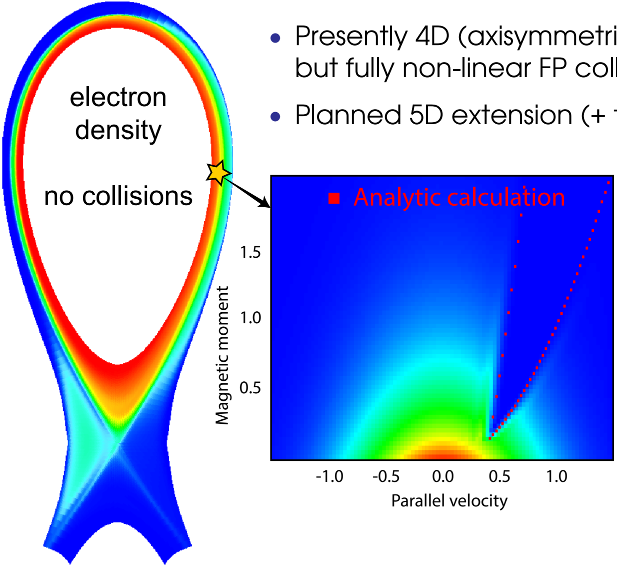
Two integration strategies:

① Work is under way to integrate SOLPS, BOUT++, and COGENT within OMFIT

② Enable HPC capabilities by coupling individual SOLPS components within IPS (ORNL)

ATοM is accelerating development of COGENT — a full-f continuum gyrokinetic code for the edge

- Presently 4D (axisymmetric) and electrostatic but fully non-linear FP collision operator
- Planned 5D extension (+ toroidal dimension)



- High accuracy 4th order finite-volume conservative discretization
- Adaptive velocity mesh refinement
- Born parallel and highly scalable (collaboration with ASCR FASTMath)

M.A. Dorf, M. Dorr & ESL team

AToM strategy *“to enhance and extend present modeling capabilities by leveraging and integrating existing research”* is proving effective

Milestone results

- Integrated OMFIT and IPS frameworks
- EPED1 workflow within IPS enabled new capabilities
- Self-consistent first-principles predictive core-edge modeling

Short term: validate and use core-pedestal model

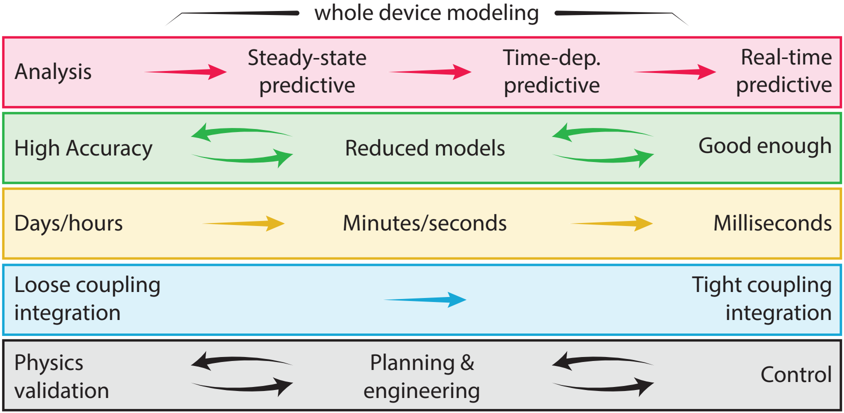
- Validate workflow for more DIII-D discharges, especially high β_N
- Optimize ITER fusion performance as a function of pedestal density and other key parameters

Longer term: Extend workflow to SOL

- EPED2 to predict pedestal structure based on $n_{e,\mathrm{sep}}$ and $T_{e,\mathrm{sep}}$
- Predict $n_{e,\mathrm{sep}}$ and $T_{e,\mathrm{sep}}$ from 2-point model first, then SOLPS/IPS
- BOUT++ and COGENT to provide transport coeff. to SOL model

AToM is working towards providing high-fidelity reduced models that are needed for functional WDM

Integrated modeling pipeline:



whole device modeling

Analysis → Steady-state predictive → Time-dep. predictive → Real-time predictive

High Accuracy ⇄ Reduced models ⇄ Good enough

Days/hours → Minutes/seconds → Milliseconds

Loose coupling integration → Tight coupling integration

Physics validation ⇄ Planning & engineering ⇄ Control

High fidelity reduced model: minutes/seconds run time simulation, where uncertainty due to physics approximation is comparable with uncertainty from inputs