Integrated modeling with TRANSP and OMFIT

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TRANSP user group

PPPL, March 23rd 2015

Outline

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One Modeling Framework for Integrated Tasks

OMFIT is an integrated modeling framework that:

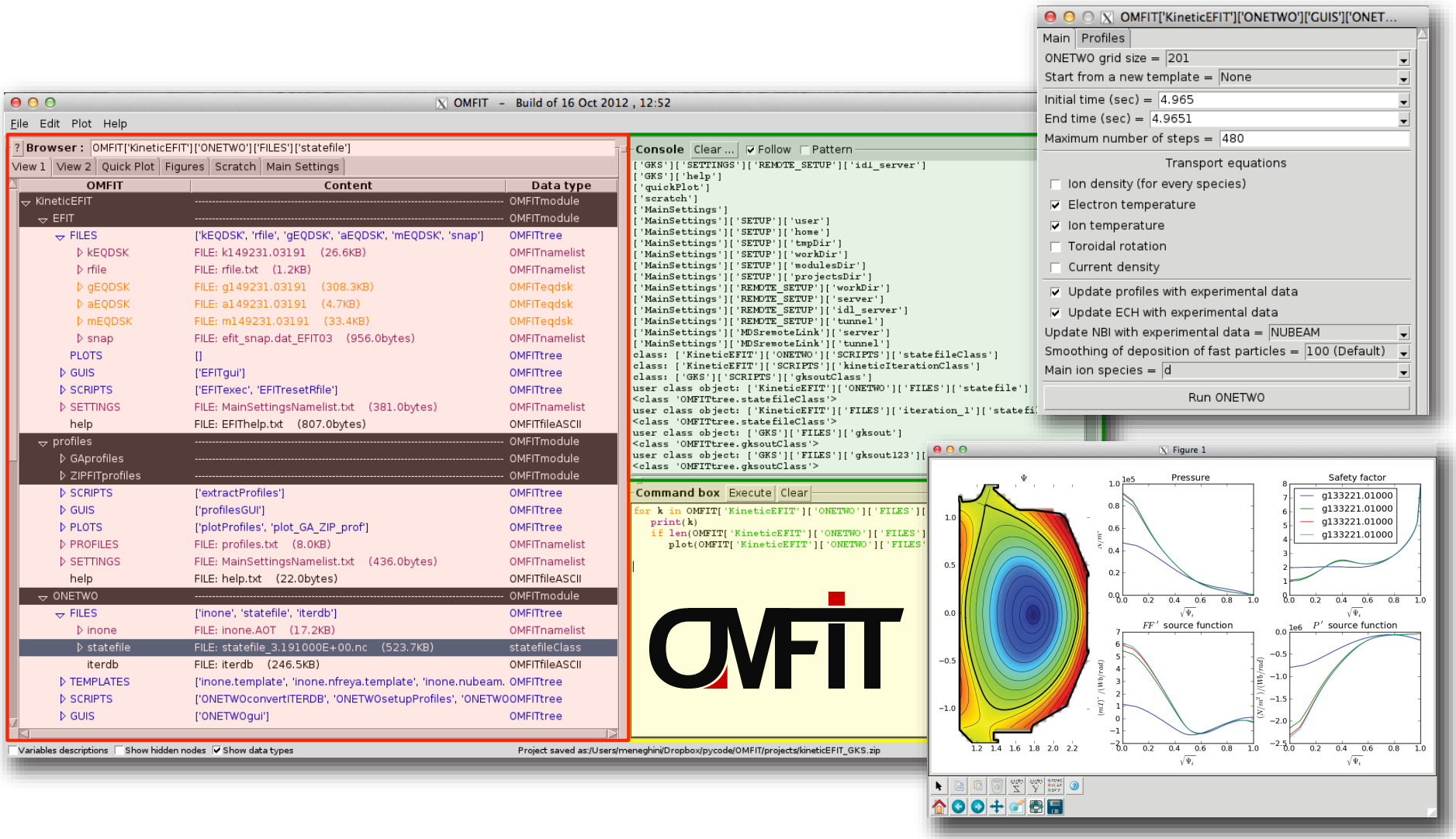
1. **Enables code to interact in complicated workflows**
   Managing complexity of data exchange and codes execution

2. **Facilitates all stages of the modeling cycle**

   Workflow execution, but also: simulation setup, code development, debugging, comparing to other codes or experiments, data management, post-processing, plotting, ...

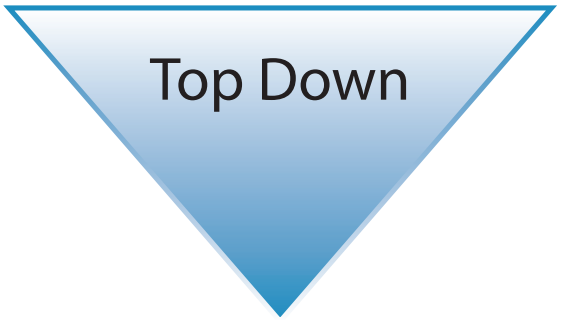
How? OMFIT is a hybrid between a workflow manager and an integrated development environment

O. Meneghini and L. Lao, Plasma and Fusion Research, **8** 2403009 (2013)



OMFIT adopts a 'bottom-up' development approach

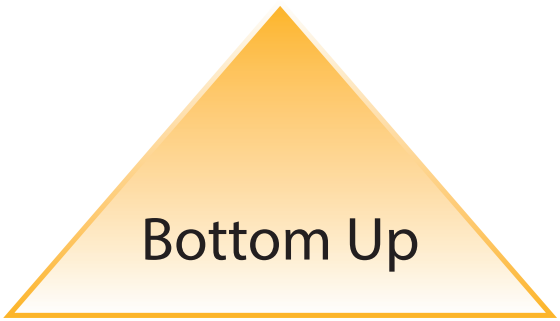
Assume design requirements are well known and immutable



Structured development process

- *Waterfall* 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

- *Agile* methodology
  - Start simple
  - Incremental deliveries
  - Embed users feedback
- Easy to change
- Lower investment risk

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

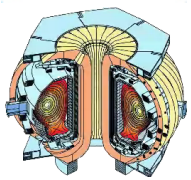
Lightweight, pure-Python framework is easy to install, maintain, and expand

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

OMFIT is an integral element of the *Advanced Tokamak Modeling* (AToM) SciDAC project

Not a new physics code, but rather a concept:

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

GENERAL ATOMICS

OAK RIDGE National Laboratory

UCSD

Lawrence Livermore National Laboratory

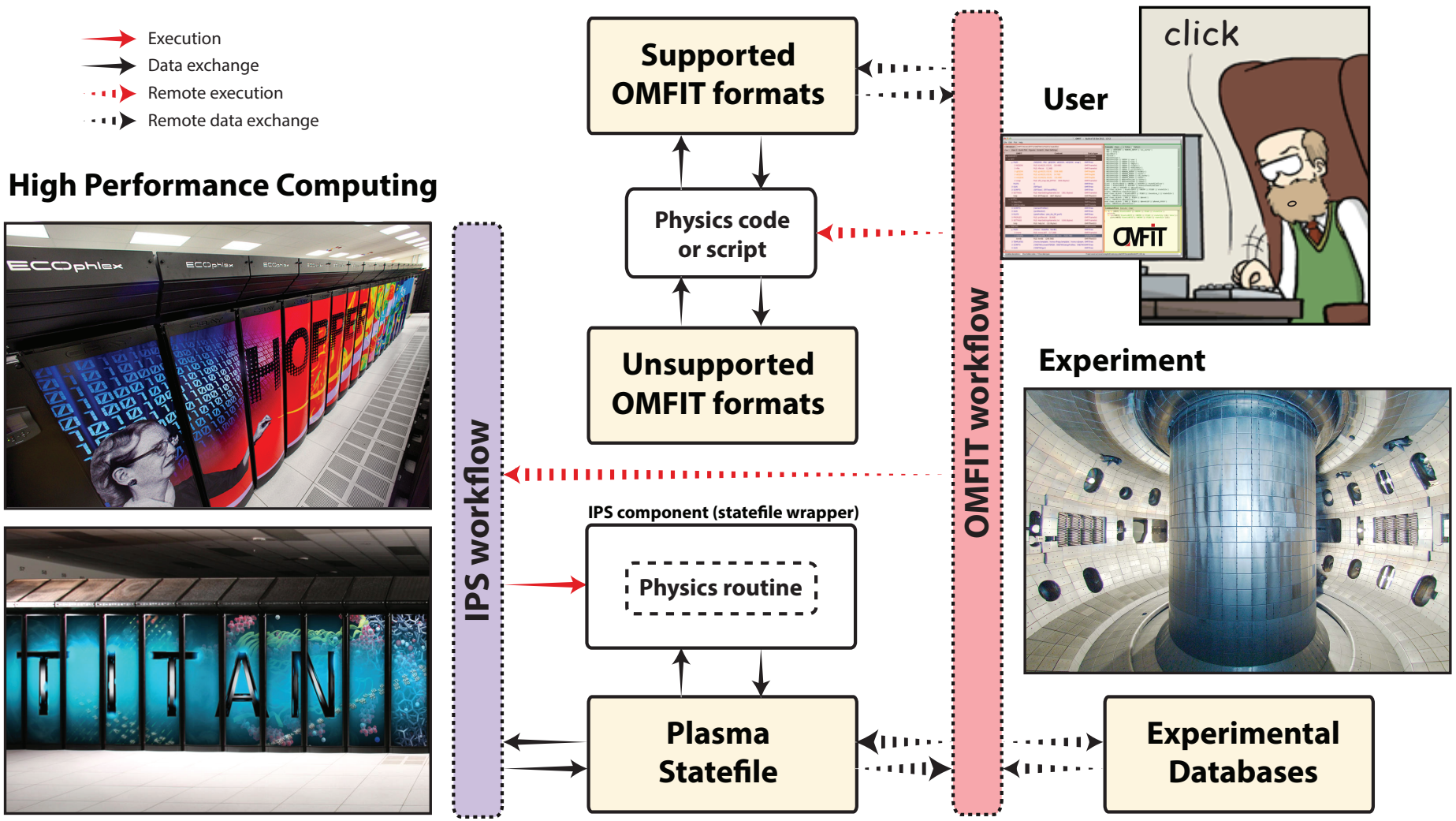
FASTMATH

SUPER

1. Bridge gap between *experimental data analysis* and *high performance simulation* communities
2. Performance engineering of critical HPC components
3. Study coupled core, pedestal, and scrape-off layer physics eg.: TGYRO $\leftrightarrow$ EPED $\leftrightarrow$ COGENT

As part of AToM, couple *Integrated Plasma Simulator* (IPS) and OMFIT and exploit their synergy

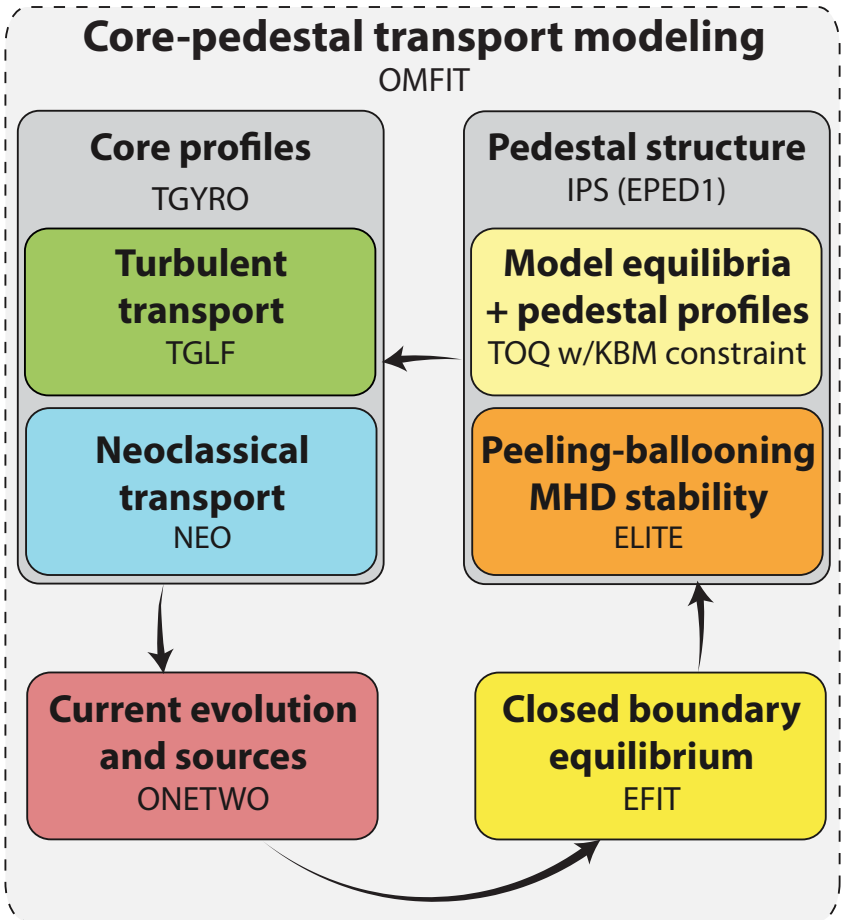
- IPS provides powerful HPC scheduling capabilities
- OMFIT provides interface to users, experiments and codes

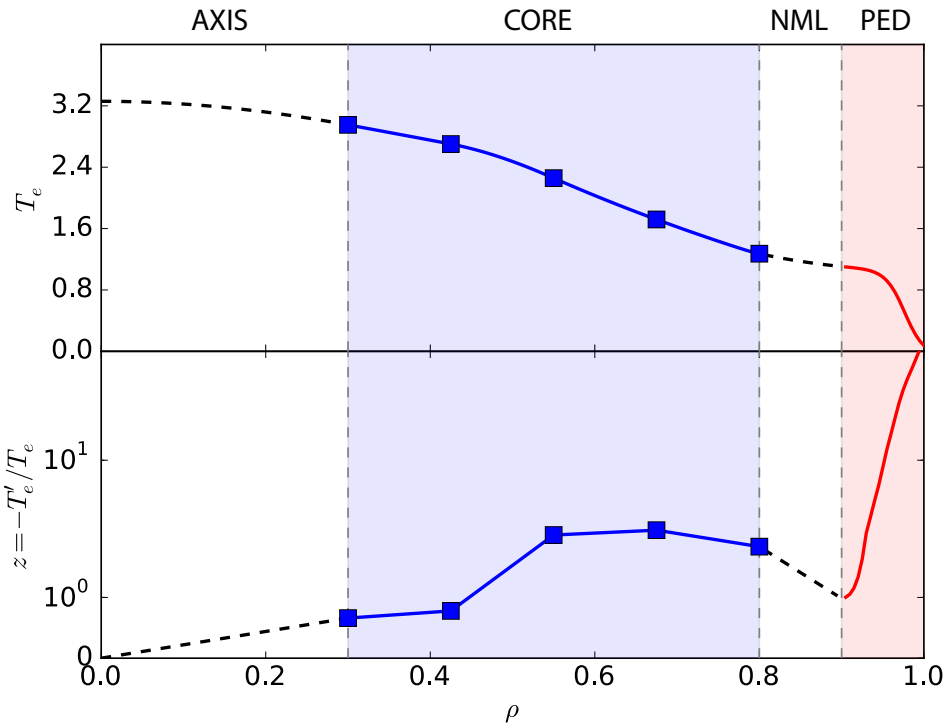


Outline

AToM project enabled first-principles self-consistent equilibrium, core transport, and edge stability studies

Separation of MHD, transport, and current diffusion timescales





Four radial zones:

PED Pedestal structure model (PB+KBM)

NML Linear scale-length interpolation

CORE Reduced gyrokinetic model

AXIS Linear scale-length to zero

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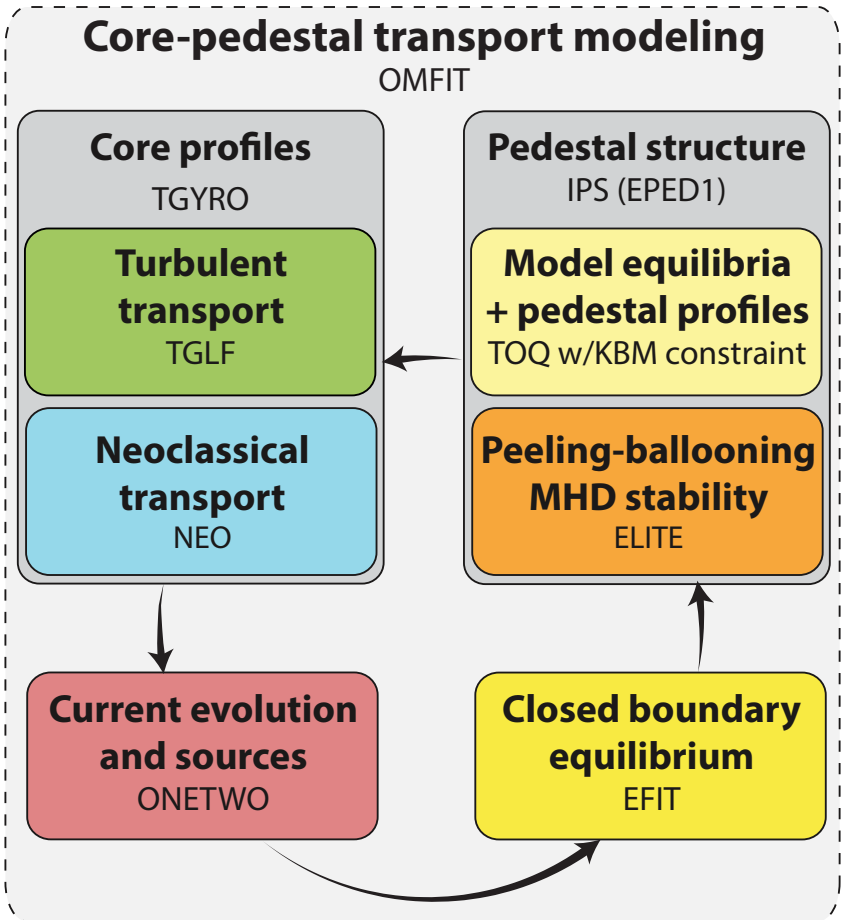

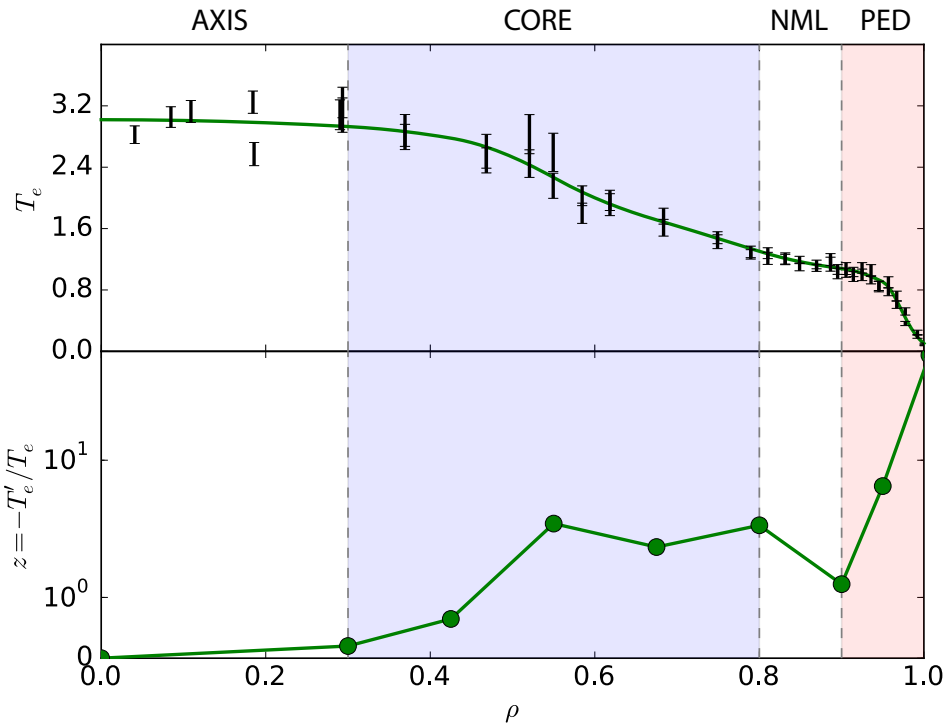

Linear scale-length fitting of experimental data supports choices of:

- Radial zone locations
- Using few TGLF calculation points

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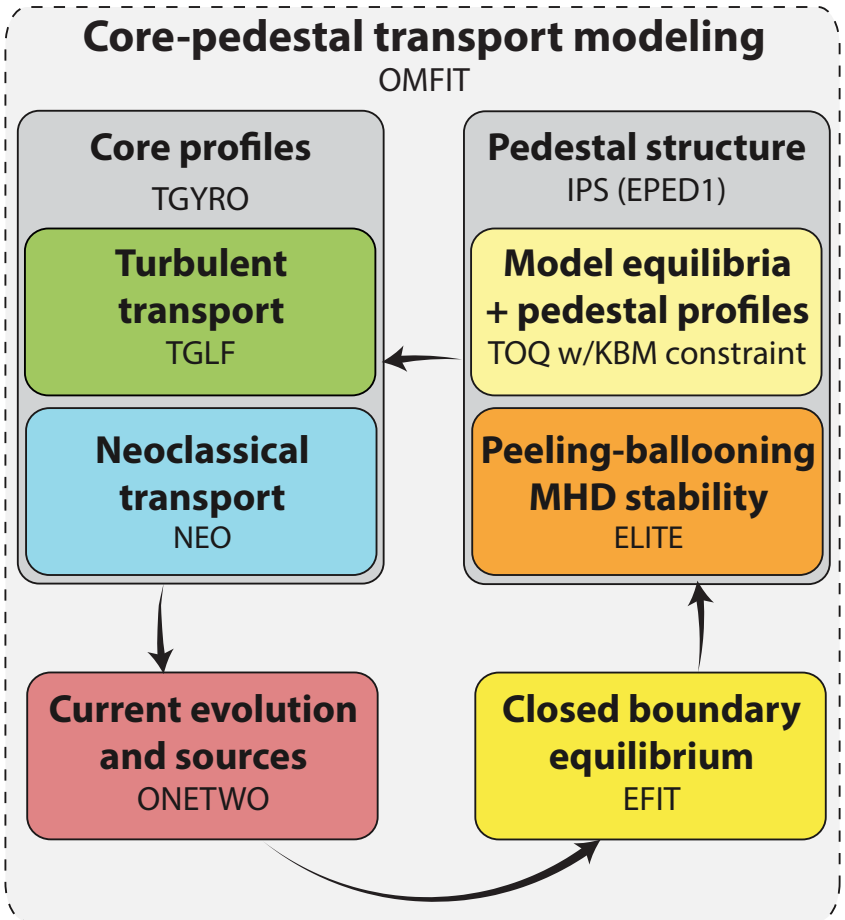

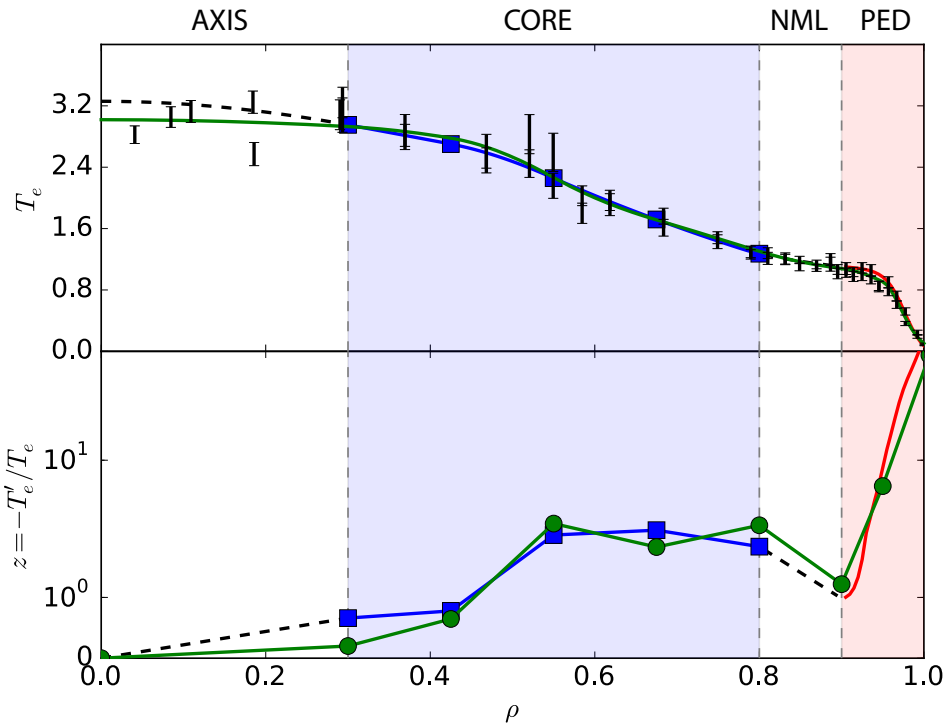

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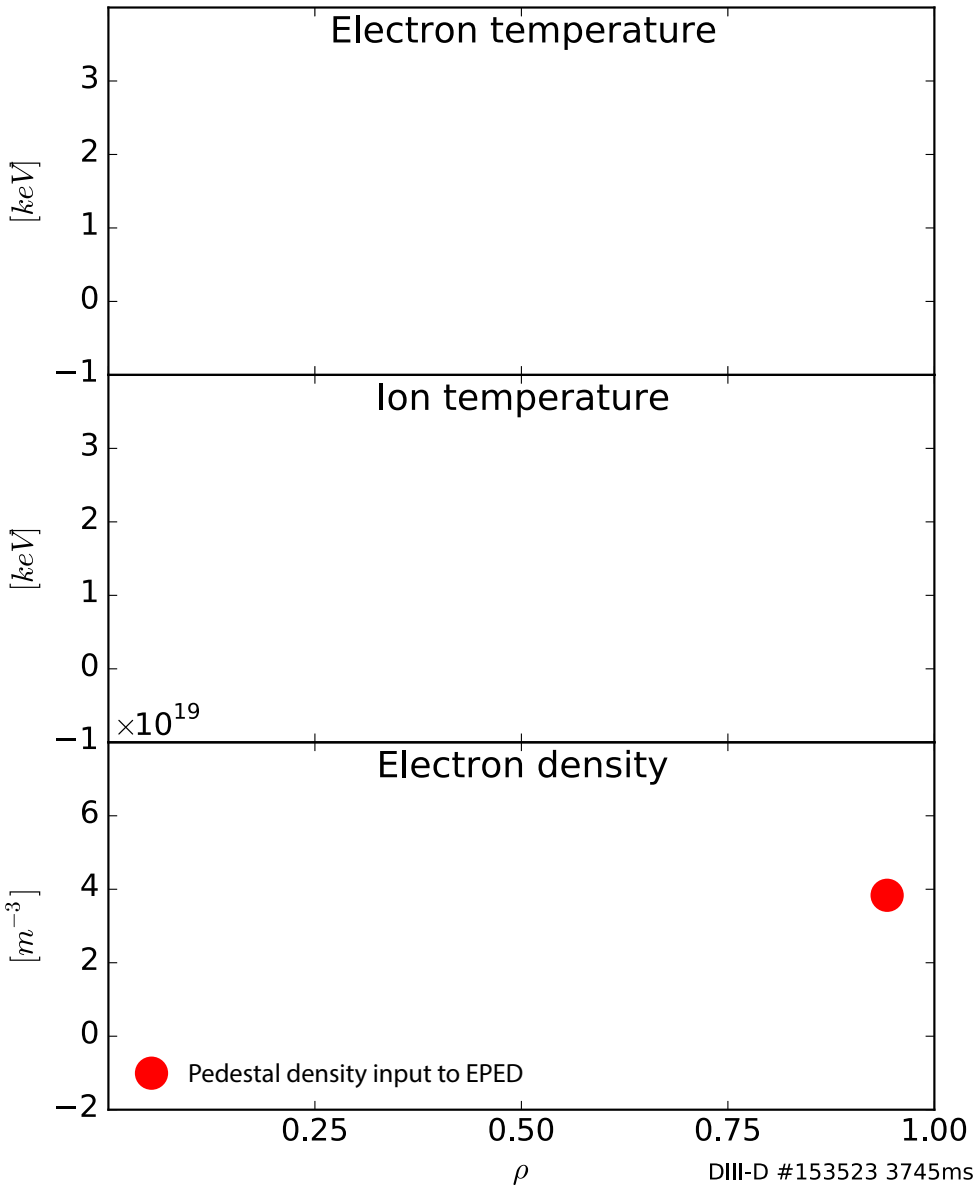
First applied this workflow to DIII-D ITER baseline scenario with low torque and electron heating

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



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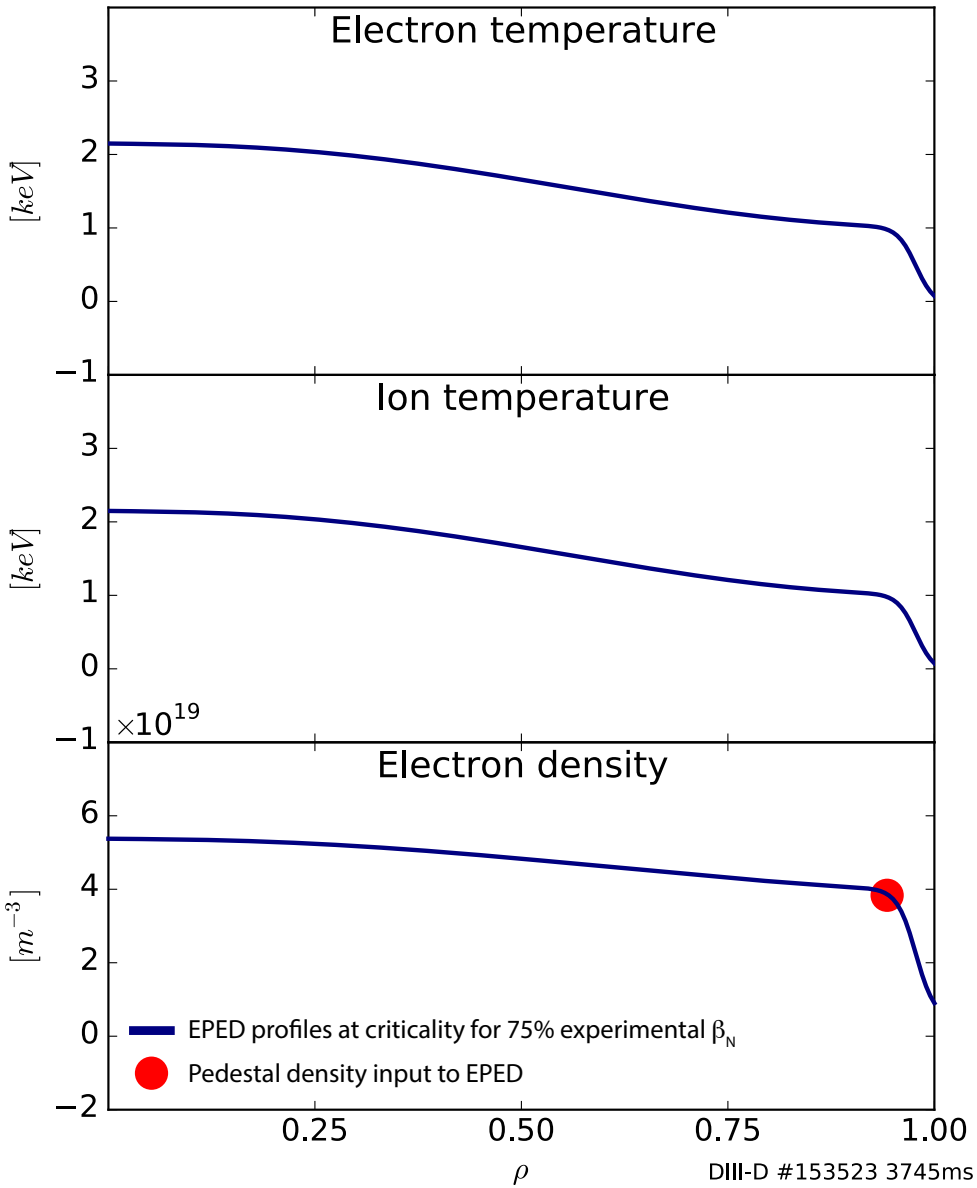

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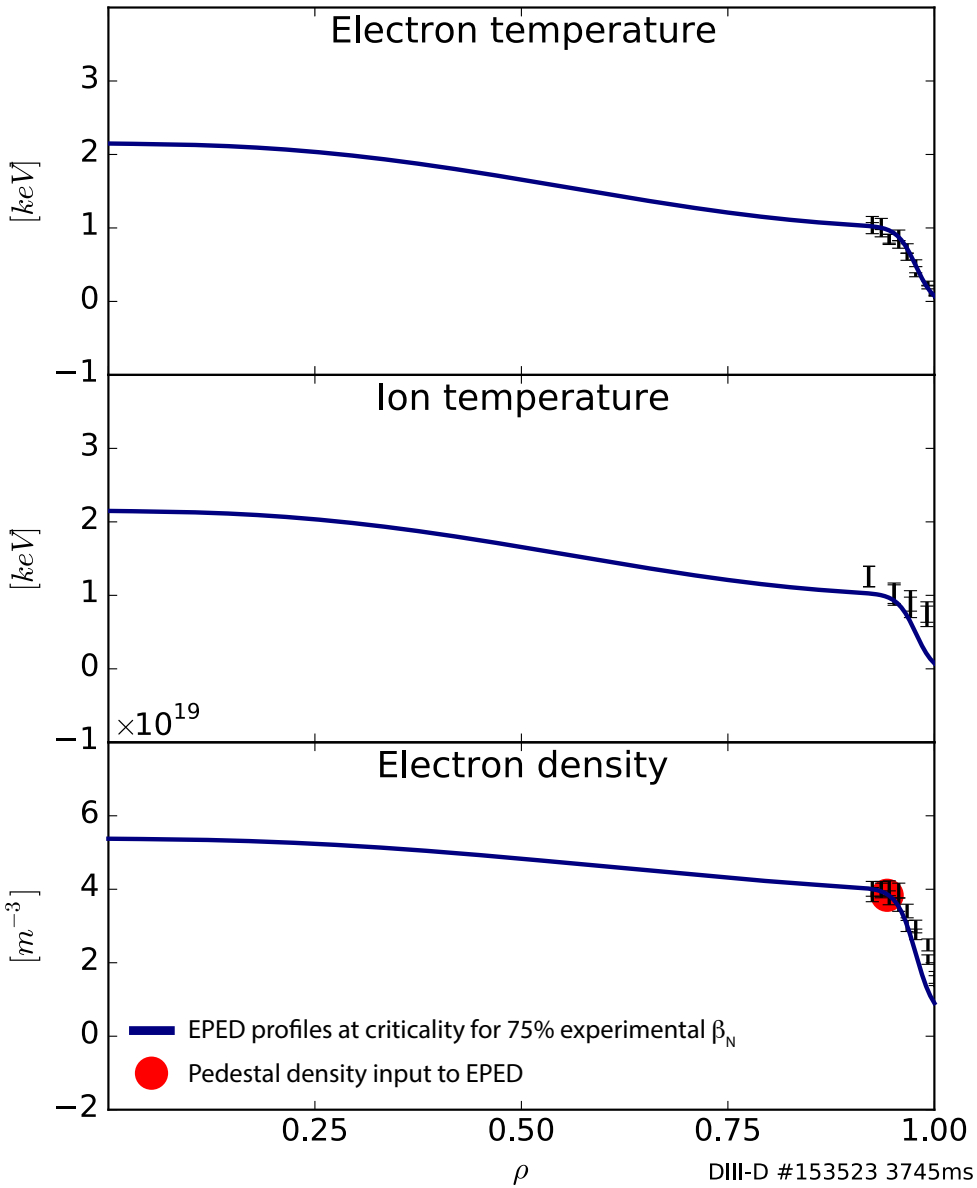

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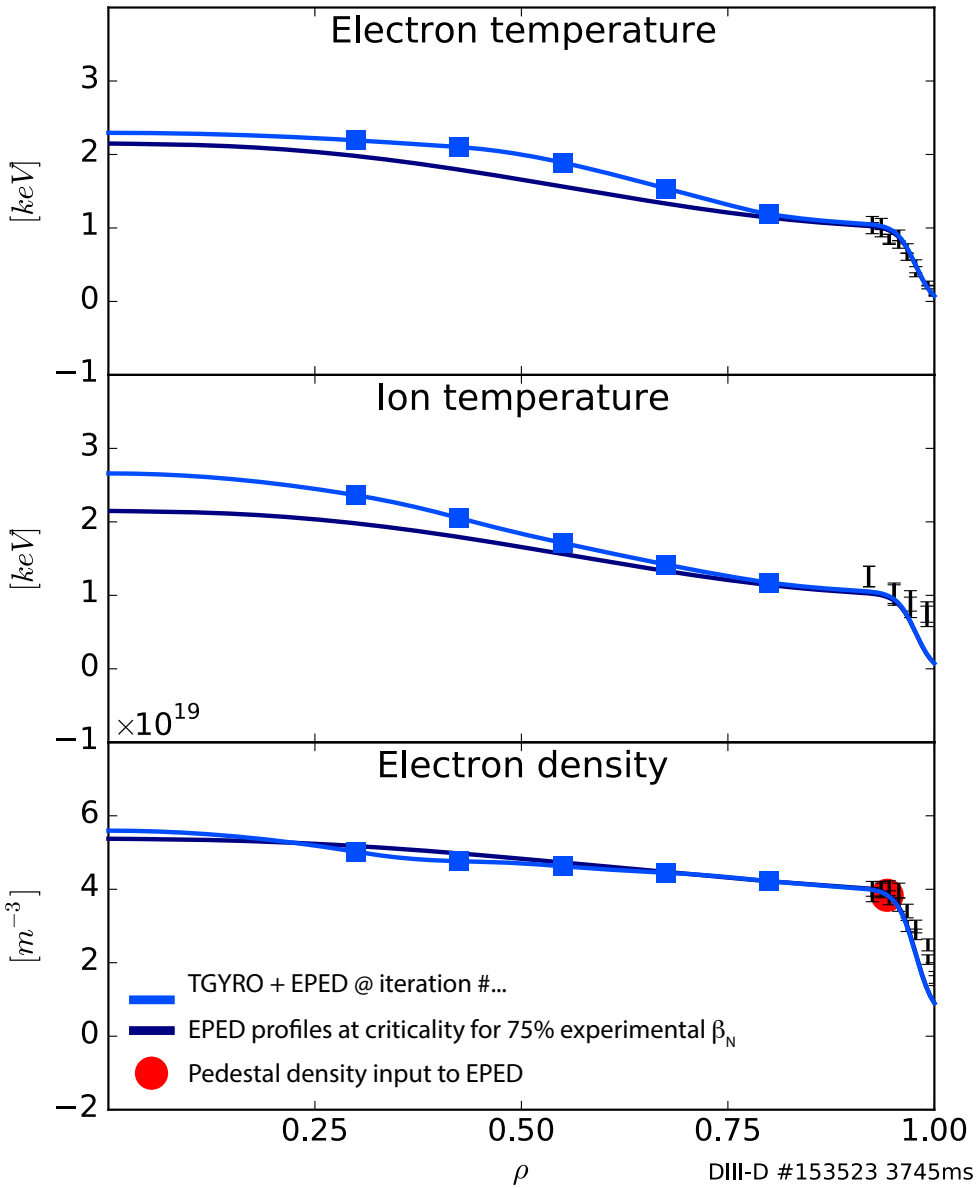

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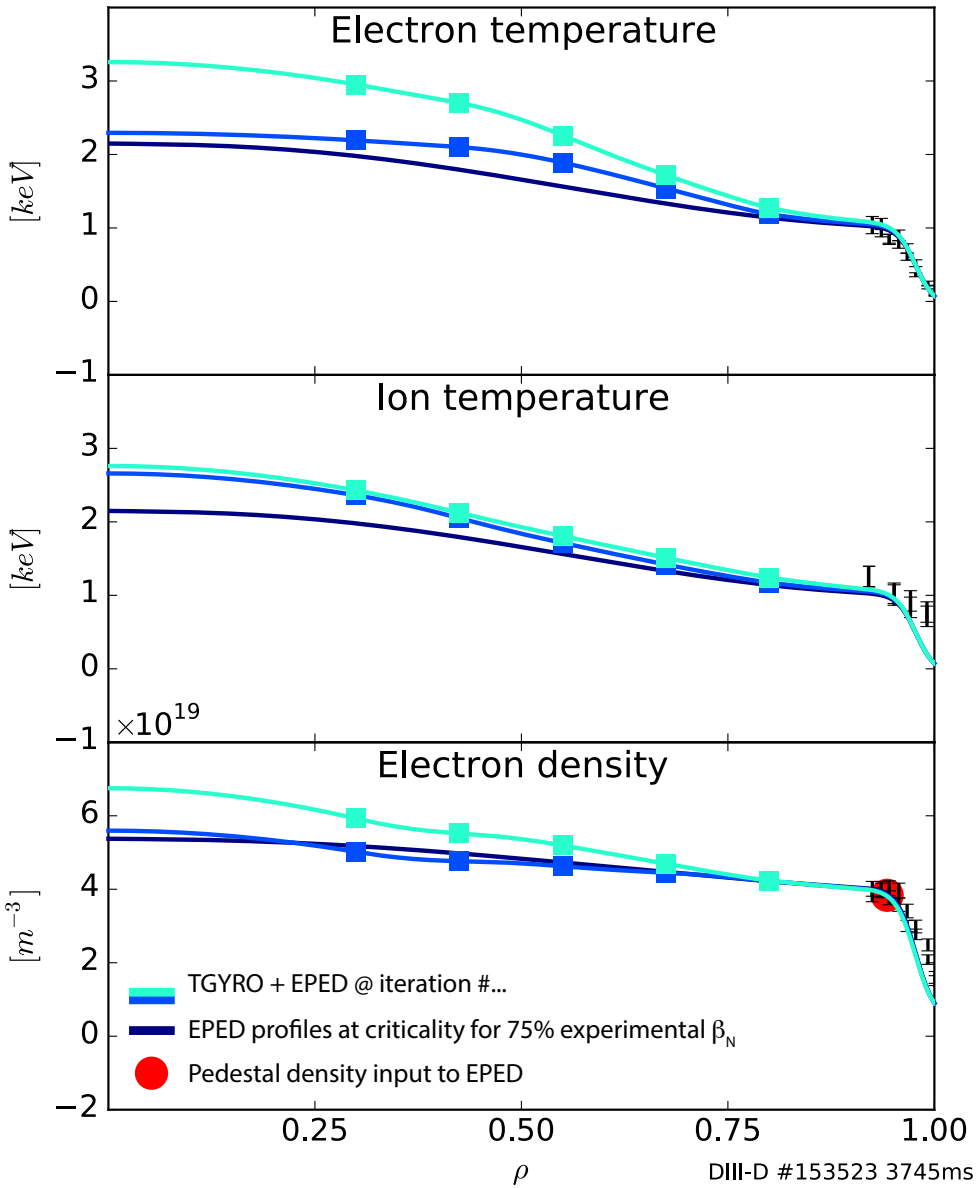

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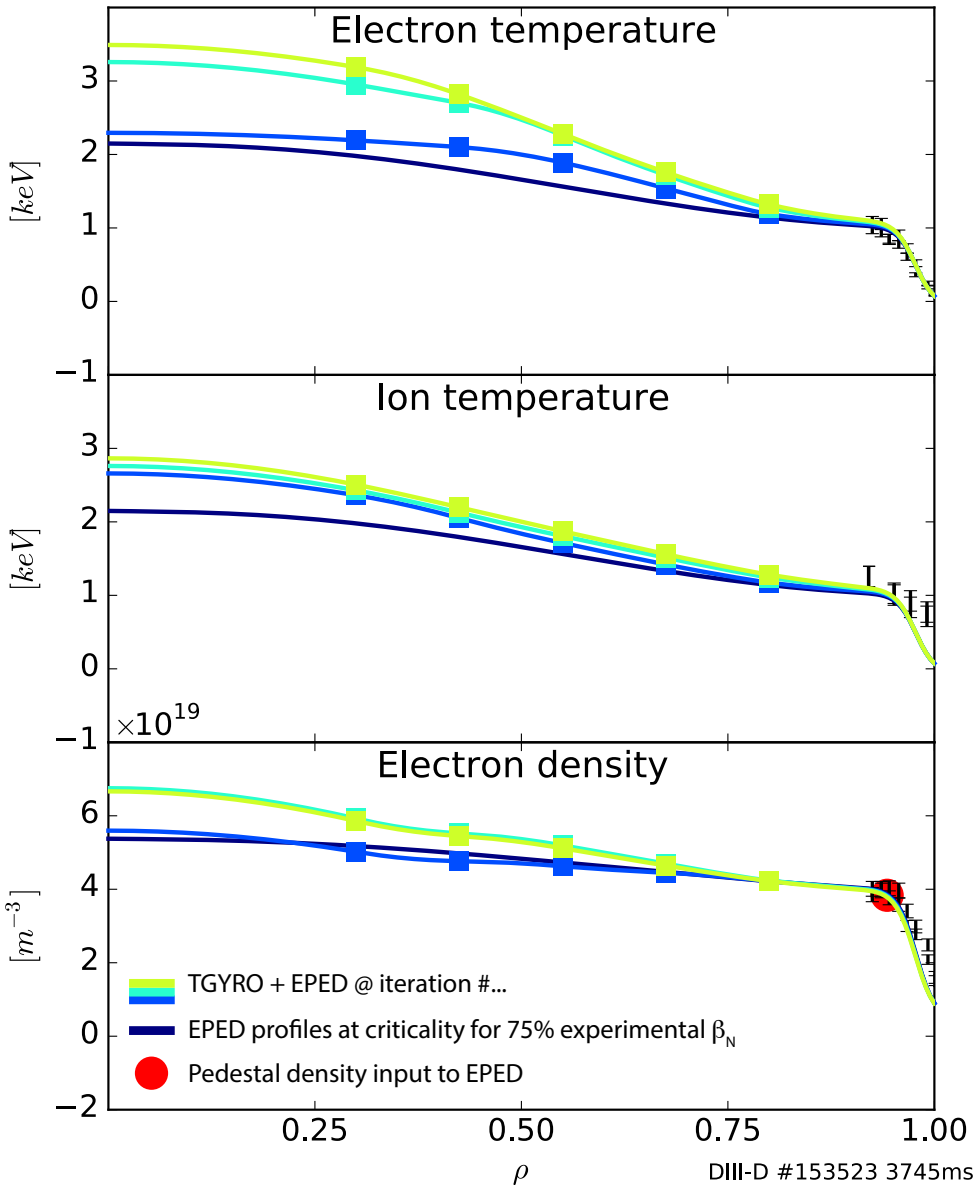

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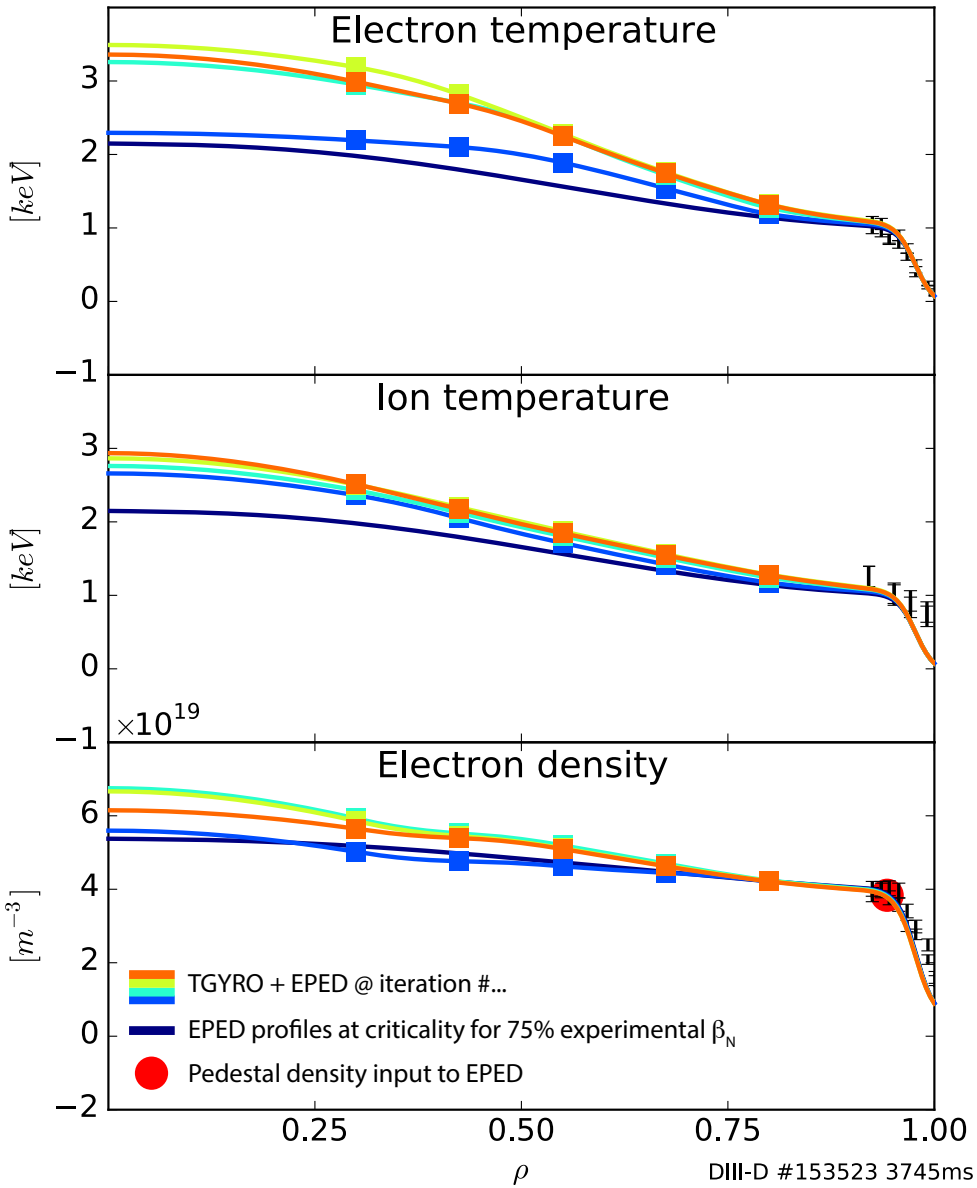

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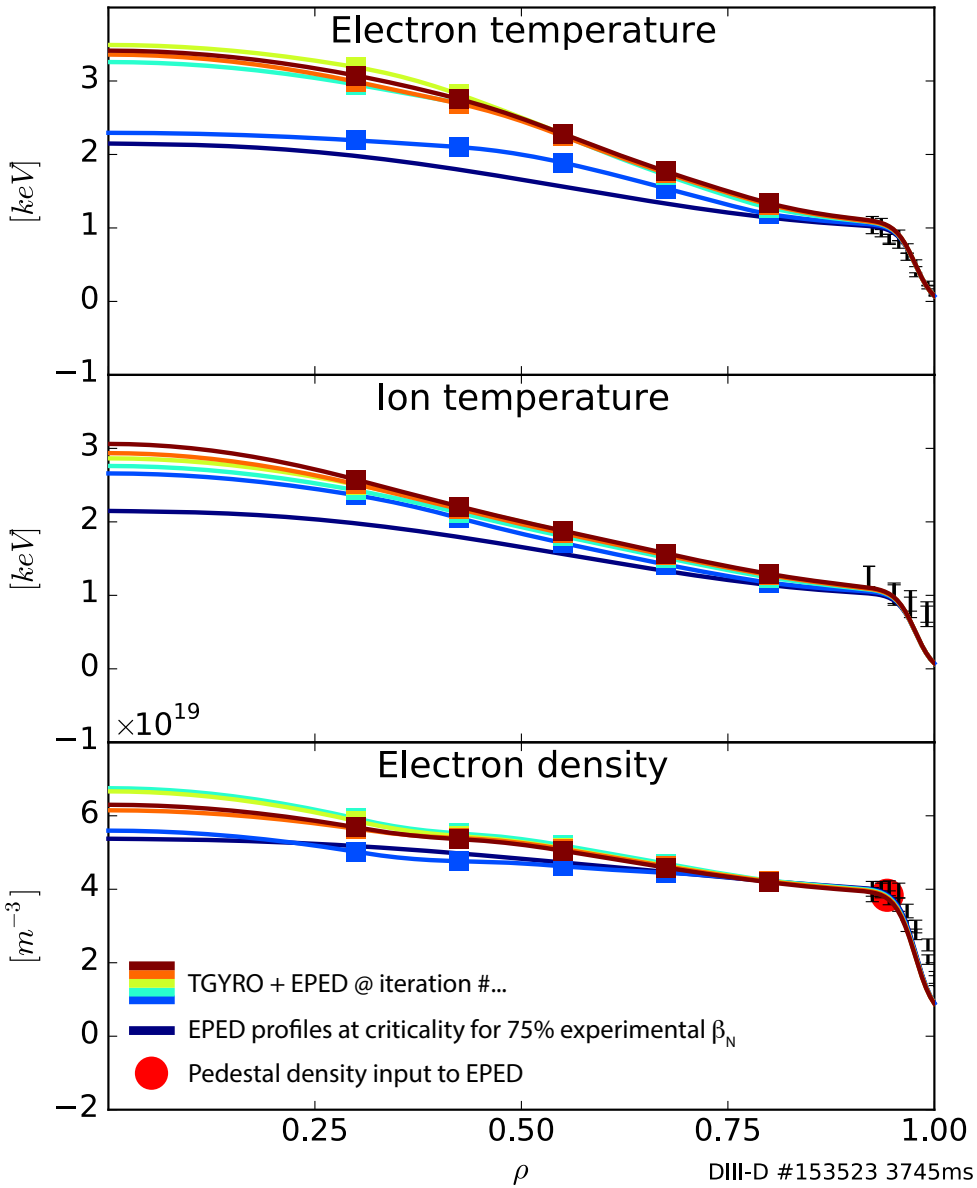

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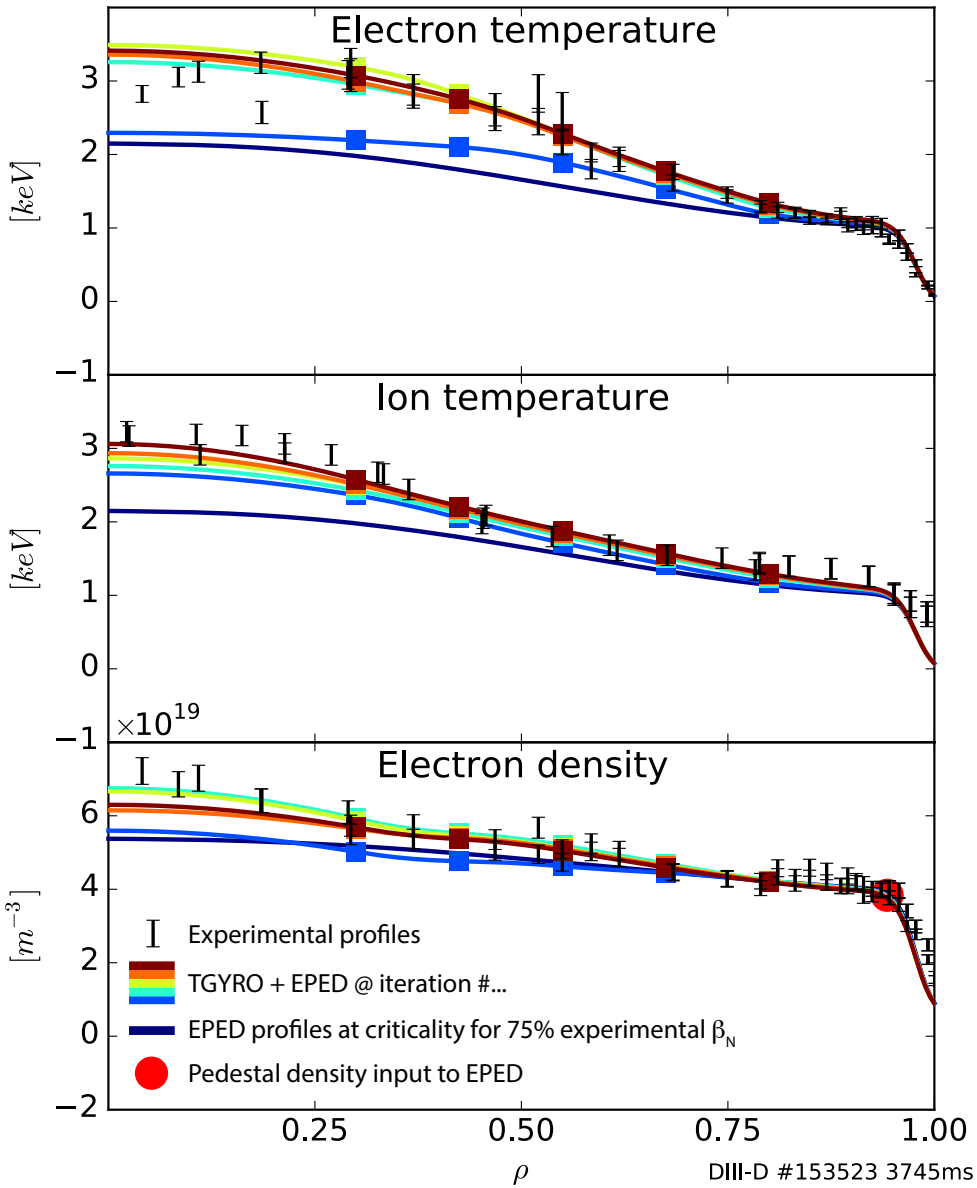
- Start with EPED. First run uses (poor) initial guess for β_N
- TGYRO to predict profiles and β_N. Then iterate...
- Measurements recovered very well across the plasma
- Pedestal prediction is weakly sensitive to β_N Shafranov shift stabilization



Outline

Running TRANSP from OMFIT is in line with AToM philosophy

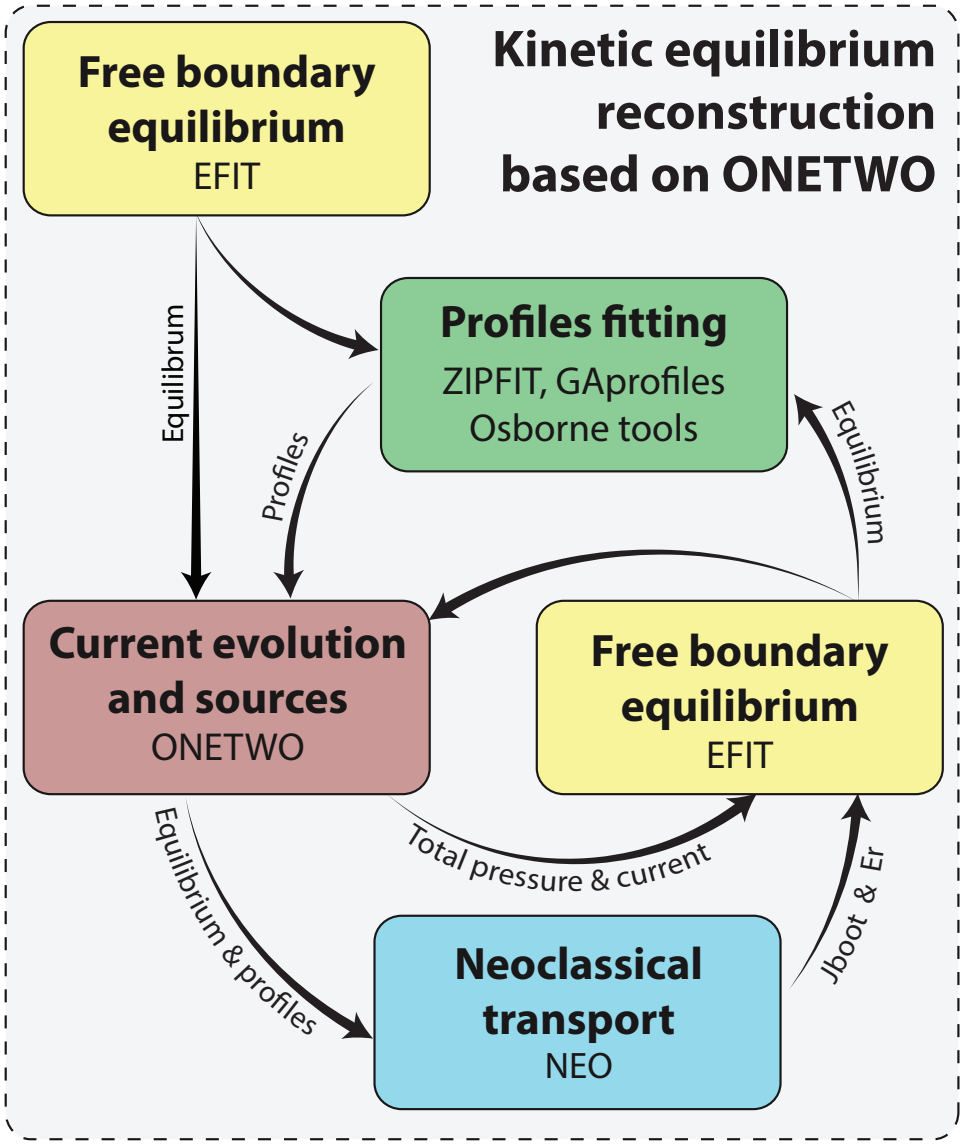
TRANSP is a comprehensive transport code

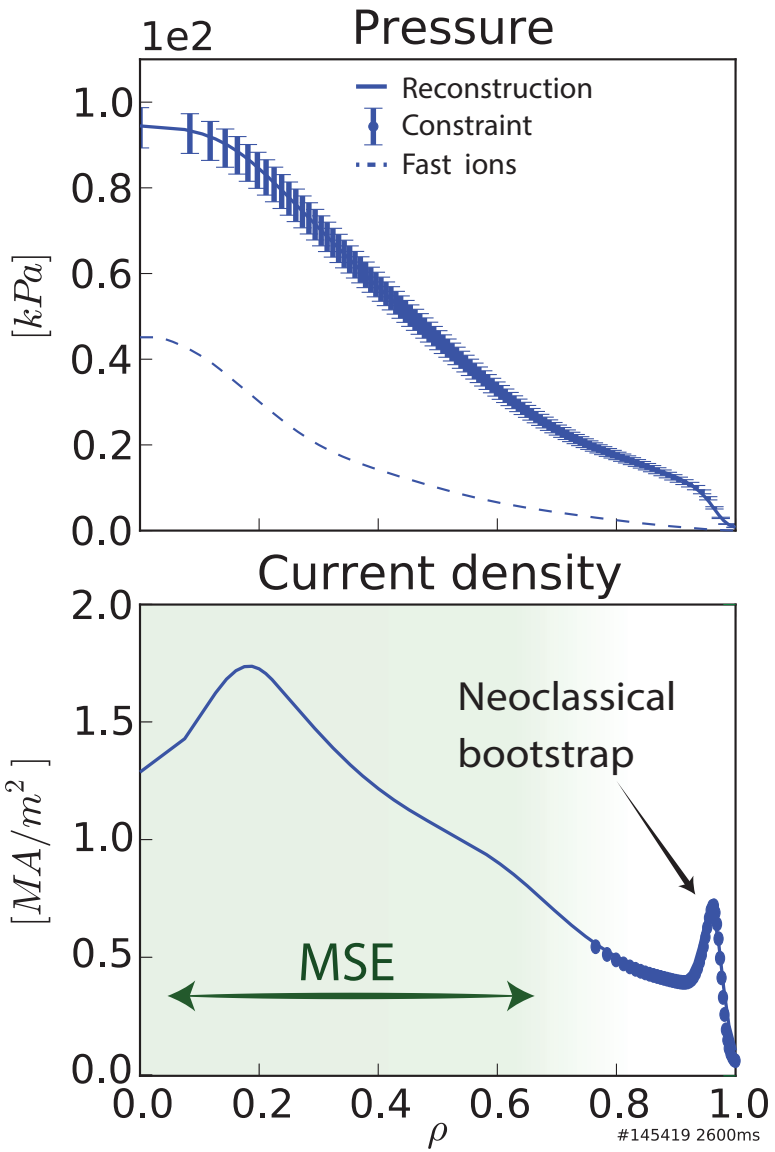
- Widely adopted
- Validated on numerous devices
- Solid infrastructure $\rightarrow$ TRANSP grid
- Responsive support

OMFIT can provide a convenient interface to user, experimental data and codes outside of TRANSP

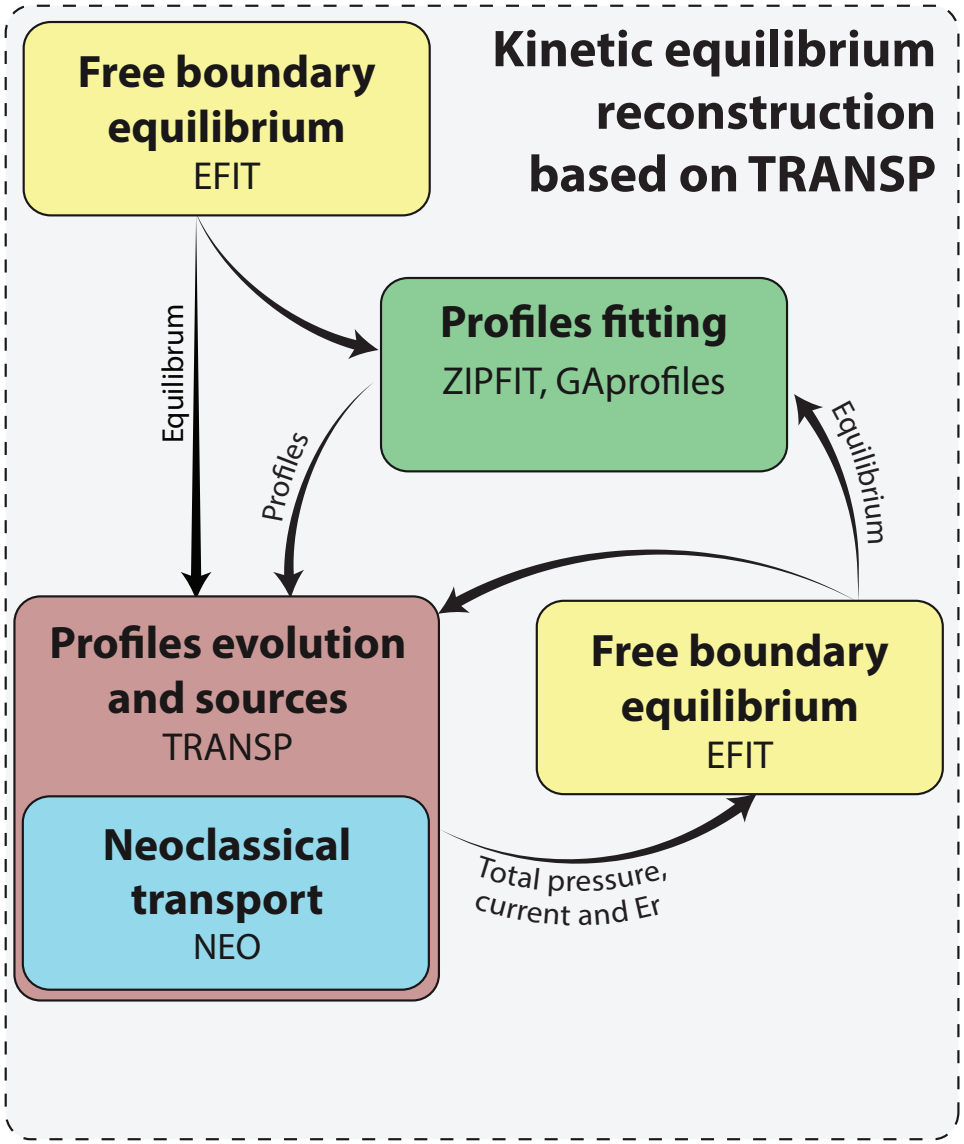
Initial OMFIT-TRANSP integration sparked by need to generate time-dependent DIII-D kinetic equilibrium reconstructions based on TRANSP runs (B. Grierson)

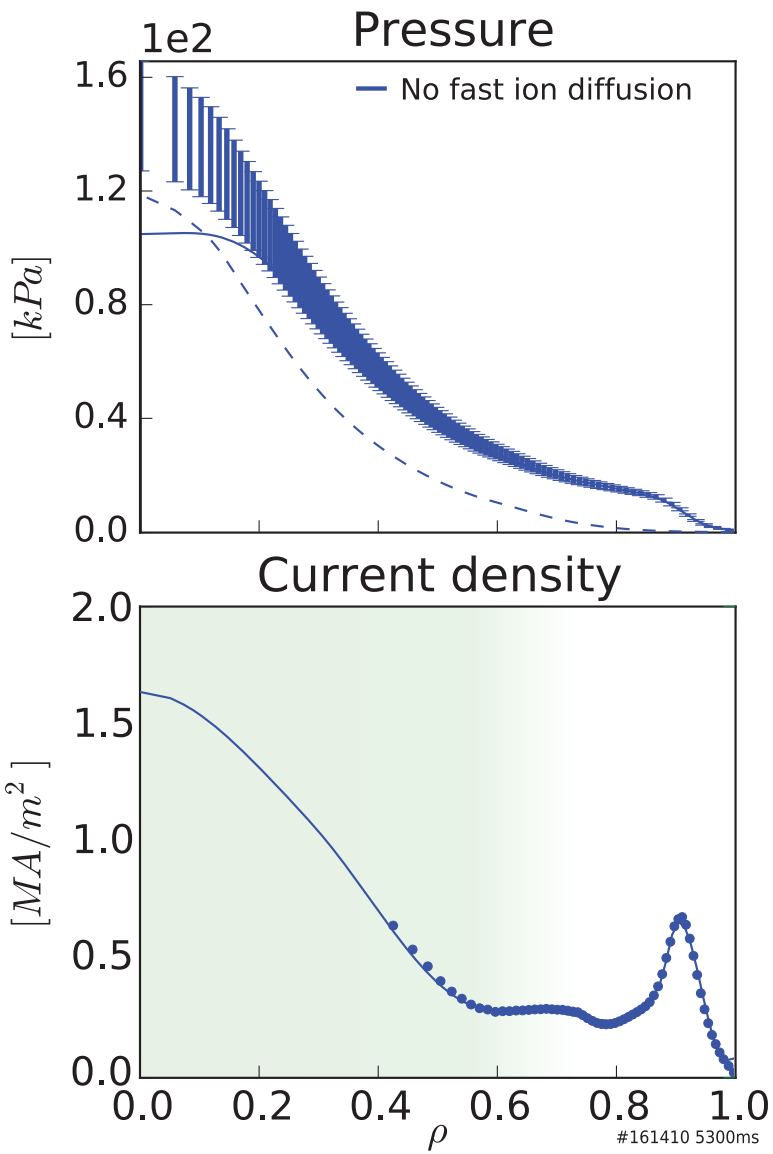
DIII-D kinetic EFIT analysis originally based upon ONETWO





Developed new TRANSP module and integrated it as part of the OMFIT kineticEFIT module





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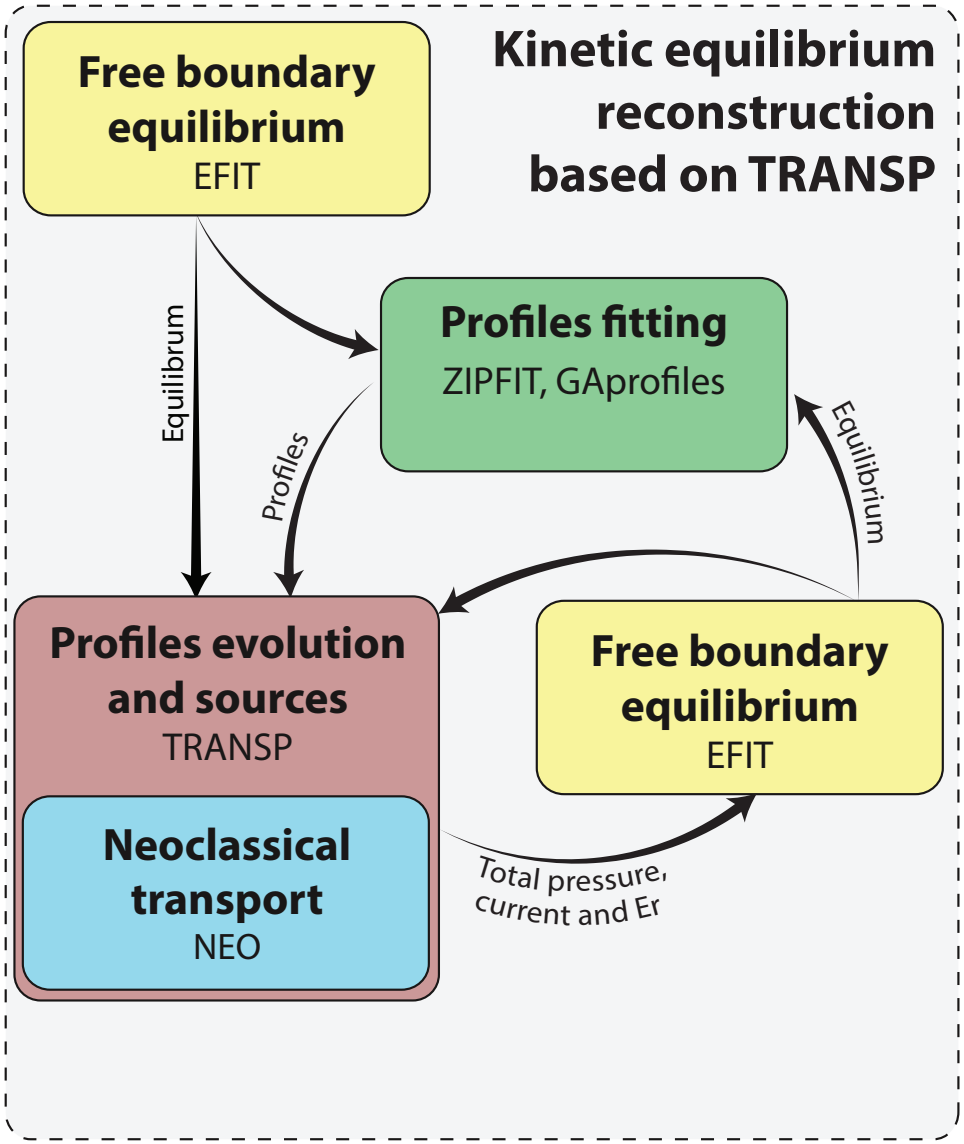

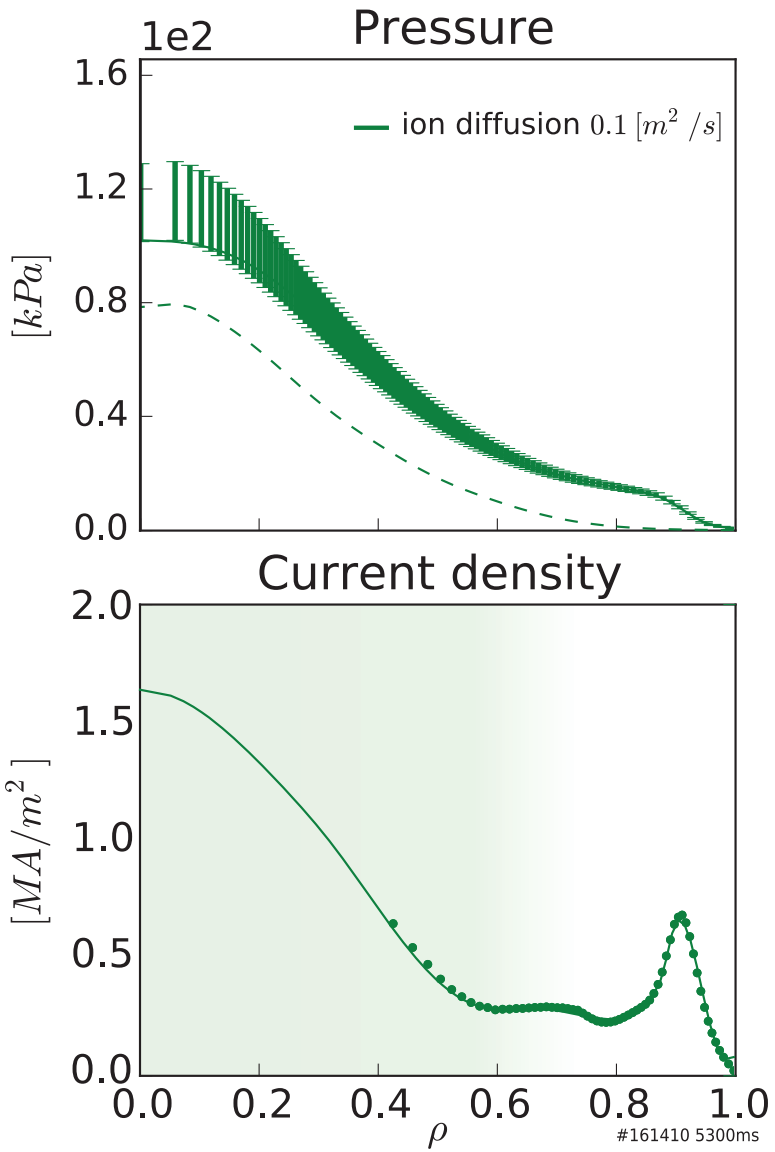

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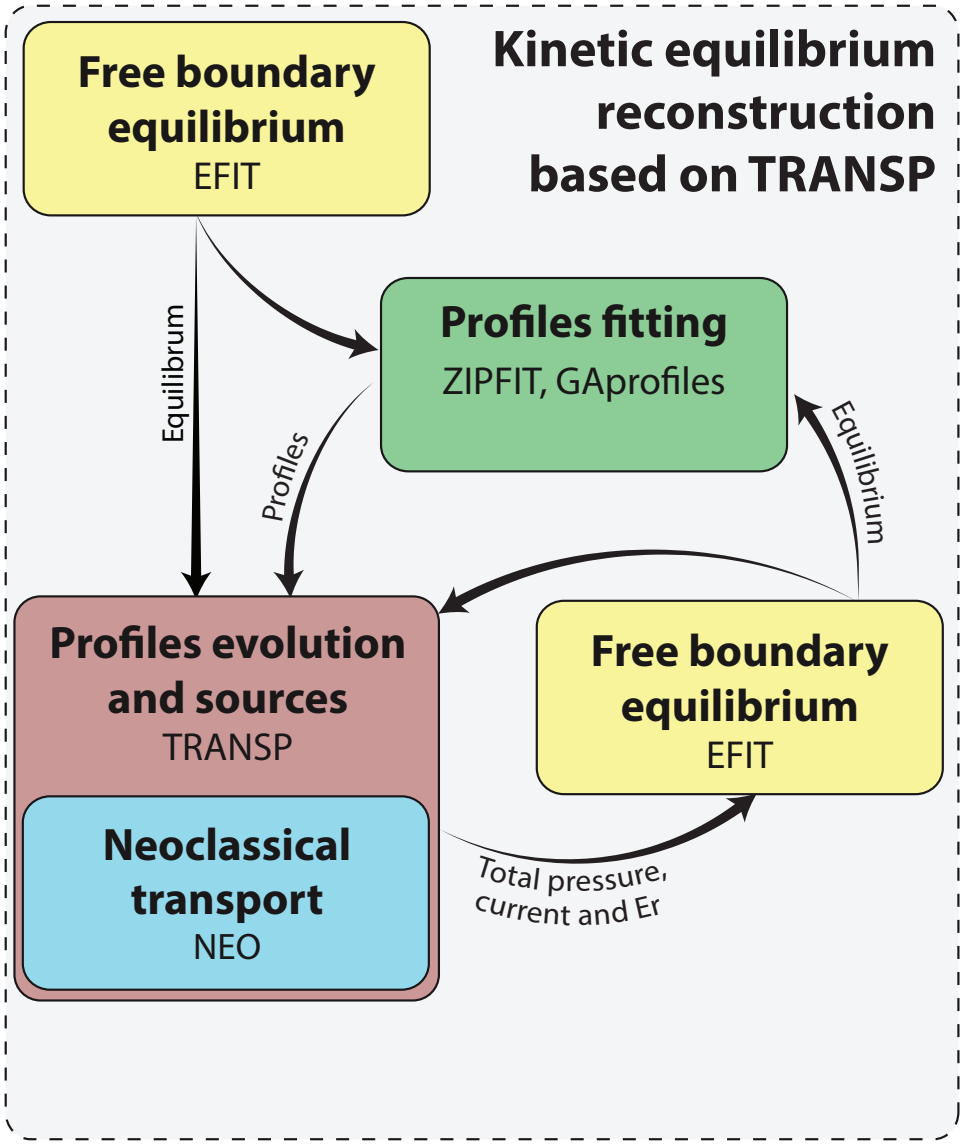

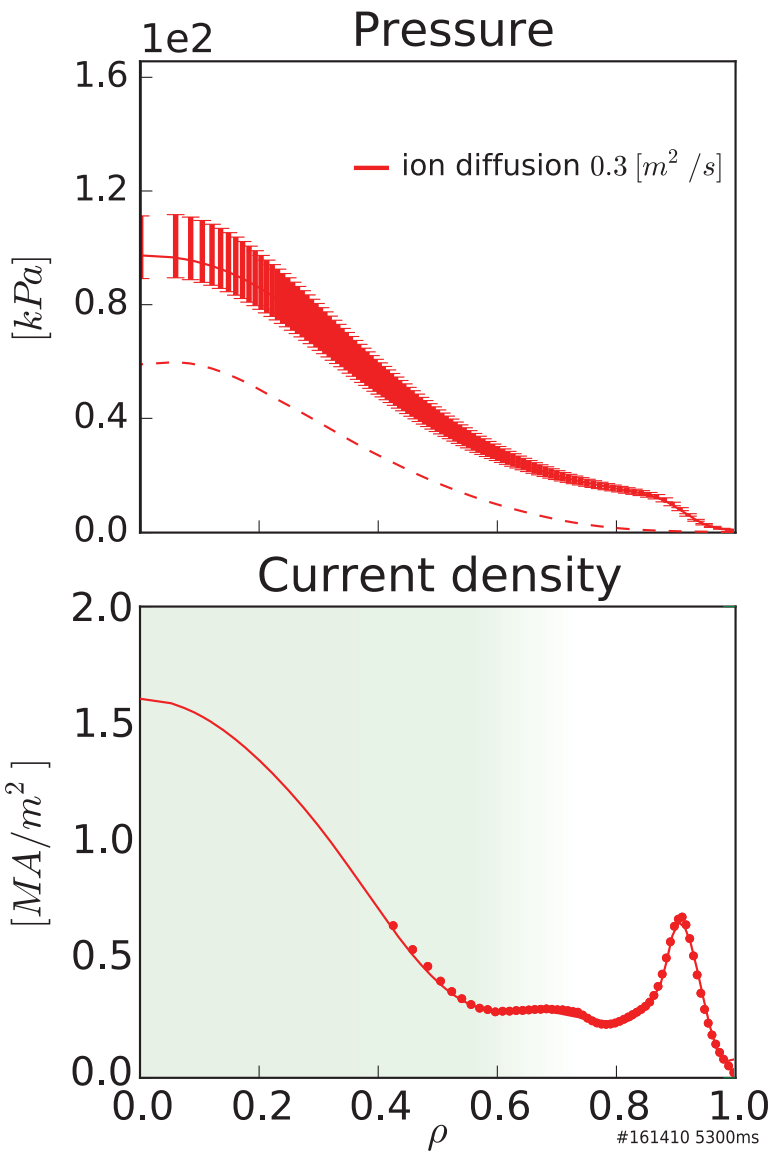

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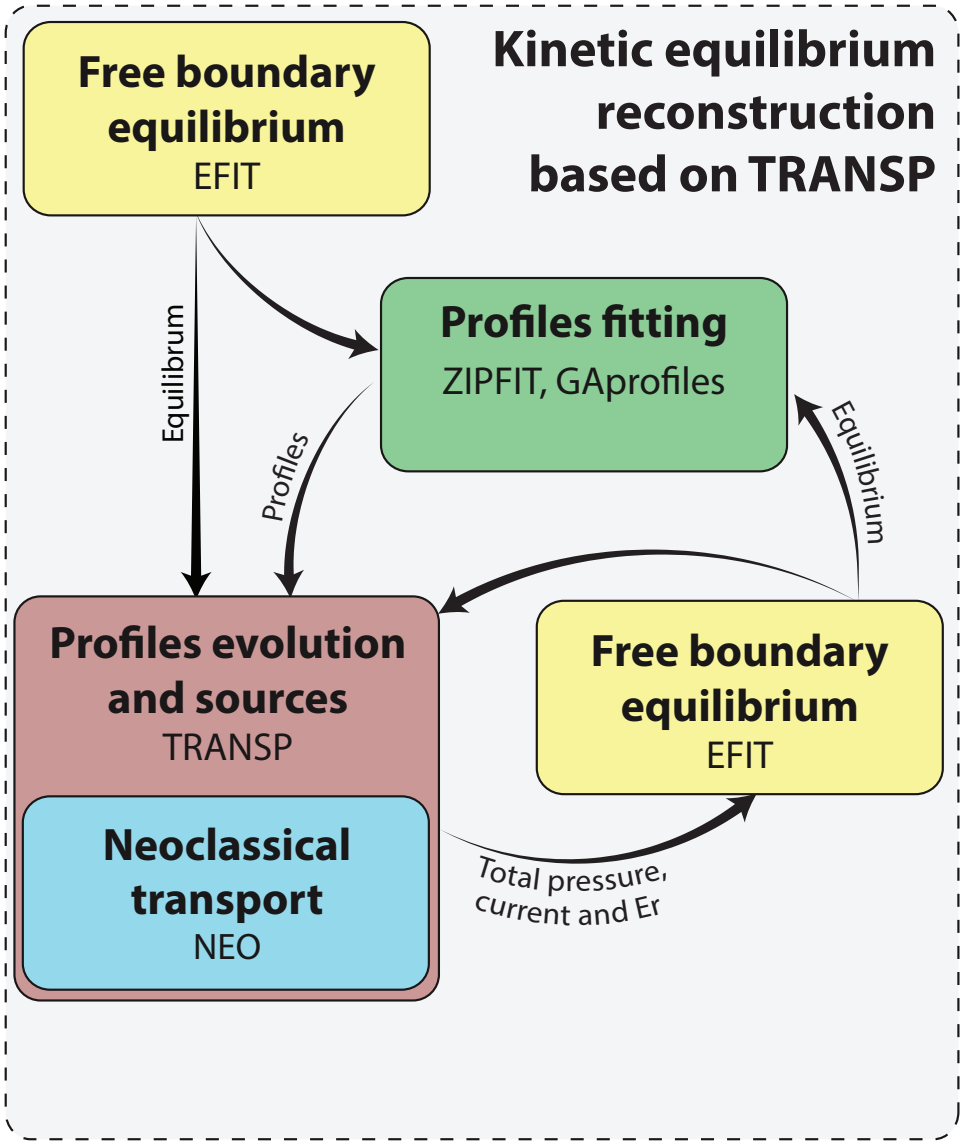

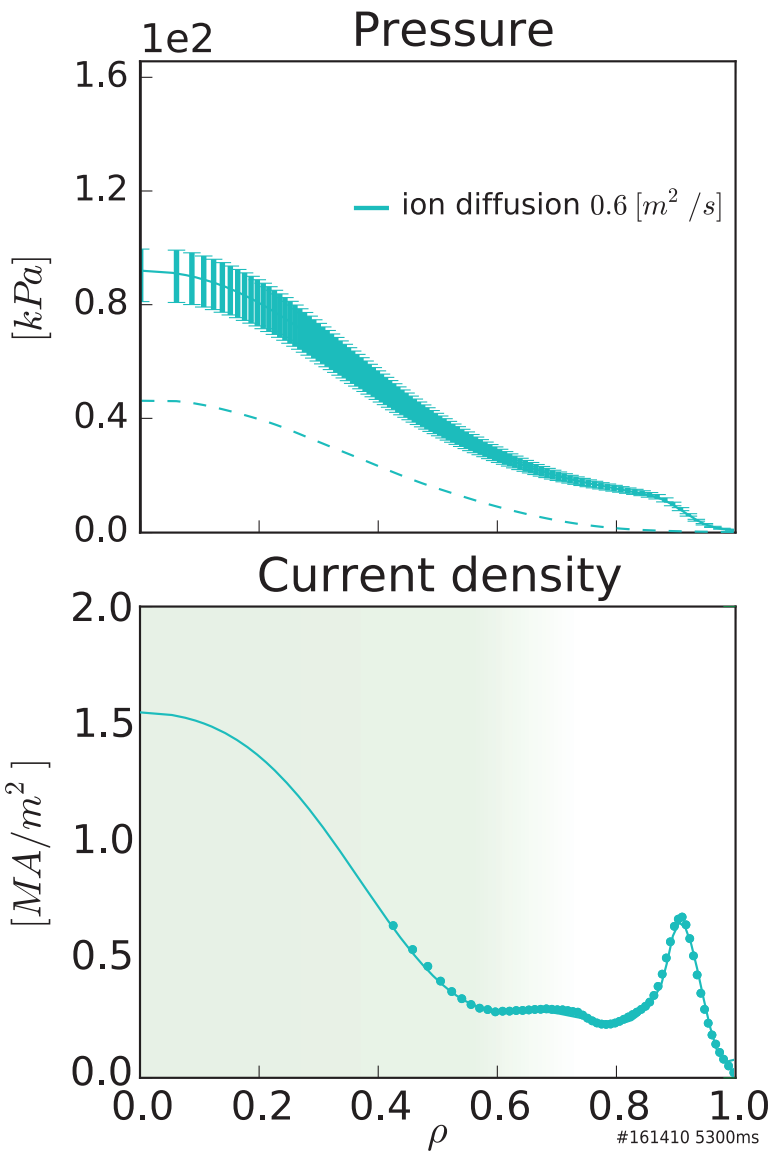

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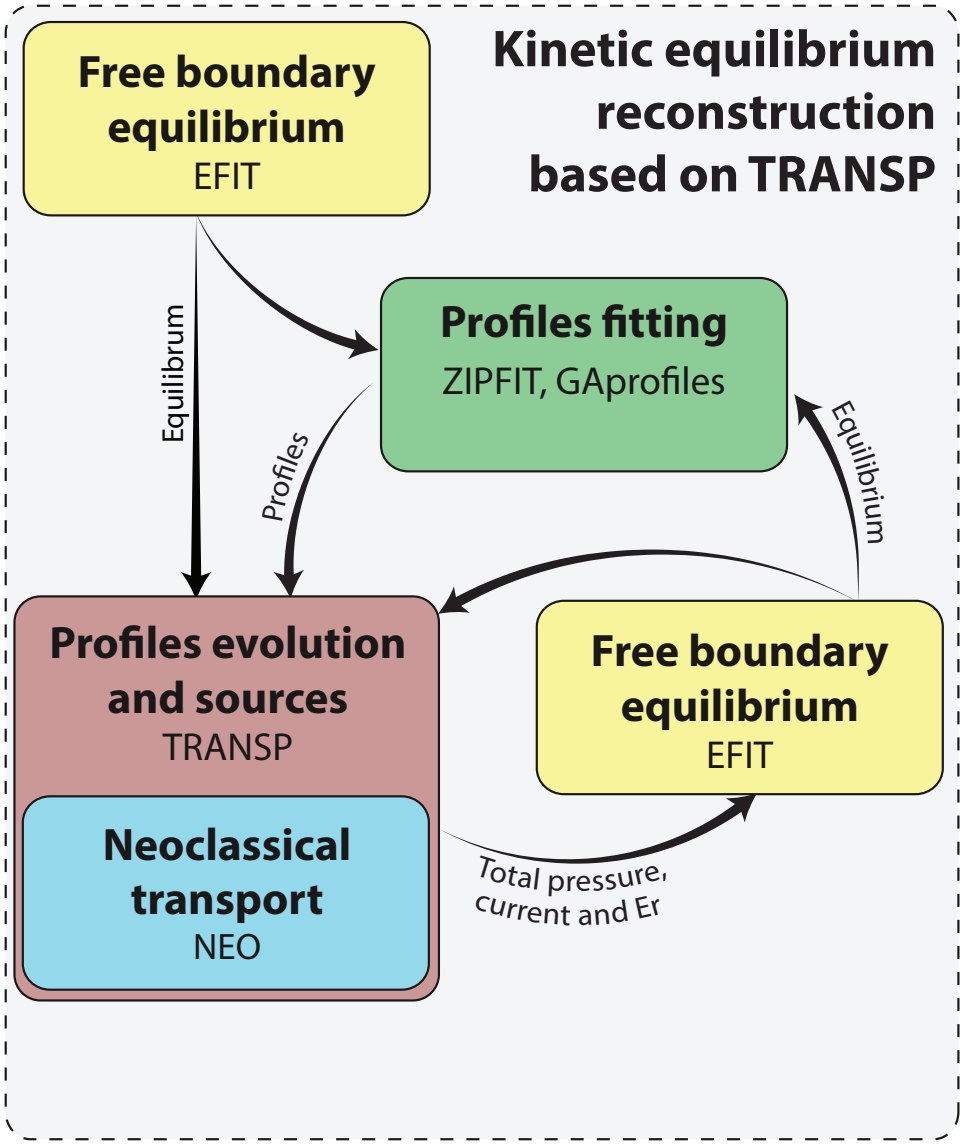

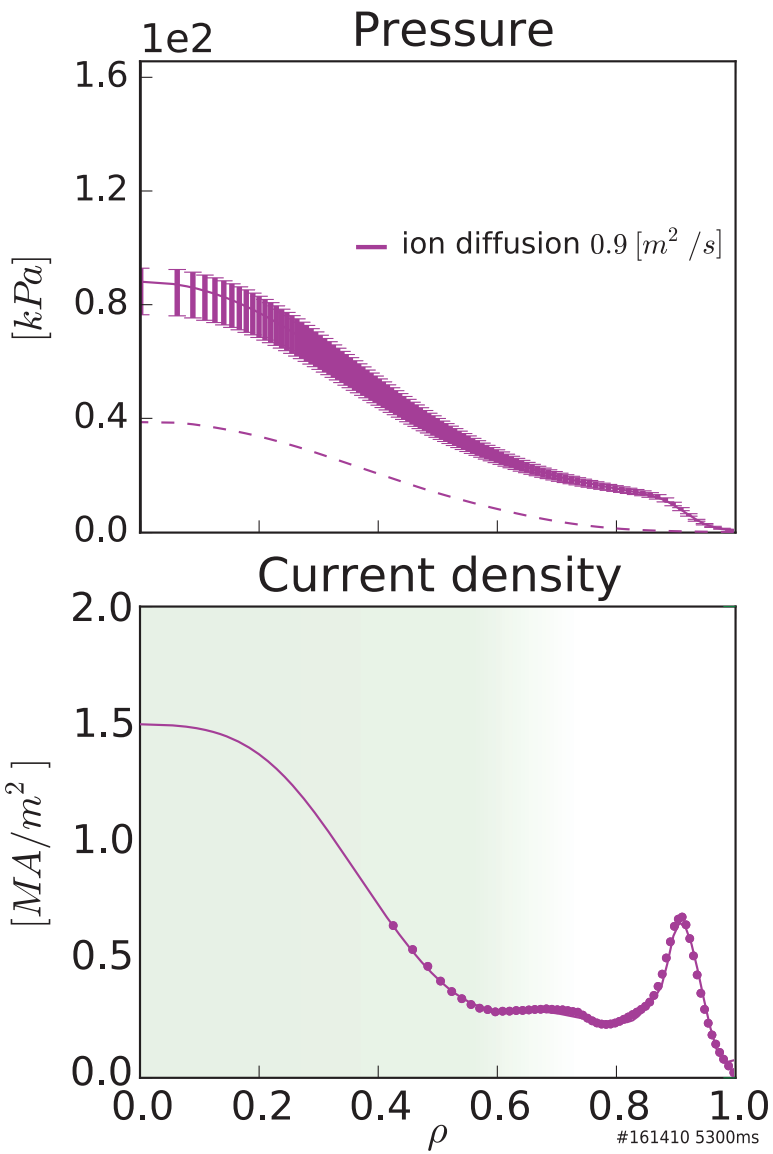

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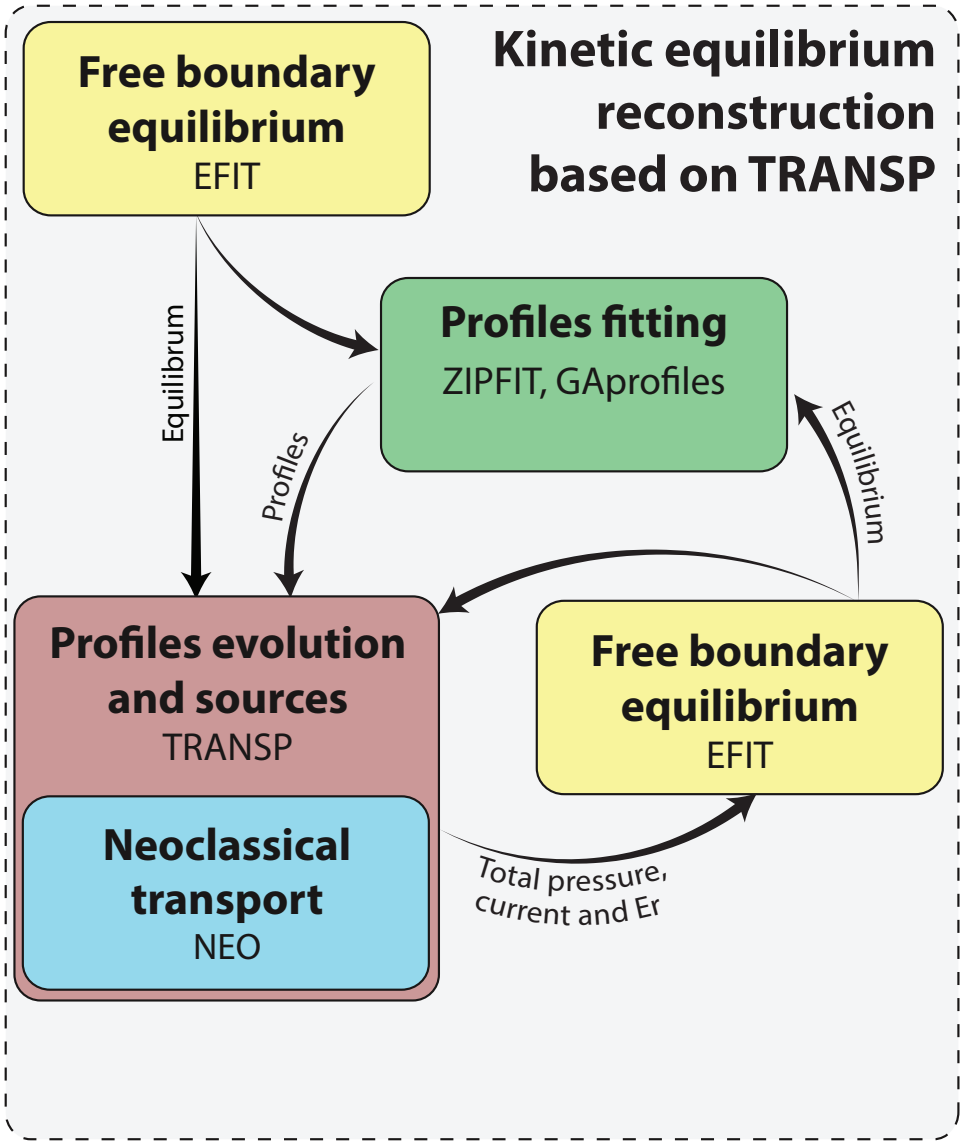
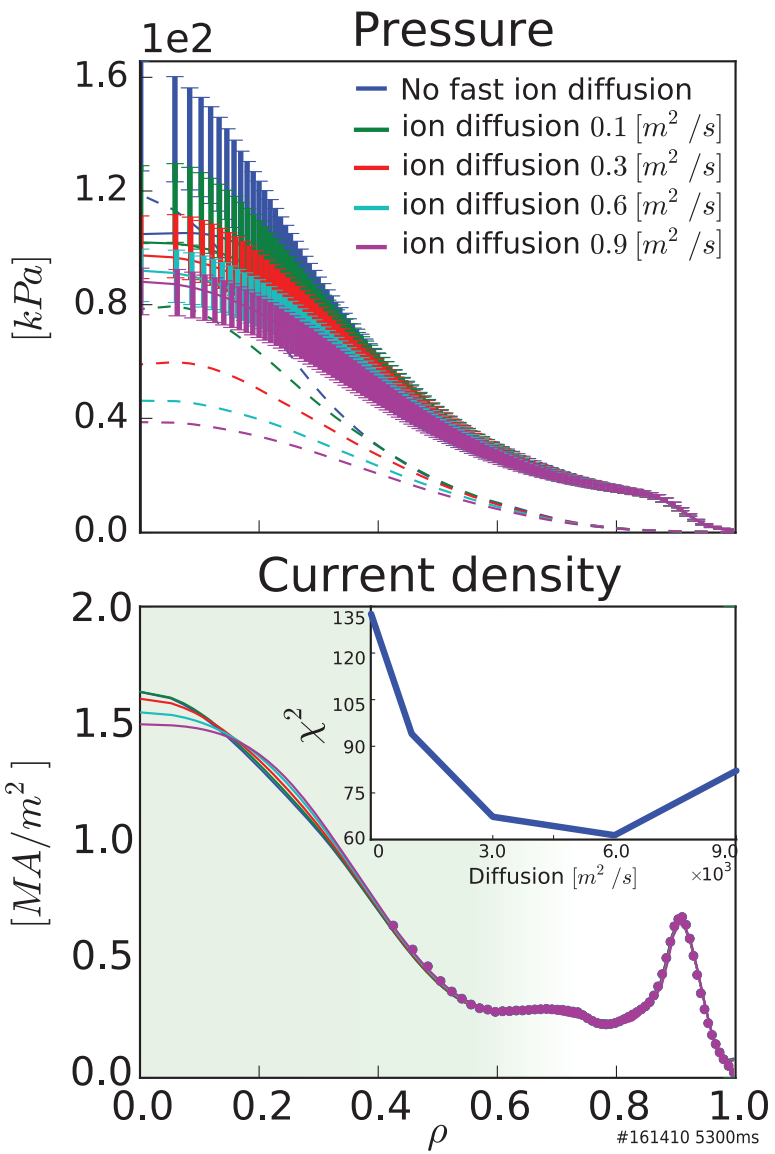
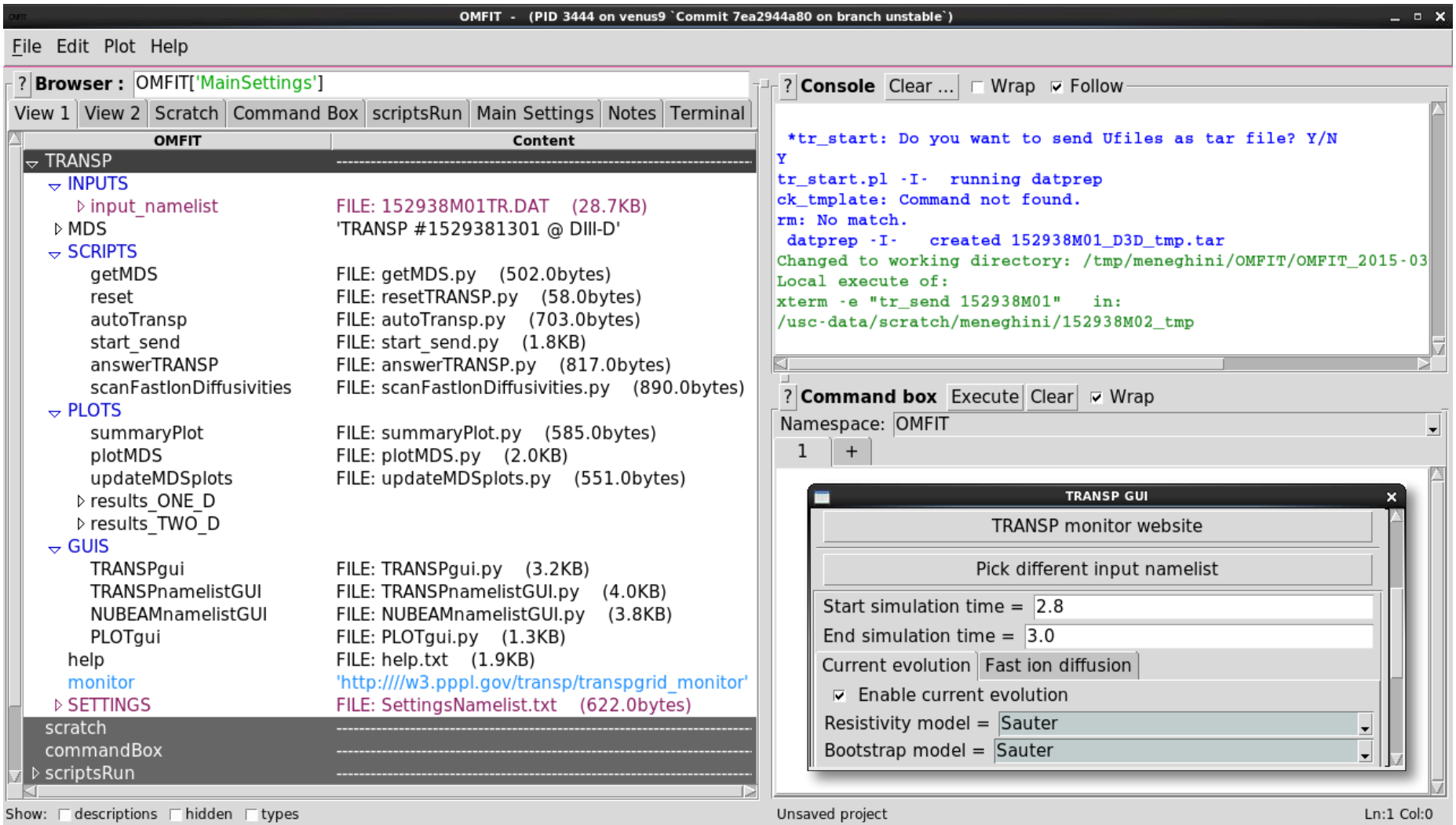




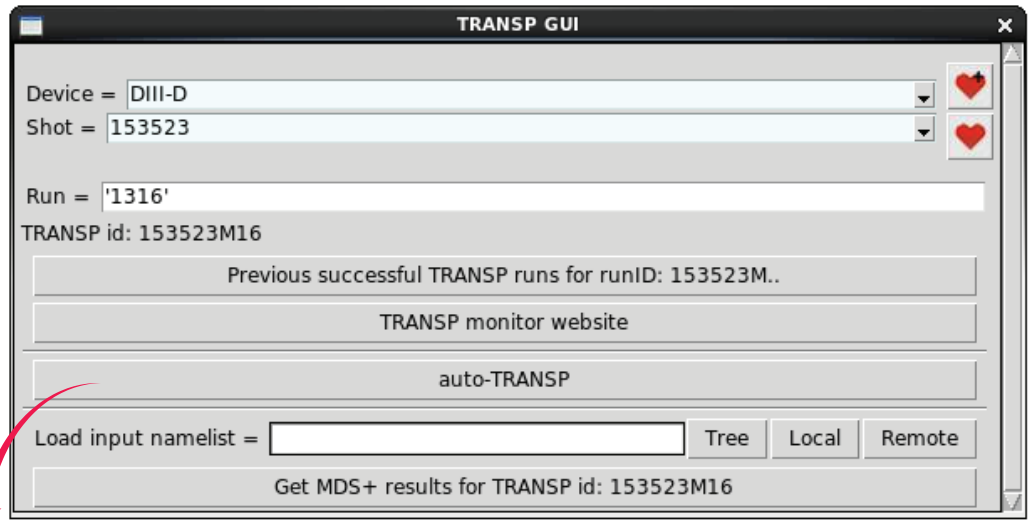
Overview of the TRANSP module in OMFIT



TRANSP module uses *auto*-TRANSP tool to setup input U-files and initial namelist

Preparing TRANSP runs is a complex problem, that is machine dependent

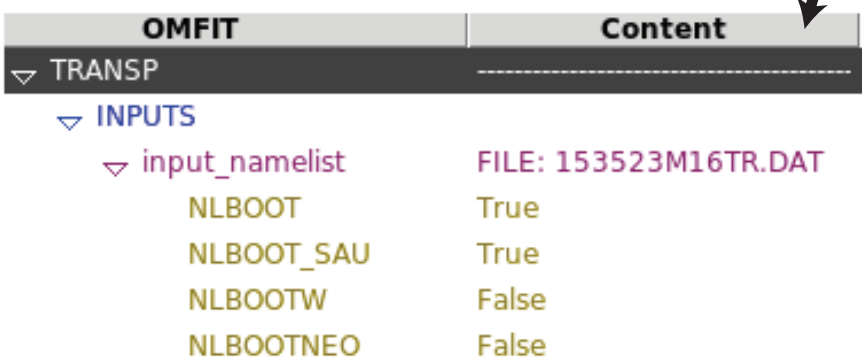
Example of how OMFIT can *"stand on the shoulders of giants"* by (remotely) executing tools that were developed over the years

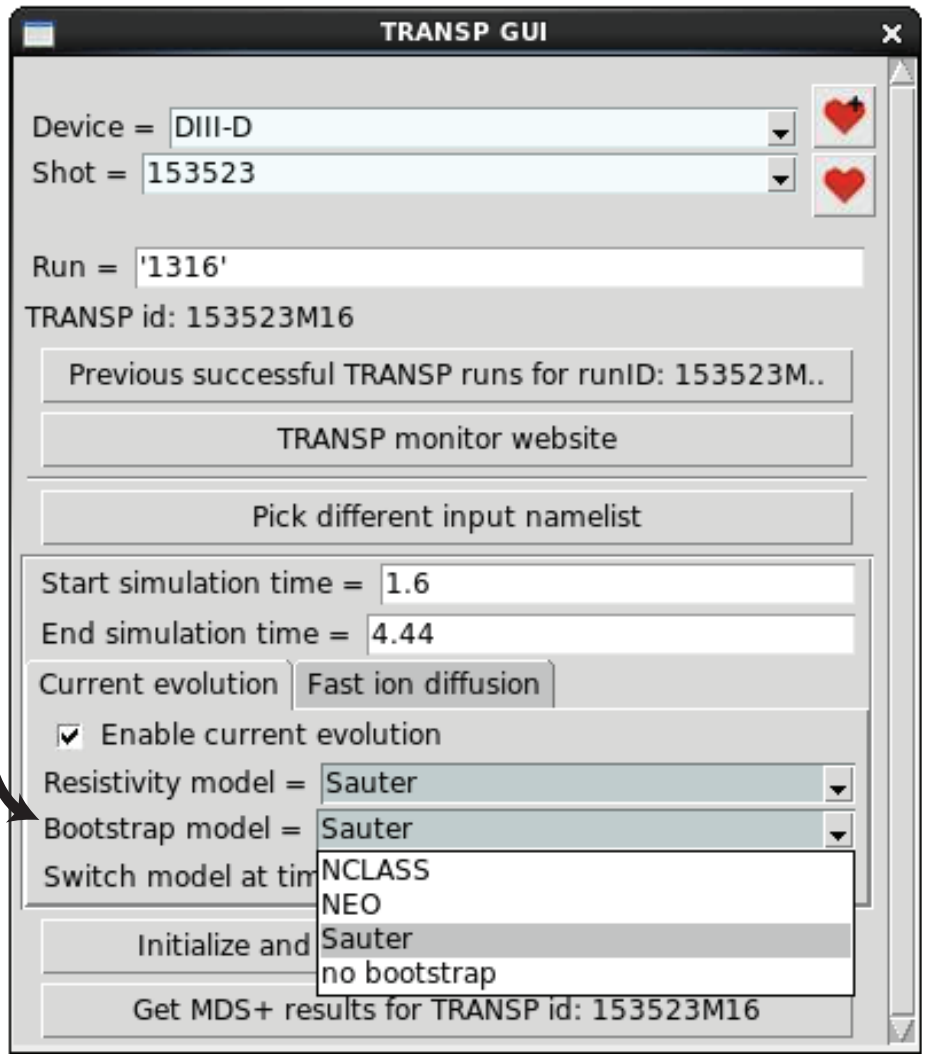


OMFIT API allows to easily build GUIs that manage the complex inter-dependencies within the TRANSP namelist

```
ComboBox(["root['INPUTS']['input_namelist']['%s']"%k for k in ['NLBOOT','NLBOOT_SAU','NLBOOTW','NLBOOTNEO']],
         {'no bootstrap':[False,False,False,False],
          'Sauter'      :[True ,True ,False,False],
          'NCLASS'      :[True ,False,True ,False],
          'NEO'         :[True ,False,False,True ]},
         'Bootstrap model')
```

e.g. set bootstrap current model

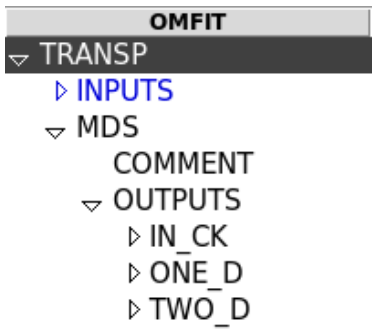


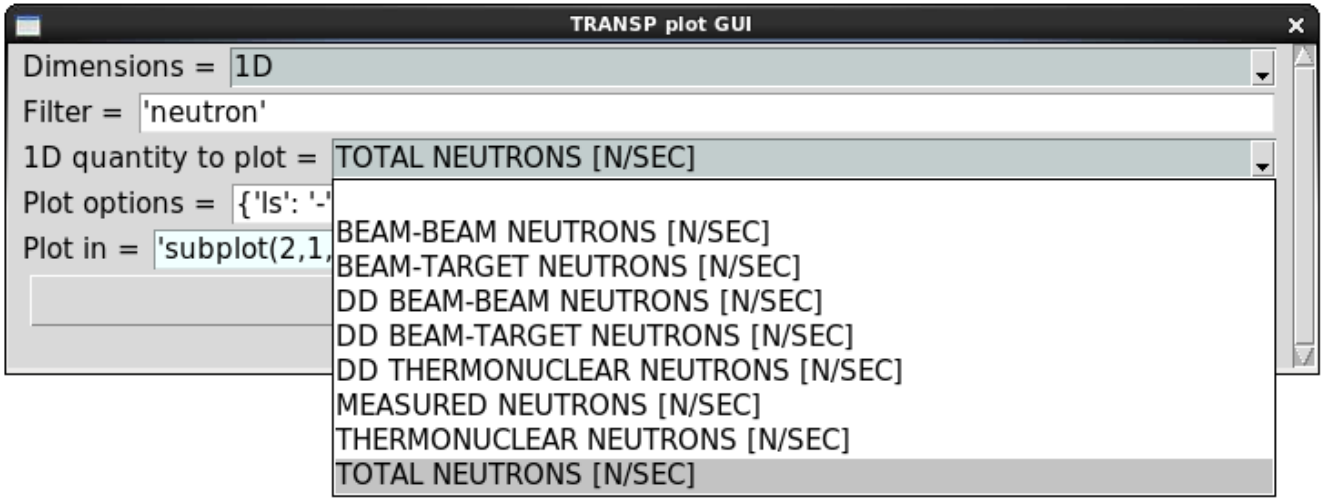


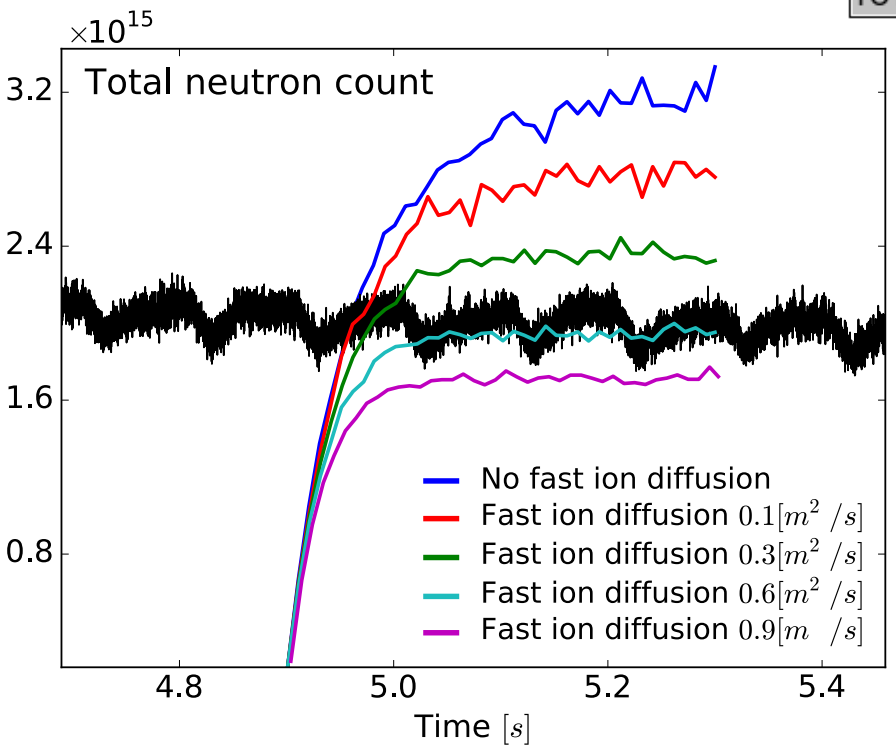
Scripting within OMFIT allows many possibilities e.g. trivial to scan fast ion diffusion

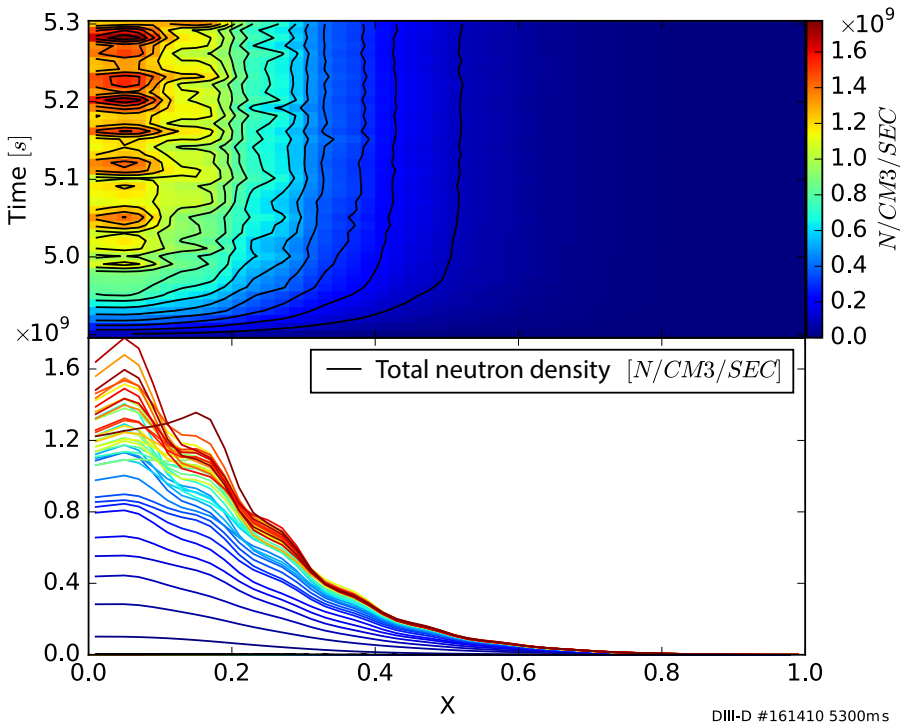
```
starting_runID=2
diffusivities=[1000,3000,6000,9000]
for k,diffusivity in enumerate(diffusivities):
    comment='fast ion diffusion %e cm**2/s'%diffusivity

    root['SETTINGS']['PHYSICS']['runID']='13'+'%02d'%(starting_runID+k)

    root['INPUTS']['input_namelist']['NMDIFB']=1
    root['INPUTS']['input_namelist']['BDIFB']=diffusivity
    root['INPUTS']['input_namelist']['CDIFB']=diffusivity

    root['SCRIPTS']['start_send'].run(send=True,
                                      interactive=False,
                                      comment=comment)
```

OMFIT can post-process results from TRANSP jobs both for plotting or use as part of a workflow



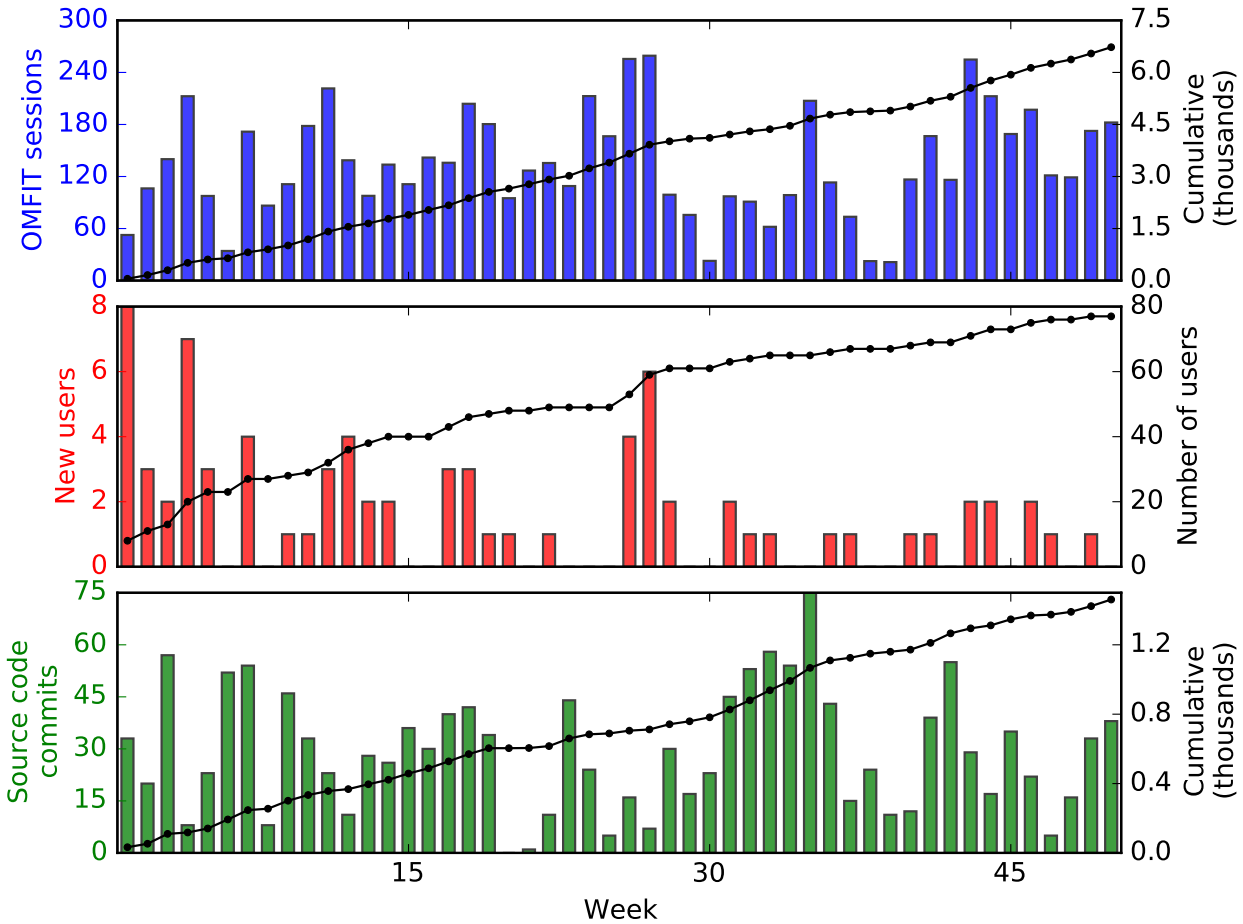






Outline

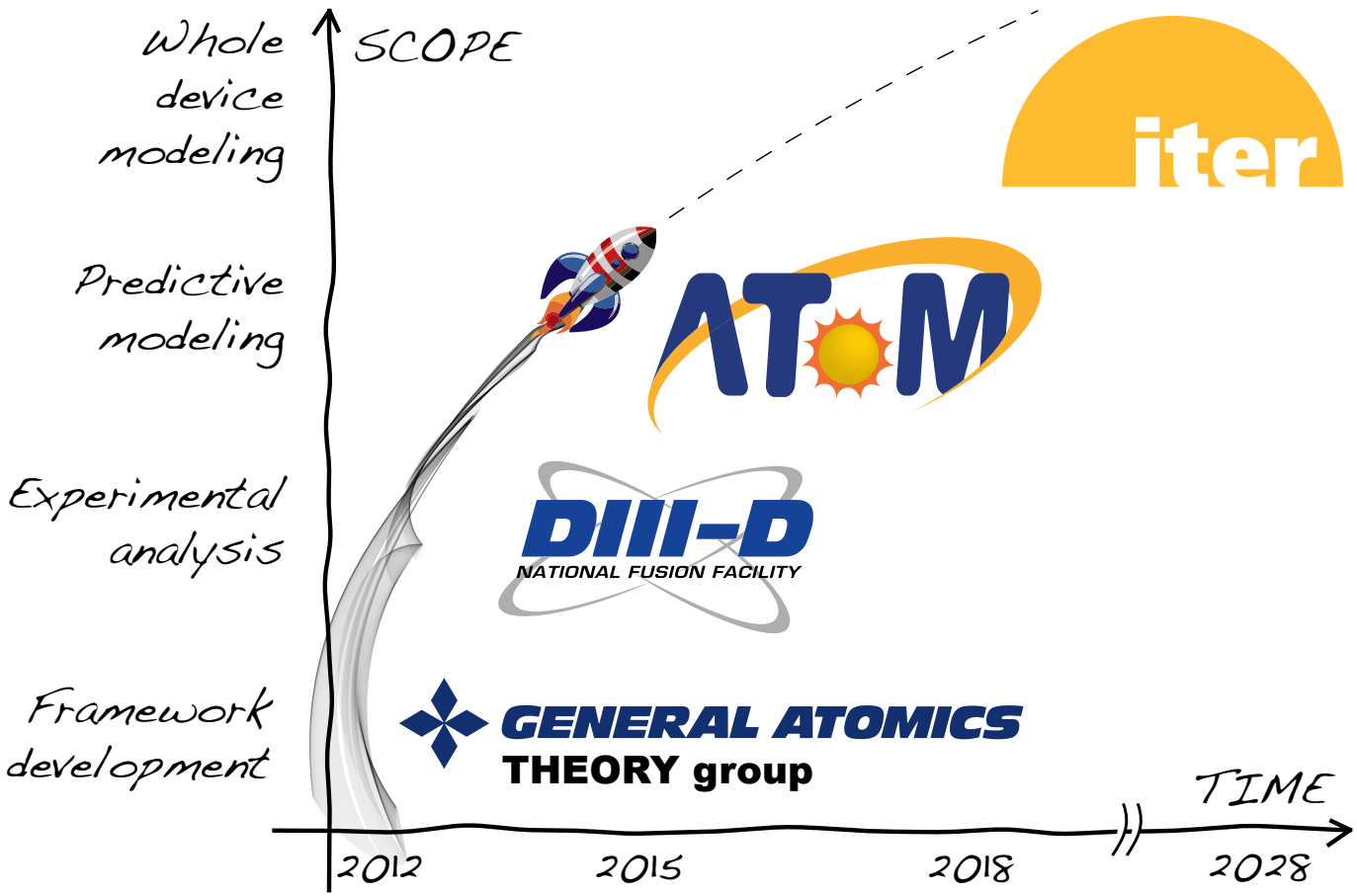
OMFIT is a vibrant project, actively used by many researchers, for a broad range of applications



- Kinetic equilibrium reconstruction
- Core stability calculations
- Edge stability diagrams
- Self-consistent steady state transport simulations
- Neoclassical theory validation
- Validation of Sauter Vs kinetic neoclassical
- Divertor design
- Helicon wave system design
- Magnetic flutter theory validation
- Neoclassical toroidal viscosity theory validation
- Building of neural network transport models
- Self-consistent study of interaction between NTM and ITG
- Experimental data analysis for transport and 3D fields
- ...

Future perspectives

- Continue *"to enhance and extend present modeling capabilities, by supporting, leveraging, and integrating existing research"*, with the aim of boosting a **bottom-up** integrated modeling vision



Future perspectives

- Continue *"to enhance and extend present modeling capabilities, by supporting, leveraging, and integrating existing research"*, with the aim of boosting a **bottom-up** integrated modeling vision

- Self-consistent core-edge modeling
  - Validate TGYRO-EPED workflow for more DIII-D discharges
  - For ITER, optimize fusion performance as a function of pedestal density and other key parameters
  - AToM plans to extend model beyond the separatrix with COGENT

- TRANSP-OMFIT integration
  - OMFIT provides a convenient interface to user, experimental data, and codes outside of TRANSP
  - No changes required to TRANSP or user workflows
  - Experiments using TRANSP could use OMFIT to generate their kinetic equilibrium reconstructions
  - Additional interesting applications: e.g. OMFIT driving TRANSP runs to minimize a cost function (optimize current profile, fusion power, ...)