Neural-network accelerated core-pedestal coupled simulations, and applications to ITER

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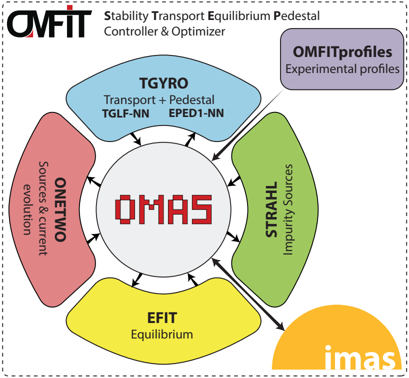


Transport Task Force
March 18-21, 2019

GENERAL ATOMICS

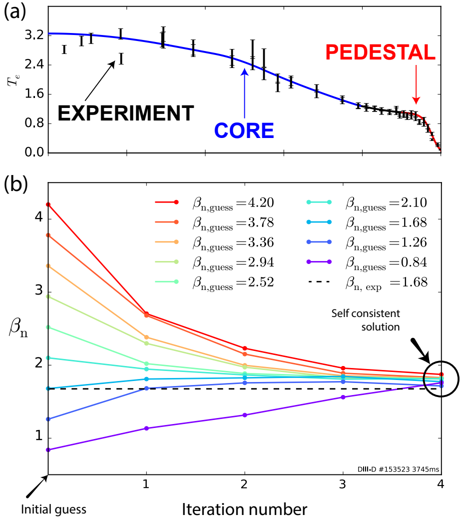
ATOM

Past core-pedestal coupled simulations developed within OMFIT assumed impurity profile to be know

O. Meneghini et al. NF 2017:

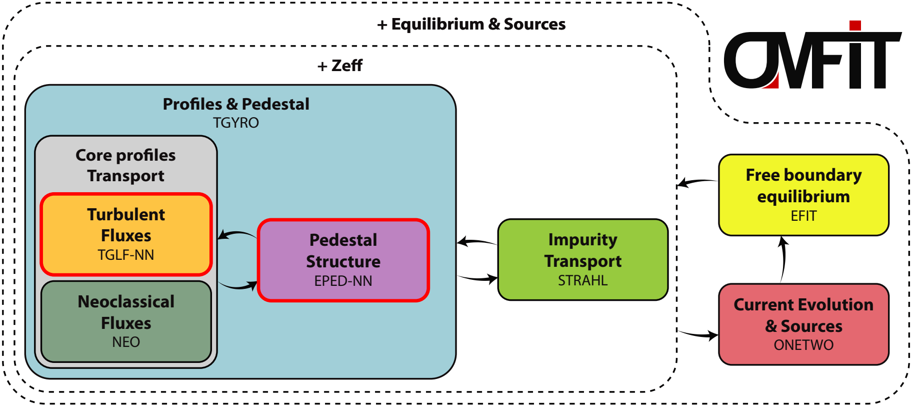
- Iterative workflow to couple core-pedestal solutions
- Speedup process by millions with neural networks
- Robustly finds self-consistent solution without pedestal height/width as free parameters
- **...BUT:** Z_{eff} profile was assumed to be know

In this work, we lift this assumption, an **allow for self-consistent transport of impurities**



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

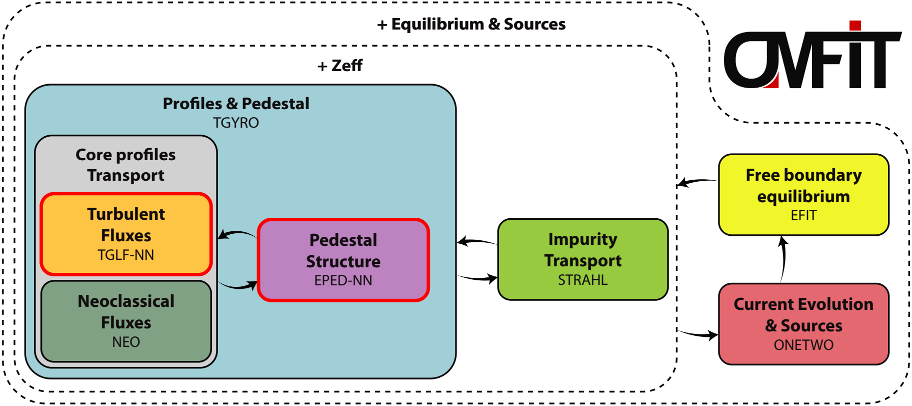
- Three nested self-consistency loops
  - core profiles **+** pedestal **+** impurities **+** equilibrium & sources
- Used NN models to speedup the most critical bottlenecks
- Compatible with ITER IMAS data structure (leveraging OMAS)



GENERAL ATOMICS

Used neural network models EPED1-NN and TGLF-NN to speedup the most critical bottlenecks in the workflow

- EPED1 pedestal model $\sim$20 CPU/h $\rightarrow$ EPED1-NN $\sim$ms
  - EPED1-NN pedestal coupling moved within core-profiles calculation
- TGLF transport model called 1000 $\times$ $\sim$10 CPU/s $\rightarrow$ TGLF-NN $\sim$ms
  - TGLF-NN embedded as part of orginal TGLF code



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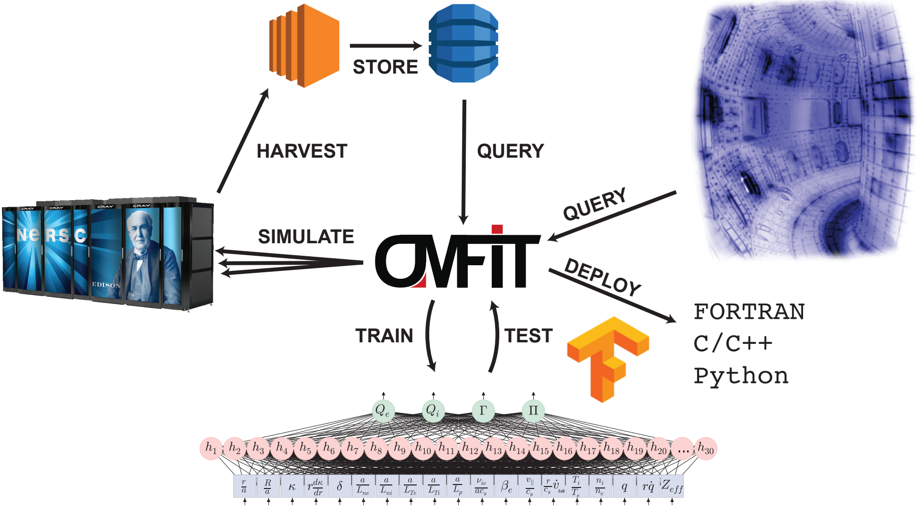
OMFIT provides a convenient environment to support machine learning applications



OMFIT module 'BRAINFUSE' gathers data, trains, tests and deploys neural network for multiple applications

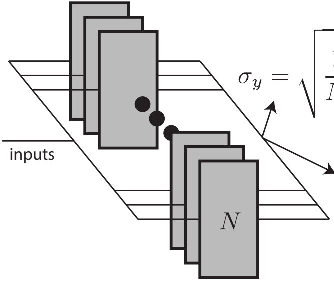
Three main domains:

1 Pedestal
- **EPED1-NN**
- **RMPED-NN**

2 Transport fluxes
- **TGLF-NN**

3 Bootstrap current
- **NEOjbs-NN**

- Regularization to avoid over-training
- Ensemble of NNs used to estimate the error in NN models prediction
  - random NN initialization
  - each NN trained on a subset of the training DB (k-fold)



$$\sigma_y = \sqrt{\frac{1}{N}\sum_i^N (y_i - \bar{y})^2}$$

$$\bar{y} = \frac{1}{N}\sum_i^N$$

EPED1-NN to predict pedestal structure for H and Super-H mode plasma regimes

Trained to reproduce results of **IPS-EPED1** model

10 input parameters to predict **12** outputs:

1. **normal H mode** solution
2. **Super-H mode** solution

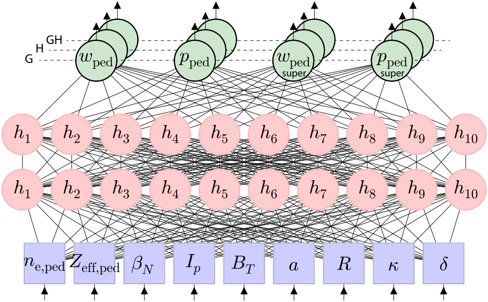
H and Super-H set to be equal when there is only one root

Extended NN model so that each root is evaluated for 3 different diamagnetic stabilization models:

G $\gamma/\omega_A > 0.03$

H $\gamma/(\omega^\star/2) > 1$

GH $\gamma^2/(\omega_A\omega^\star/2) > 0.03$



EPED1-NN model closely reproduces EPED1 predictions
Trained across input parameter range of multiple devices

Built database of $\sim$20,000 EPED1 runs (2 million CPU hours)

DIII-D: 3,000 runs

KSTAR: 700 runs

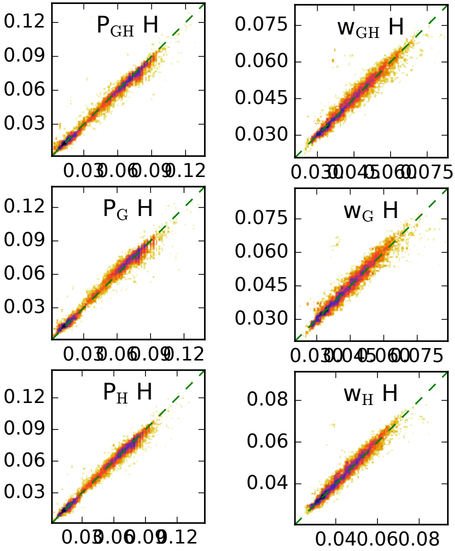
JET: 200 runs

ITER: 15,000 runs

CFETR: 1,200 runs

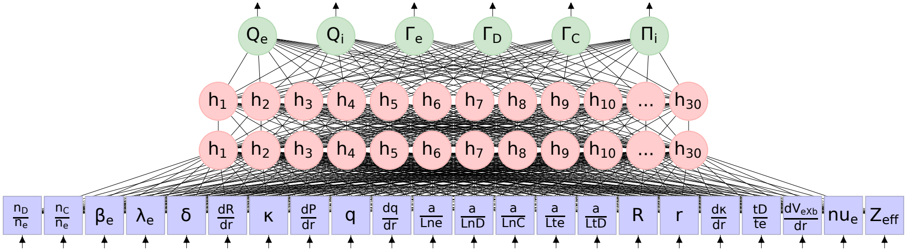
Same EPED1 runs reprocessed with different diamagnetic stabilization rules

$\times 10^9$ **speedup**



TGLF-NN predicts core turbulent fluxes

Trained to reproduce results of **TGLF** model
NOTE: TGLF is itself a reduced model of gyrokinetic simulations



For 2 ion species plasma (eg. Deuterium & Carbon for DIII-D):

- 23 dimensionless input parameters
- to predict 6 gyro-Bohm fluxes $Q_e, Q_i, \Gamma_e, \Gamma_D, \Gamma_C, \Pi_i$

+2 inputs and +1 output for every additional ion species:

- 25 inputs, 7 outputs for DT, He4, Ne plasma (eg. ITER)

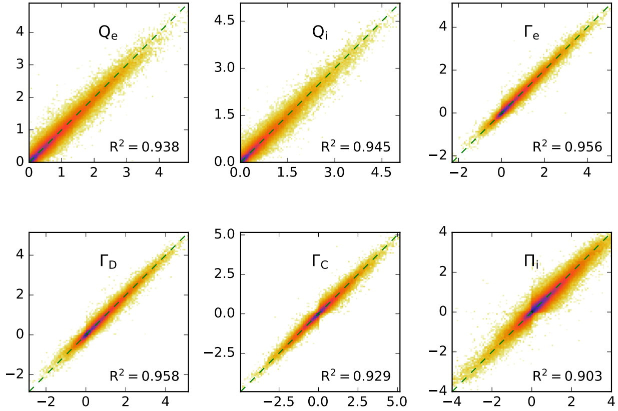
TGLF-NN model closely reproduces TGLF predictions

Training data generated making random variations around points of interest

DIII-D: 1M runs

ITER: 500k runs

$\times 10^5$ **speedup**



GENERAL ATOMICS

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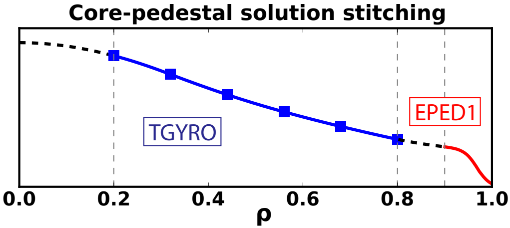
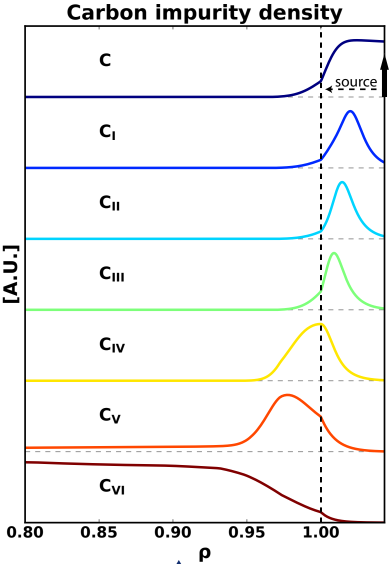
Self-consistent impurity transport done with STRAHL





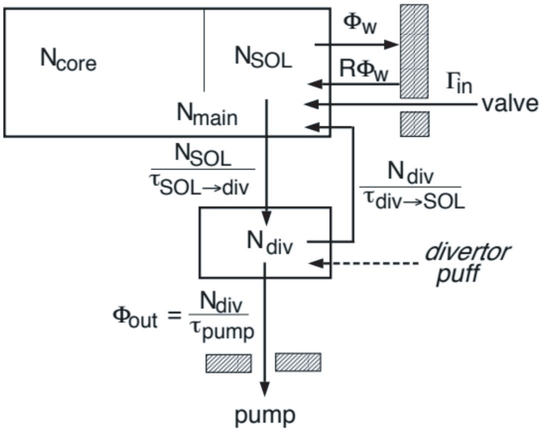
STRAHL is a 1D impurity transport code:

- IN Influx of neutral species (rate and energy)
- IN Transport coefficients
- IN Background plasma density and temperature
- OUT Profiles for each ionized state of the impurity

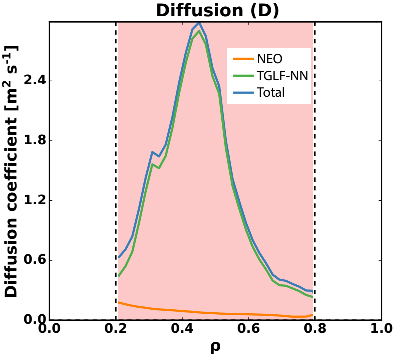
For the purpose of core impurity transport we are not focusing on physics of the divertor chamber in STRAHL

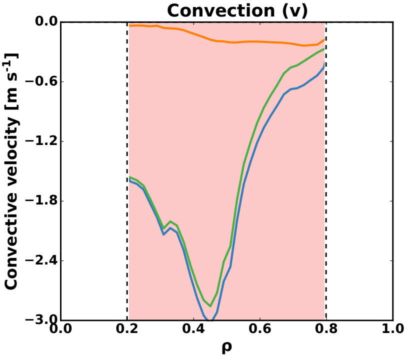
- Set artificially short SOL/divertor/pump confinement times for simulations to reach steady-state fast
- **Neutrals source scaled** to match Z_{eff} at one radial location, or total plasma impurity particle content
- **STRAHL uses a diffusive and convective transport ansatz:**

$$\Gamma_I = -D\frac{\partial n_I}{\partial r} + v\, n_I$$



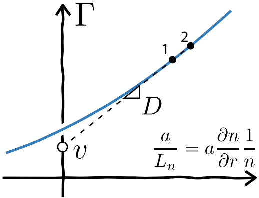
Diffusion and convection coefficients for impurity transport CORE region:





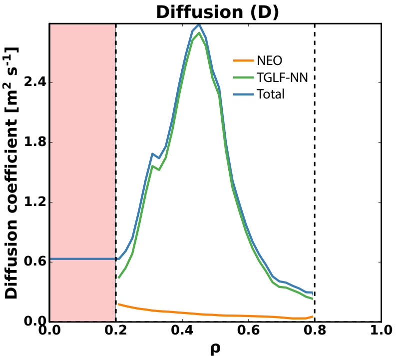
In the core D and v can be calculated from TGLF(-NN) and NEO fluxes:

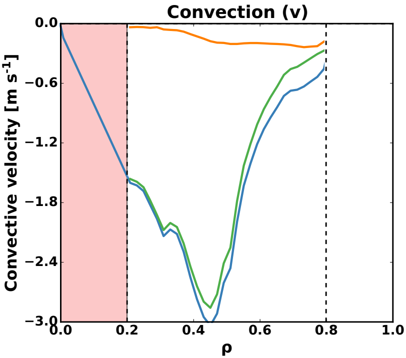
$$D = \frac{\Gamma_1\, n_2 - \Gamma_2\, n_1}{n_2'\, n_1 - n_1'\, n_2} \qquad v = \frac{\Gamma_1\, n_2' - \Gamma_2\, n_1'}{n_2'\, n_1 - n_1'\, n_2}$$



GENERAL ATOMICS

Diffusion and convection coefficients for impurity transport AXIS region:



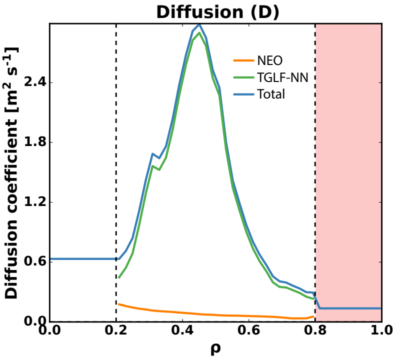


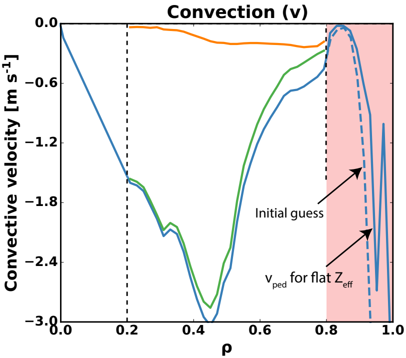
Near the axis impurity particle source is zero, thus in stationary regime:

$$\frac{\partial n_I}{\partial r}\frac{1}{n_I} = \frac{v}{D}$$

- Fix $D_{axis} = D|_{\rho=0.2}$
- Set v_{axis} such that v_{axis}/D_{axis} linearly goes to zero at $\rho = 0$

Diffusion and convection coefficients for impurity transport PEDESTAL region:

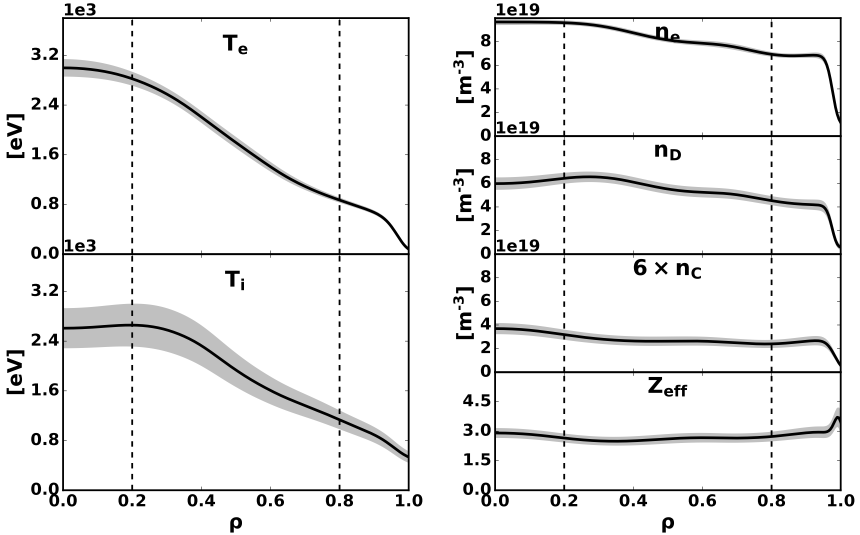




Alignment of impurity, main ion and electron density profiles (ie. flat Z_{eff}) is a reasonable physical constraint for the pedestal region

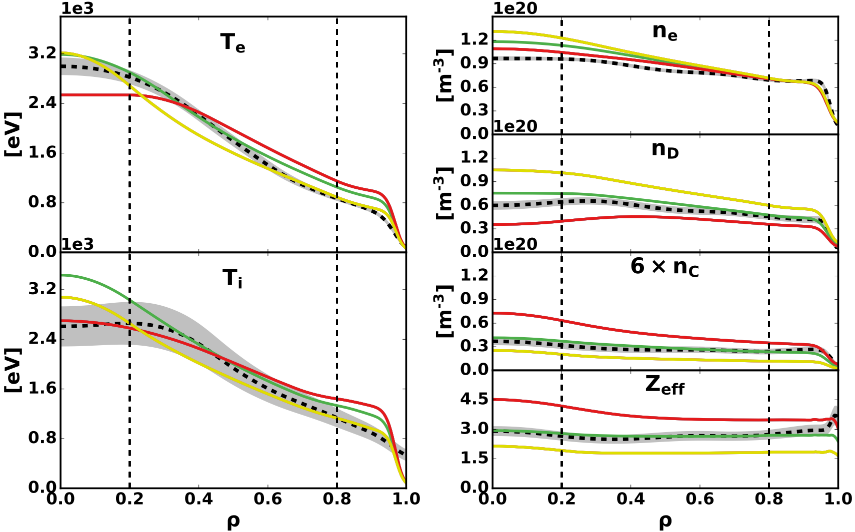
- Fix $D_{axis} = D|_{\rho=0.8}$
- Initial guess $v_{ped} = \frac{\partial n_e}{\partial r}\frac{1}{n_e} D_{ped}$ (inexact because sources are not zero)
- Iteratively run STRAHL and find v_{ped} so that $Z_{ped} = Z|_{\rho=0.8}$

Benchmark case: DIII-D H-mode discharge 168830



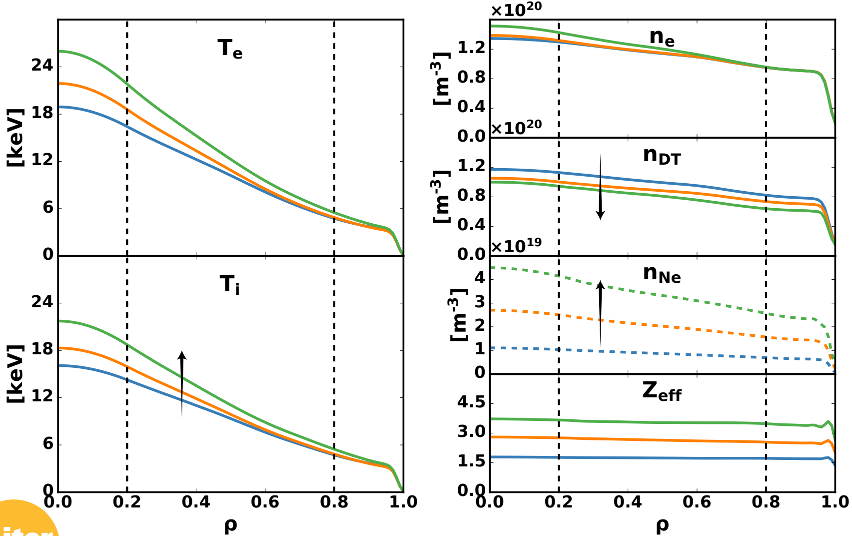
GENERAL ATOMICS

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



GENERAL ATOMICS

Initial ITER simulations show small dependency of Q on Z_{eff}: increased Z_{eff} benefits pedestal but adds to core dilution



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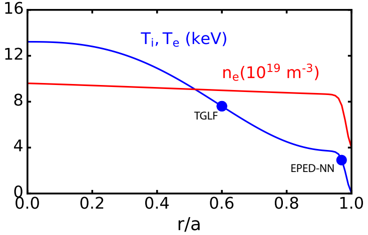
Minimal theory predictive model
0D $\rightarrow$ 1D profiles by assuming known functional form

J.McClenaghan APS 2018

- **Pedestal profiles** from EPED-NN prediction
- **Core profiles** from TGLF(-NN) prediction at one radial location
  - T_e(r=0), T_i(r=0) iterated until flux matched at r/a=0.6
- **Equilibrium** and **sources** based on input global parameters
  - R, a, B_T, I_p, $n_{e,ped}$, P_{aux}, κ, δ, q_0, Z_{eff}



$$T_e(r) = Te,ped + (T_{e,0} - T_{e,ped}\left(1 + (r/a)^{2.6}\right)^{2.6}$$

$$n_e(r) = ne,ped + (n_{e,0} - n_{e,ped}\left(1 + (r/a)^{1.1}\right)^{1.1}$$

$$Z_{eff} = \text{const}$$

$$\omega_0 = 0$$

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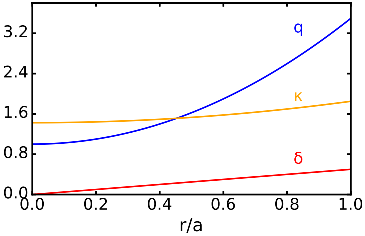

$$q = q_0 + (q_{95} - q_0) r^2$$

$$q_{95} = \frac{5a^2 BS}{RI_p}$$

$$k = k_0 + (k_s - k_0) r^2$$

$$\delta = \delta_s r/a$$

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J.McClenaghan APS 2018

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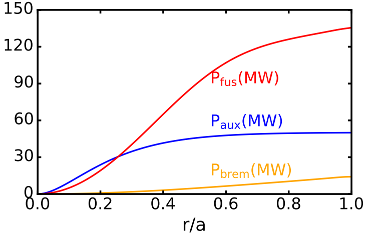

$$P_{aux} \propto \int \exp\left(-4r/a\right) dr$$

$$P_{fus} \propto \int n_i^2 r \exp\left(k_0 + k1 \log(T_i) + ...\right) dr$$

$$P_{brem} \propto Z_{eff} n_e^2 \sqrt{T_e} r dr$$

Applied model for theory-based confinement scaling Showing good agreement with ITPA experimental database

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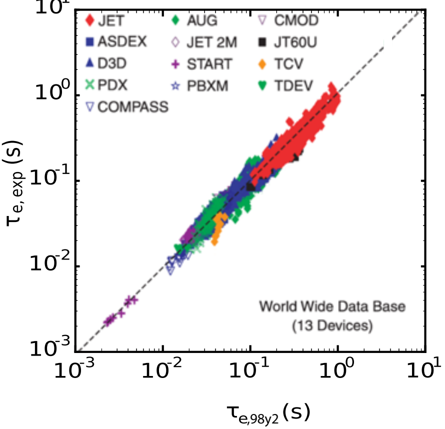
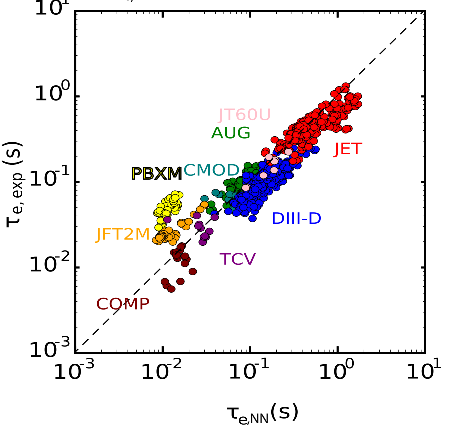
Power law fit to experimental data



$\tau_{e,NN}$ theory-based prediction



GENERAL ATOMICS

ITER prediction of theory-based model is slightly more pessimistic than $\tau_{98,y2}$ power law scaling

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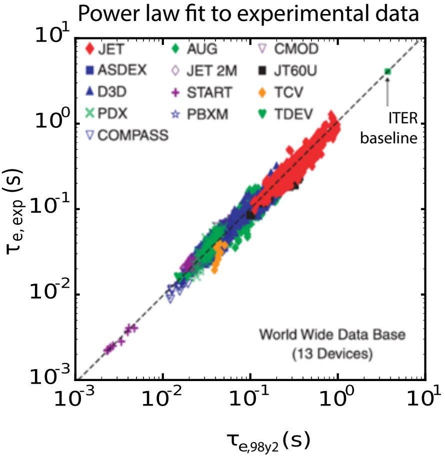

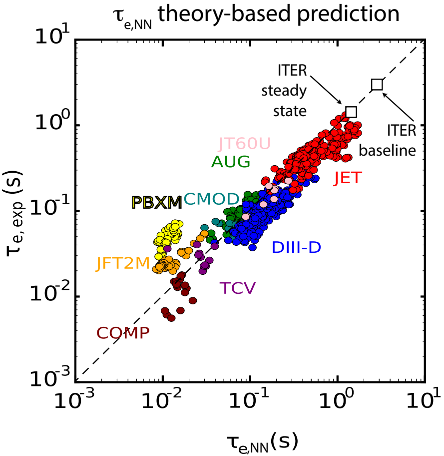

- TGLF+EPED known to be more pessimistic than $\tau_{98,y2}$ (Kinsey NF '11)
- Zero rotation and D-C TGLF-NN also more to pessimistic

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EPED-NN and TGLF-NN accelerated models enable rapid core-pedestal coupled predictions, both applied to ITER

1. Predictive simulations with self-consistent transport of impurities
   - STEP module in OMFIT, which leverages OMAS to combine codes (“*steps*“) in arbitrary workflows
   - Novel coupling strategy for impurity transport

2. Machine confinement scaling with minimal theory-based model
   - Good agreement with ITPA experimental database

Going forward:

- Apply higher fidelity predictive workflow to ITPA database
- Improve minimal theory-based predictive model to include rotation and DT-He4-Ne