Experimental Inference of Particle Transport in Tokamak Plasmas

F. Sciortino

MIT Department of Physics
Plasma Science & Fusion Center

Ph.D. Defense

sciortino@psfc.mit.edu

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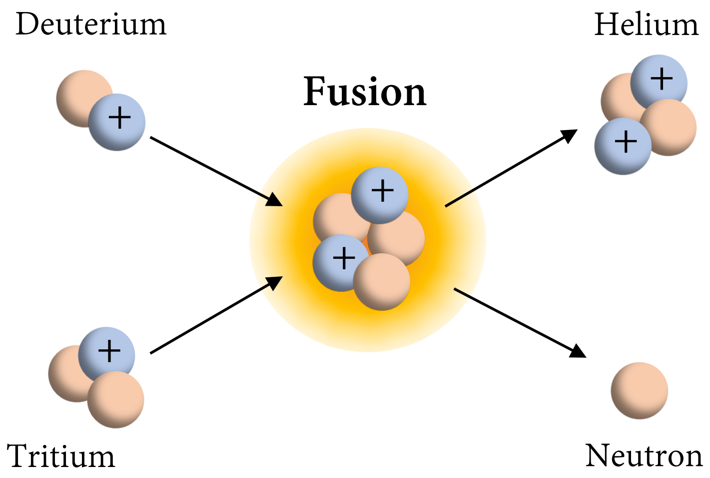
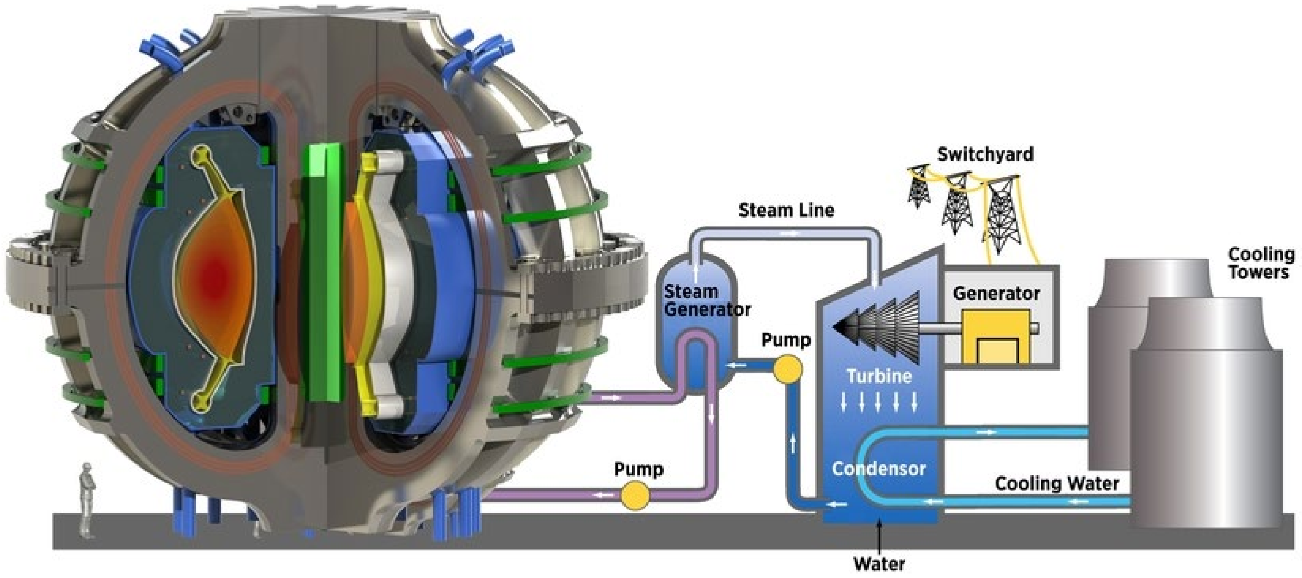
Fusion energy and plasma physics

- Fusion energy could be key to fulfilling energy demands in a sustainable way
  - “Burns” light nuclei, releasing large amounts of energy
  - Enabling technologies must be **safe**, **clean**, **economical**

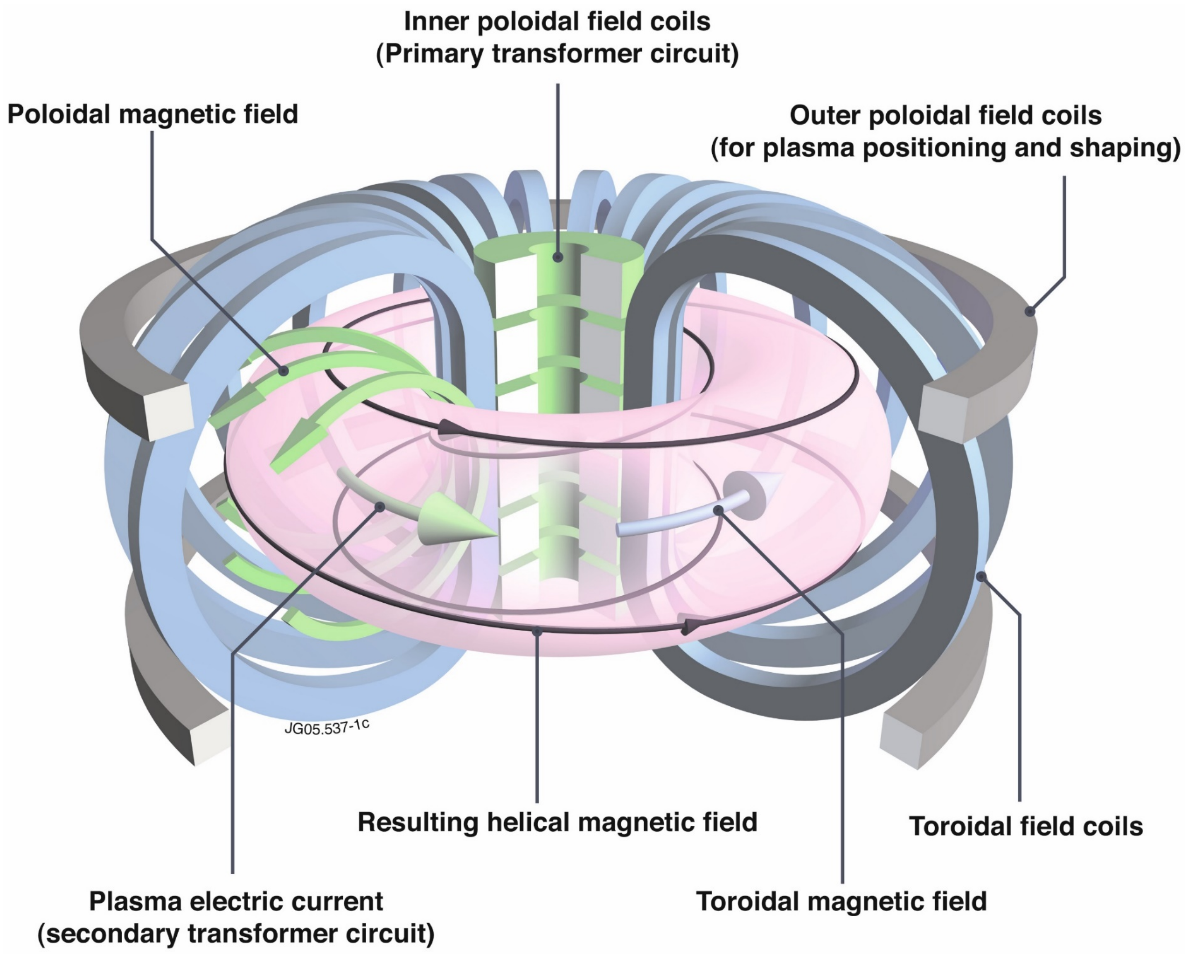




Source: Courtesy of PSFC, adapted from Wikimedia Commons

Magnetic confinement fusion & the tokamak

- Tokamaks confine hot, ionized matter (plasma) on helical magnetic field lines



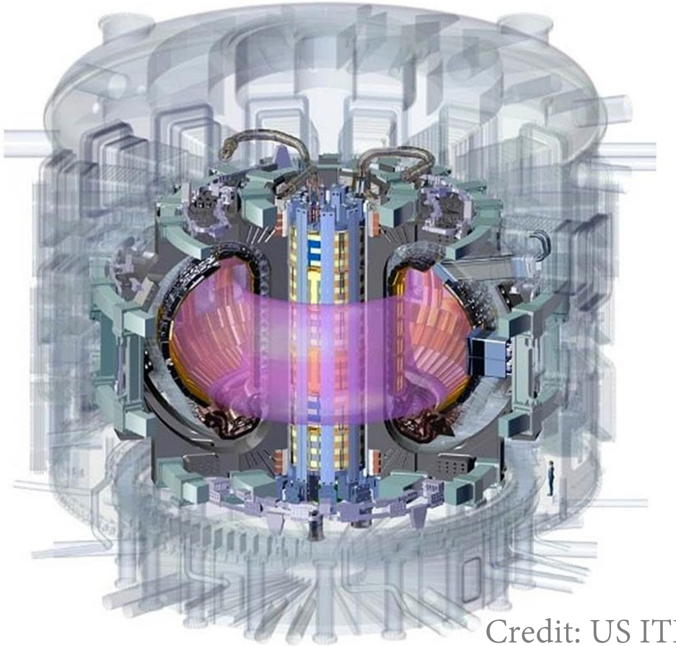
Source: EUROfusion

The future: *technology* and *scale* are leading us to breakthroughs

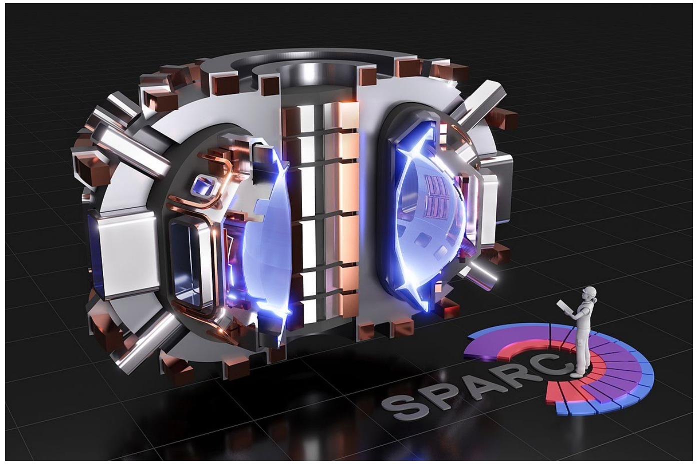
ITER & SPARC are now on their way to break-even:

$$E_{out} > E_{in}$$

- ITER is *more of everything*: an international collaboration to build the most complex device of its kind
- SPARC leverages new *high-temperature superconductors* for high-field operation at reduced scale and cost



Credit: US ITER



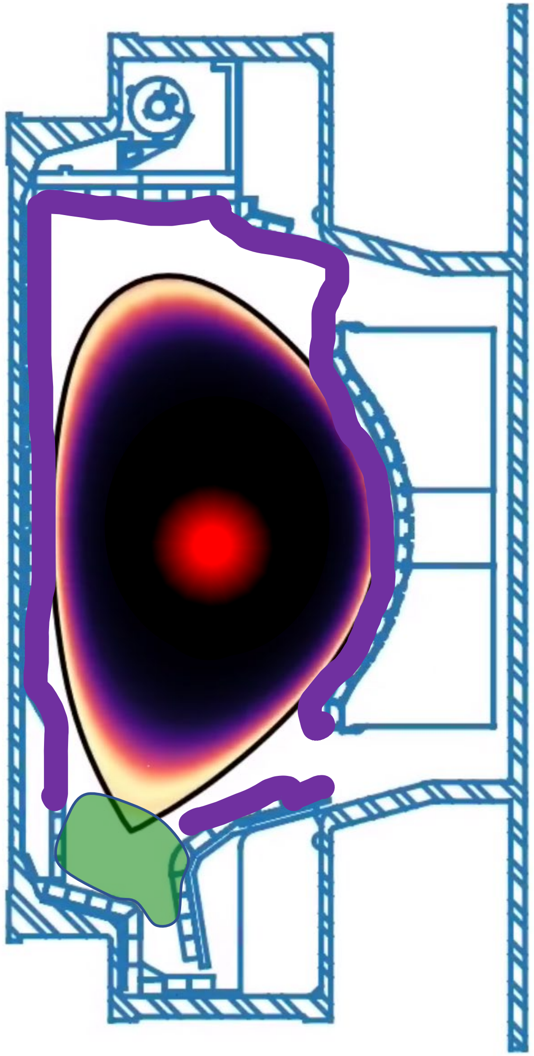
Credit: T. Henderson, CFS/MIT-PSFC

Fueling, impurities, radiation & neutrals are key to fusion performance

Performance is determined by a complex interplay of geometry, atomic and transport physics…

In this thesis, we consider the role of particle transport (*collective particle dynamics*) in determining

- Core fuel density vs. impurity accumulation
- Radiation of power
- Interactions with the device wall & neutrals



Core accumulation

Divertor radiators

Wall interactions

Main thesis contributions

1. Development of the open-source **Aurora** package for particle transport and radiation[4]

2. Quantification of the impact of **charge exchange** with background neutrals for pedestal impurity studies[4,5]

3. Creation of **HPC** frameworks for **Bayesian** inference of **experimental** particle transport coefficients[2,3,4,5,6]

4. On both Alcator C-Mod and DIII-D, contributions for **analysis of spectroscopic data**[1,2,5]

5. Comparisons of transport coefficients between **theory and experiment** for both C-Mod[2,5] and DIII-D[6]

Generally favorable theory validation; some discrepancies for flat/hollow impurity profiles

1. F. Sciortino and N. M. Cao, *IEEE Trans. Plasma Science*, vol. 48, no. 1, 2020
2. F. Sciortino et al., *Nuclear Fusion*, vol. 60, no. 12, 2020
3. F. Sciortino et al., *Review of Scientific Instruments* (invited), 92, 053508, 2021
4. F. Sciortino et al., *submitted to Plasma Physics & Controlled Fusion*, 2021
5. F. Sciortino et al., *submitted to Nuclear Fusion*, 2021
6. F. Sciortino et al., *in preparation*, 2021

Contents

1. *Aurora*
2. *Charge exchange between neutrals and impurities*
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4. *Highlights from research on*
    a) *Alcator C-Mod*
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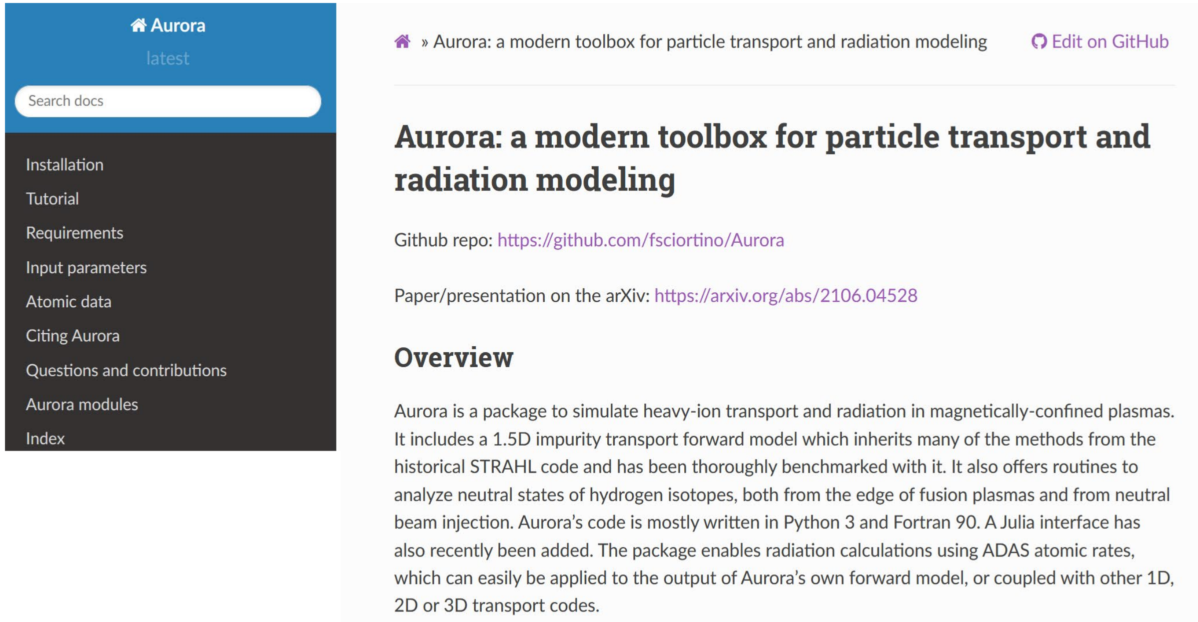
Aurora: a toolbox for impurity transport, neutrals and radiation modeling

- Initially based on the STRAHL code, used for benchmarks

- Modern high-level interface between Python, Fortran and Julia
    - Open-source : https://aurora-fusion.readthedocs.io



Aurora fresco, by Guido Reni (circa 1612-1614)

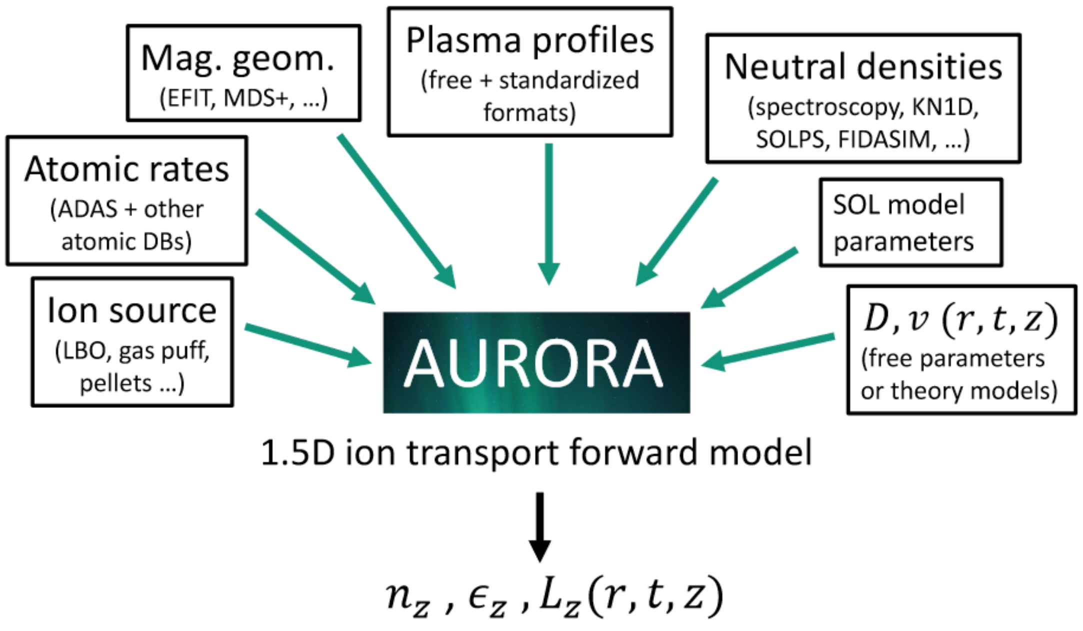
- User-friendly and flexible atomic radiation model using ADAS rates

- Impurity transport simulations
    - Efficiently parallelized when attempting to infer transport coefficients
    - Options to model ion superstages, charge exchange, arbitrary Z dependence of transport …

Aurora's forward model of particle transport

- Objective: compute spatio-temporal evolution of all charge states from a given ion source

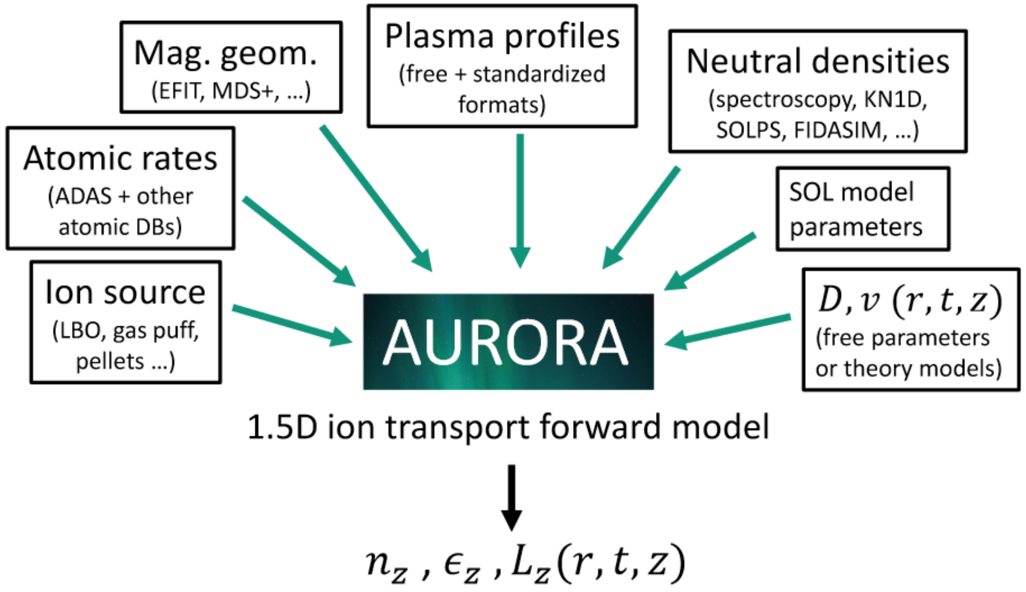
- 1.5D geometry: use 1D radial coordinate defined from (2D) flux surface volumes



n_z : charge state densities
ϵ_z : spectral line emissivities
L_z : radiated power coefficients

Sciortino et al. 2021, submitted to PPCF - https://arxiv.org/abs/2106.04528

Aurora's forward model of particle transport



- Coupled continuity equations for all ionization stages using a diffusive-convective ansatz

$$\frac{\partial n_{I,Z}}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}\overset{\text{flux}}{(r\,\Gamma_{I,Z})} + Q_{I,Z} \quad \text{atomic sources/sinks}$$

$$\Gamma_{I,Z} = -D\,\frac{\partial n_{I,Z}}{\partial t} + v\,n_{I,Z}$$

$$\begin{aligned} Q_{I,Z} = -\,&\left(n_e S_{I,Z} + n_e \alpha_{I,Z} + n_n\,\alpha^{cx}_{I,Z}\right) n_{I,Z} \\ &+ n_e S_{I,Z-1}\, n_{I,Z-1} \\ &+ \left(n_e \alpha_{I,Z+1} + n_n\,\alpha^{cx}_{I,Z+1}\right) n_{I,Z+1} \end{aligned}$$

S : ionization rate
α : radiative + dielectronic recombination rate
α^{cx} : charge exchange recombination rate
n_n : atomic background neutral density

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Charge eXchange (CX) between heavy ions and neutral particles

CX has strong impact on ionization equilibrium in the SOL, but is **often taken as negligible for core/pedestal modeling**

- *Dux et al. NF 2020* illustrated importance of this effect experimentally, but no measurements of D neutrals on AUG

$$\frac{\partial n_{I,Z}}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}\left(r\,\Gamma_{I,Z}\right) + Q_{I,Z}$$

$$\begin{aligned} Q_{I,Z} = &-\left(n_e S_{I,Z} + n_e \alpha_{I,Z} + n_n\, \alpha^{cx}_{I,Z}\right) n_{I,Z} \\ &+ n_e S_{I,Z-1}\, n_{I,Z-1} \\ &+ \left(n_e \alpha_{I,Z+1} + n_n\, \alpha^{cx}_{I,Z+1}\right) n_{I,Z+1} \end{aligned}$$

On DIII-D, D neutrals come from the tokamak edge + from Neutral Beam Injection (NBI)

On C-Mod, all D neutrals are typically from the tokamak edge

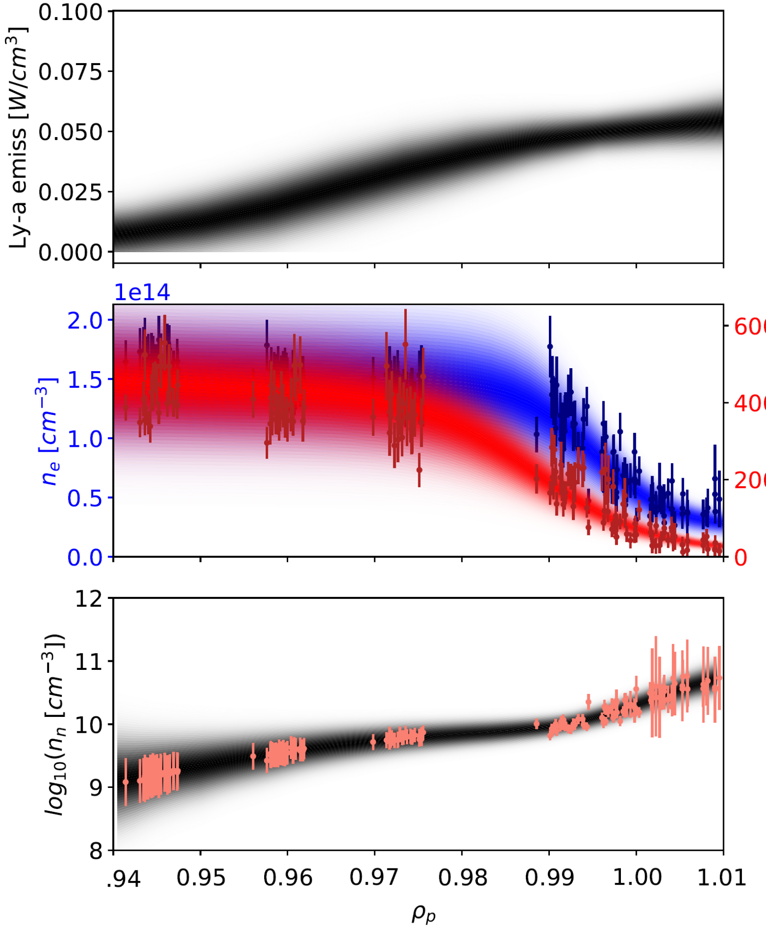
measured via a Ly_α midplane array

(H-like ion $n = 2 \rightarrow 1$ transition)

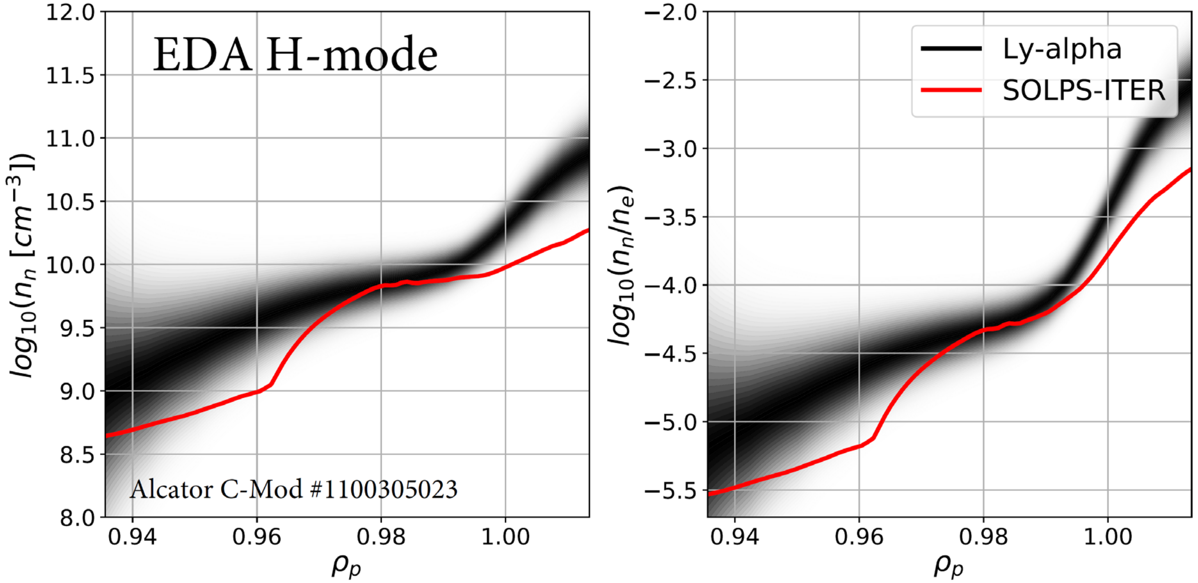
On C-Mod, we compare experimental Ly_α outer midplane signals with SOLPS-ITER

- D Ly_α brightness is Abel-inverted to obtain local emissivity

$$n_n = \frac{\varepsilon_{Ly_\alpha}}{\Delta E_{Ly_\alpha}\ n_e\ PEC_{Ly_\alpha}(n_e, T_e)}$$

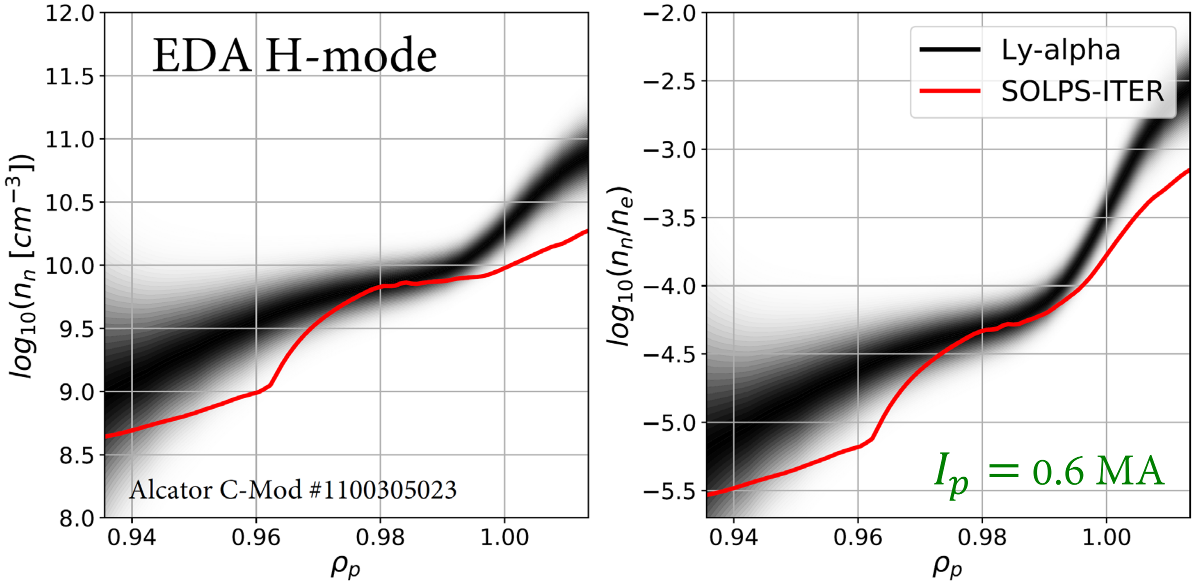


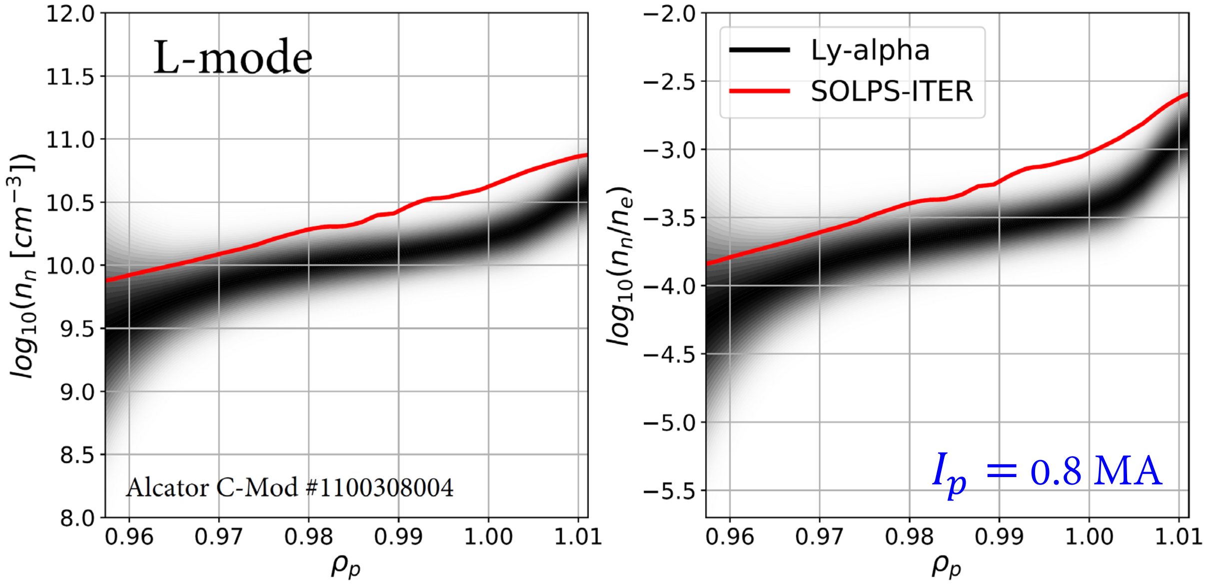
Favorable comparison to SOLPS-ITER, using the EIRENE Monte Carlo neutral model:

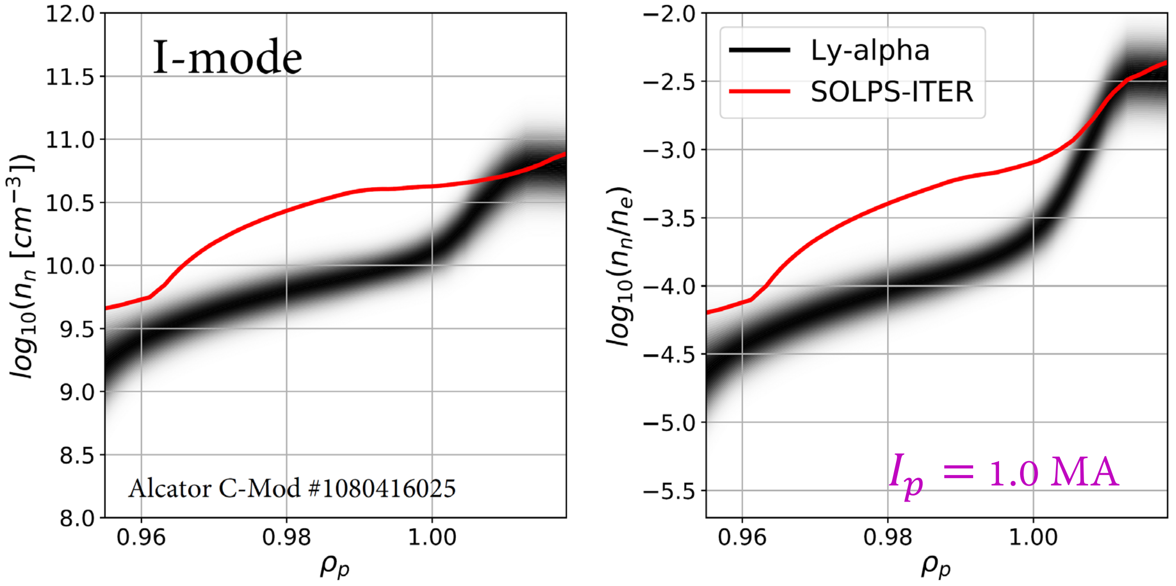


Alcator C-Mod

Good agreement between SOLPS-ITER and outer midplane Ly_α measurements



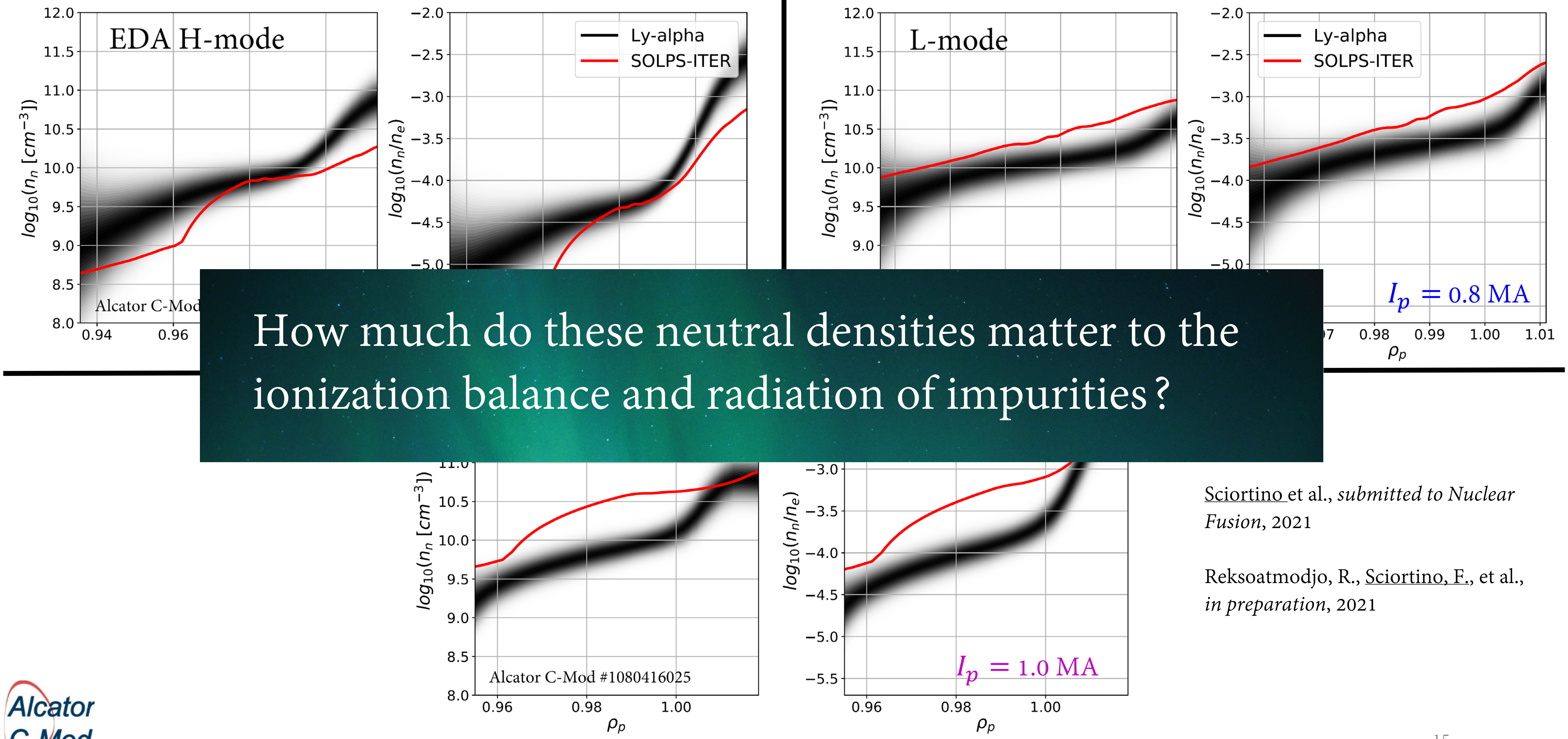




Sciortino et al., *submitted to Nuclear Fusion*, 2021

Reksoatmodjo, R., Sciortino, F., et al., *in preparation*, 2021

Good agreement between SOLPS-ITER and outer midplane Ly_α measurements



How much do these neutral densities matter to the ionization balance and radiation of impurities?

Sciortino et al., *submitted to Nuclear Fusion*, 2021

Reksoatmodjo, R., Sciortino, F., et al., *in preparation*, 2021

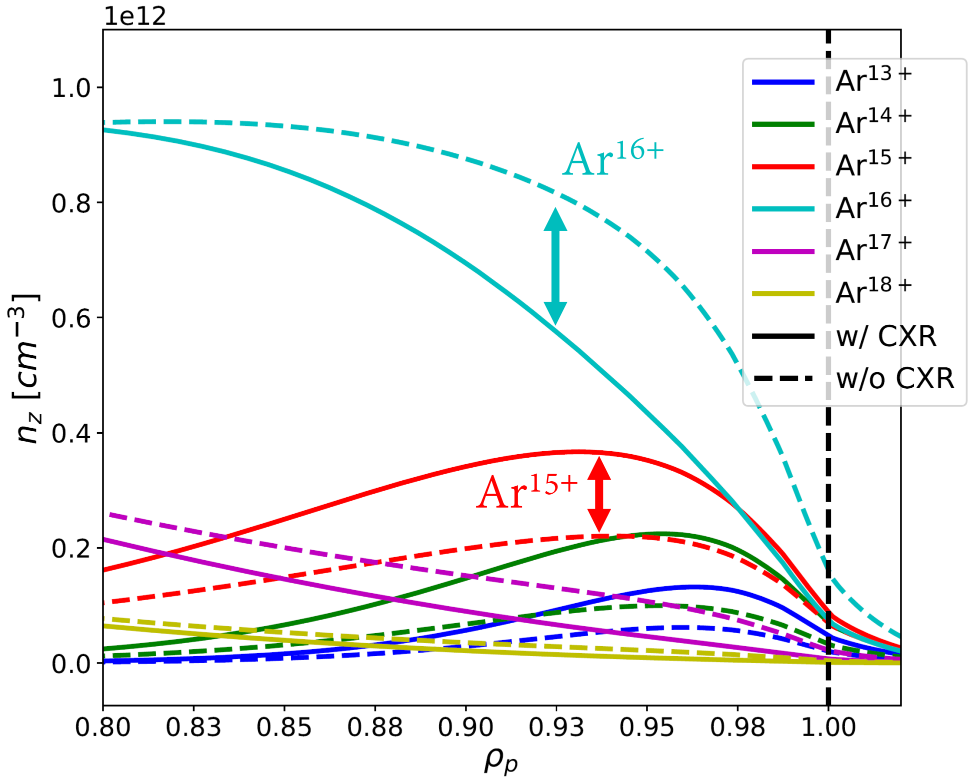
Across all regimes, edge neutrals strongly impact ionization balance and radiation

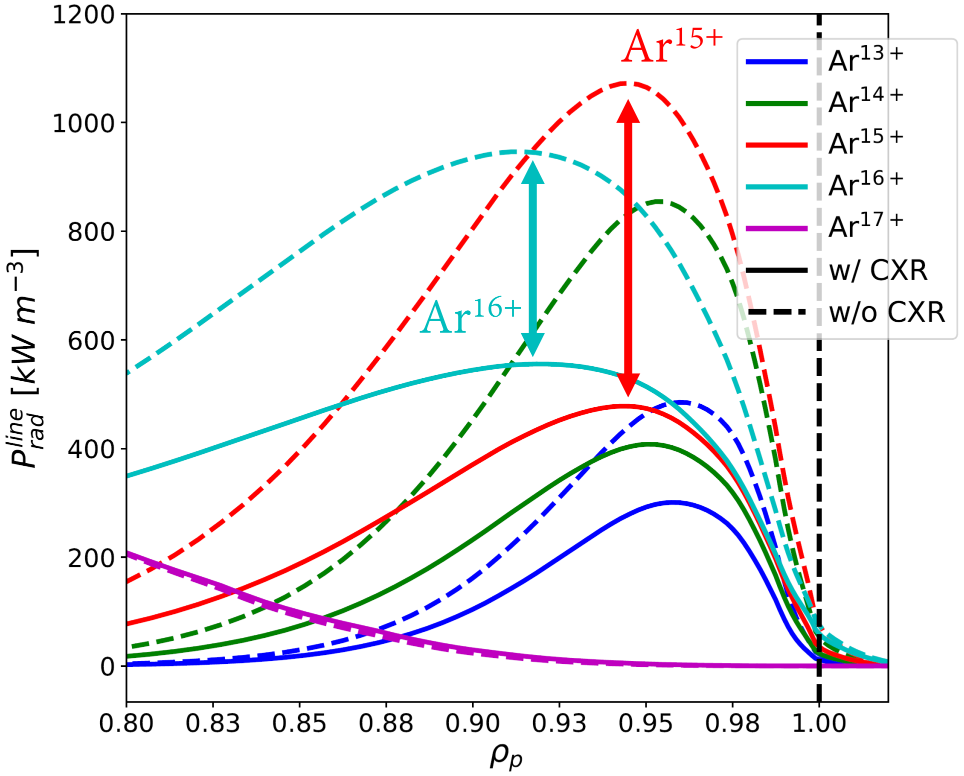
Alcator C-Mod

Identical Aurora simulations of Ar steady-state profiles, w/ and w/o CX

- Neutral densities from SOLPS-ITER/EIRENE (I-mode case)

C-Mod I-mode #1080416025





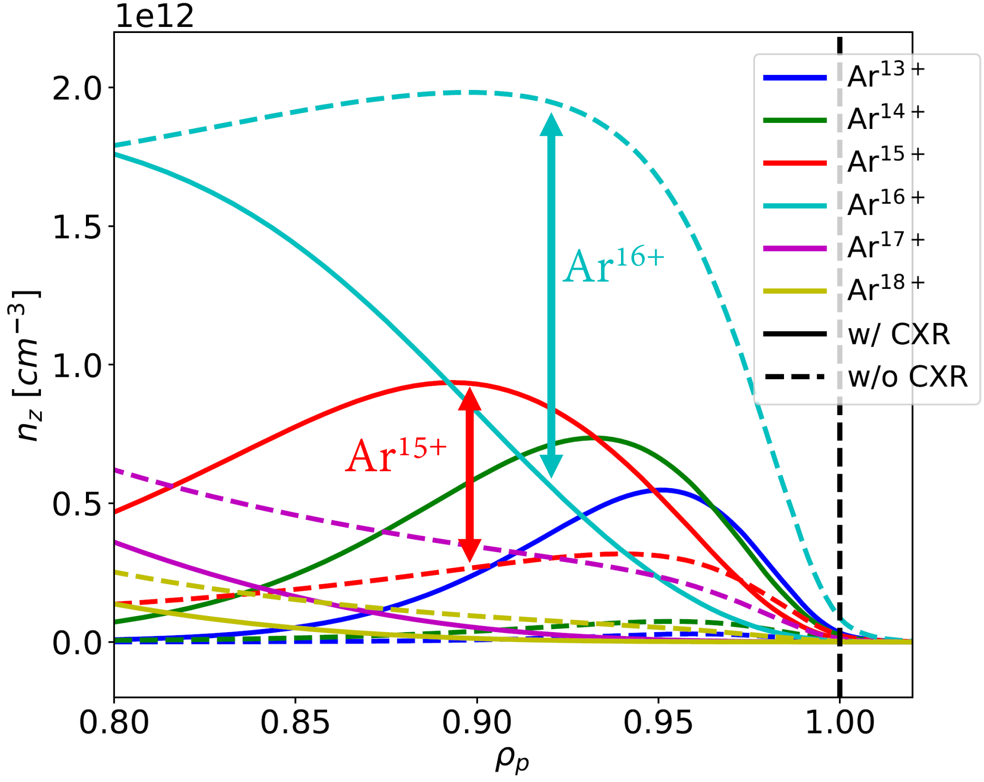
Sciortino et al., *submitted to Nucl. Fusion*, 2021

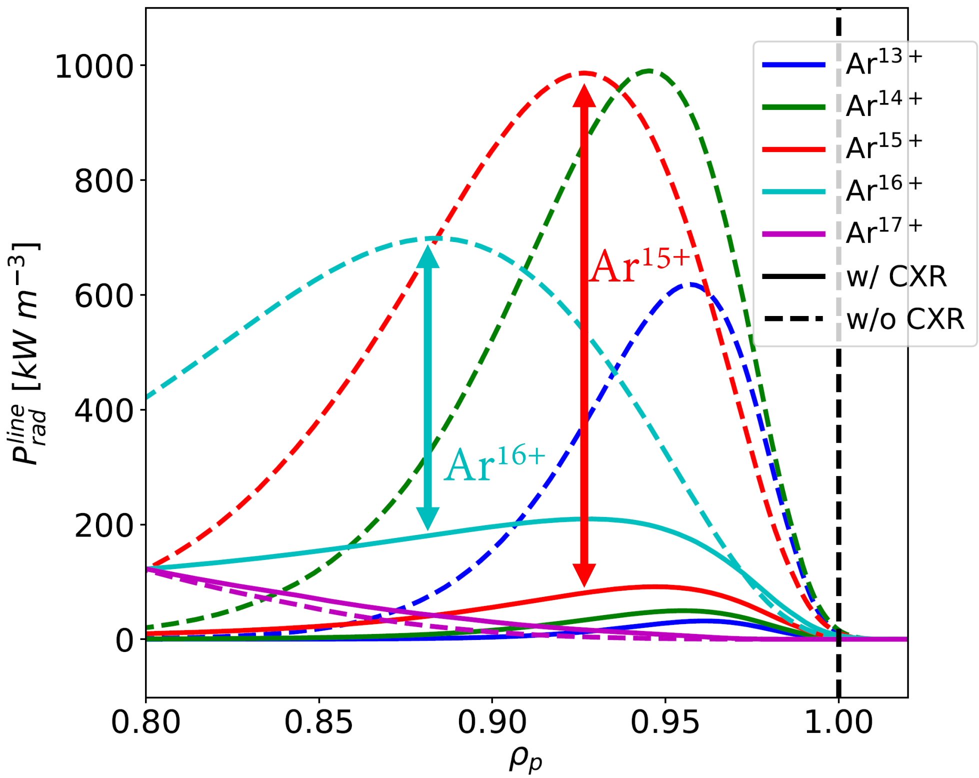
Much stronger impact of edge neutrals on DIII-D impurity studies

Identical Aurora simulations of Ar steady-state profiles, w/ and w/o CX

- Neutral densities from SOLPS-ITER/EIRENE (L-mode discharge)

DIII-D L-mode #180526





See also Dux et al 2020 *Nucl. Fusion* 60 126039

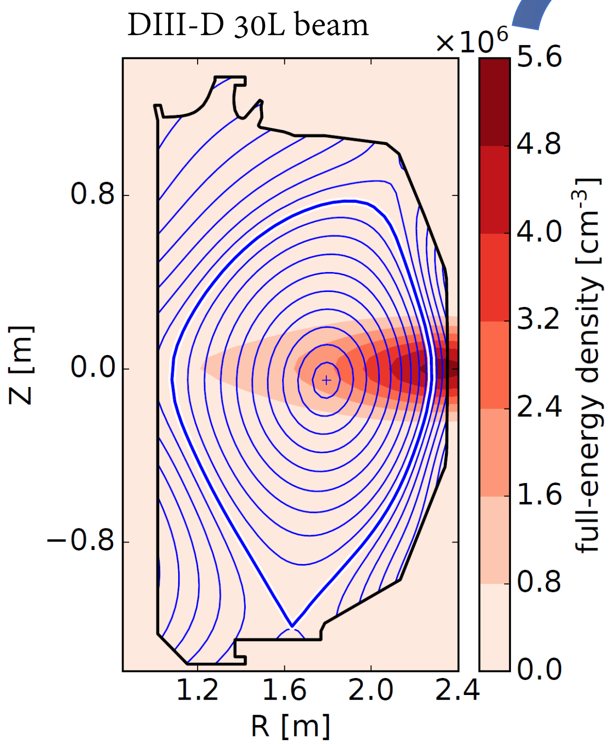
On DIII-D, NBI neutrals can also undergo CX reactions …

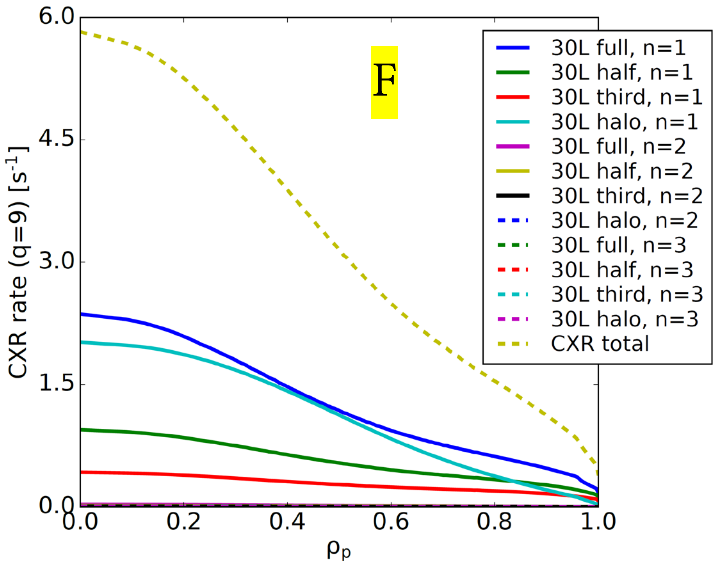
DIII-D NATIONAL FUSION FACILITY SAN DIEGO

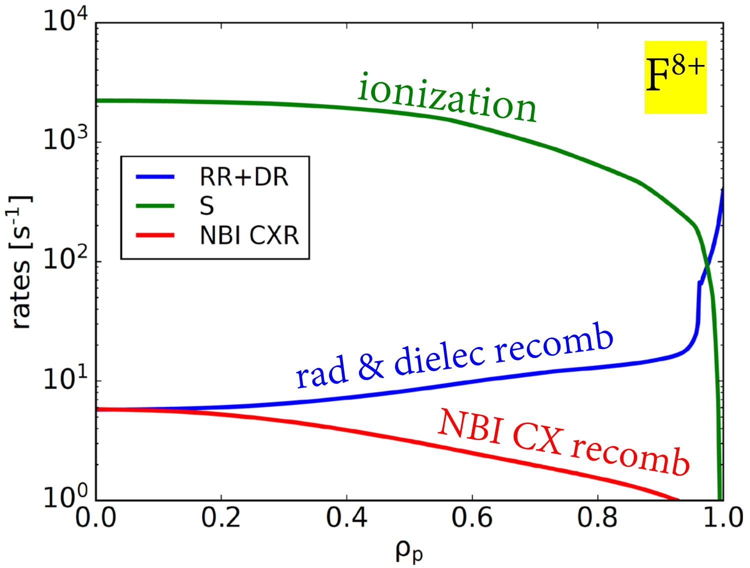
Neutral Beam Injection produces neutral populations at different energies (max ~ 80 keV)

- D atoms can also undergo multiple CX reactions, giving rise to a *halo* surrounding the beam

Using the state-of-the-art FIDASIM [1,2] Monte Carlo neutral code, we can examine all NBI neutral components







[1] Geiger *et al* 2020 *PPCF* **62** 105008
[2] Stagner, Geiger, Heidbrink - 10.5281/zenodo.1341369

On DIII-D, NBI neutrals can also undergo CX reactions with injected ions…

Neutral Beam Injection produces neutral populations at different energies (max ~ 80 keV)

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[1] Geiger *et al* 2020 *PPCF* **62** 105008
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NBI CXR never as important as edge neutrals for particle transport simulations

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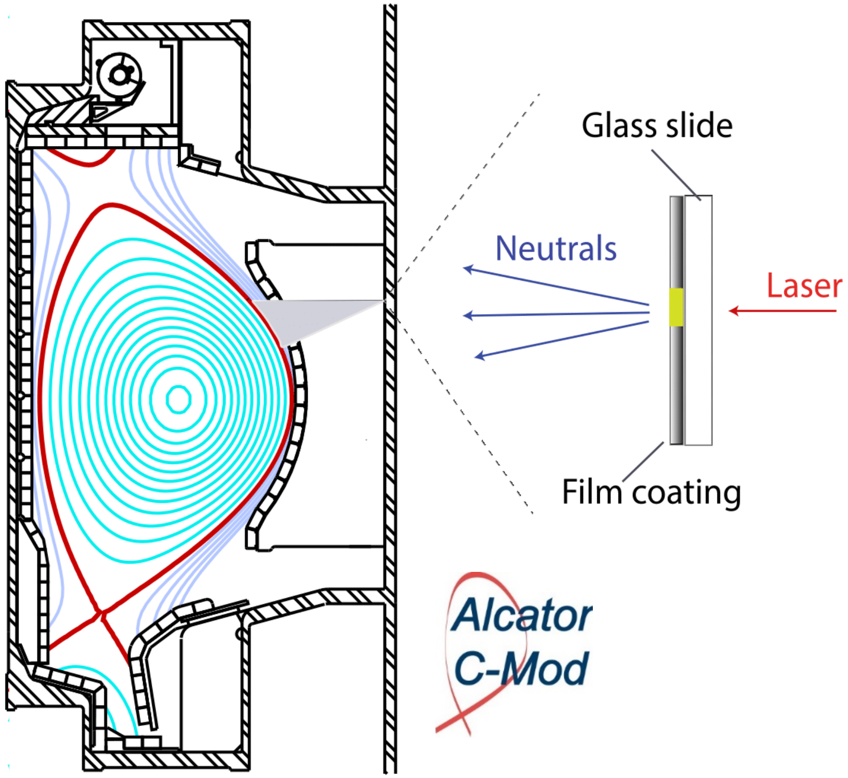
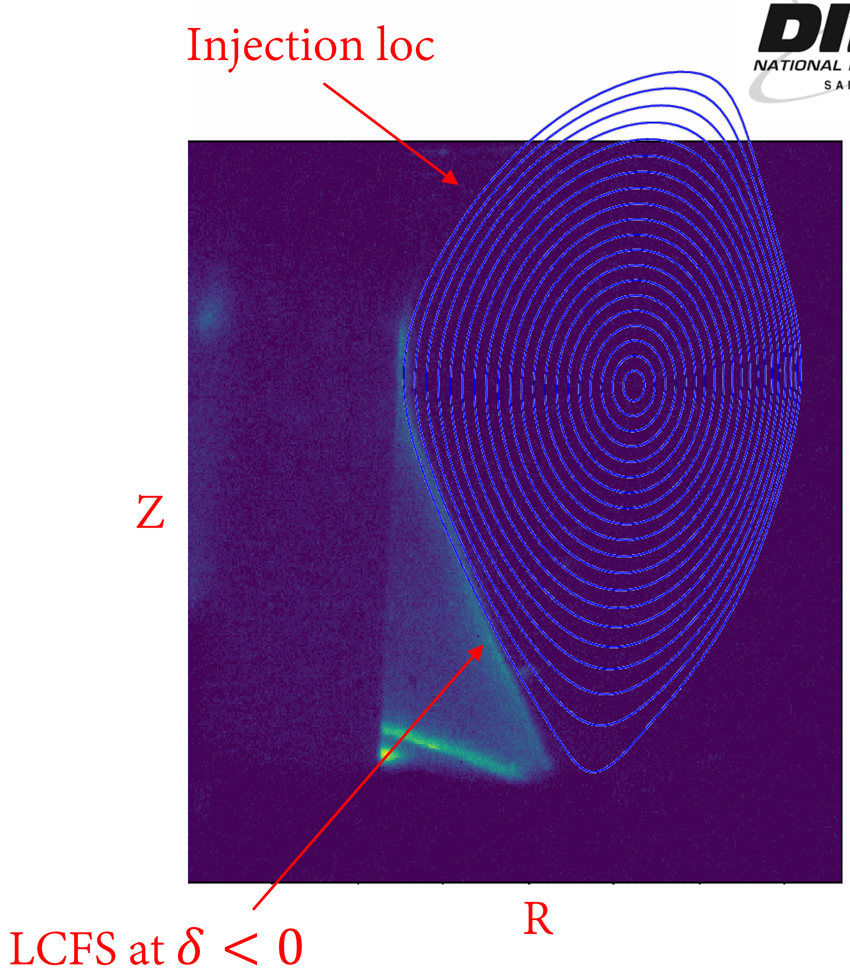
Inferring particle transport from Laser Blow-Off (LBO) injections



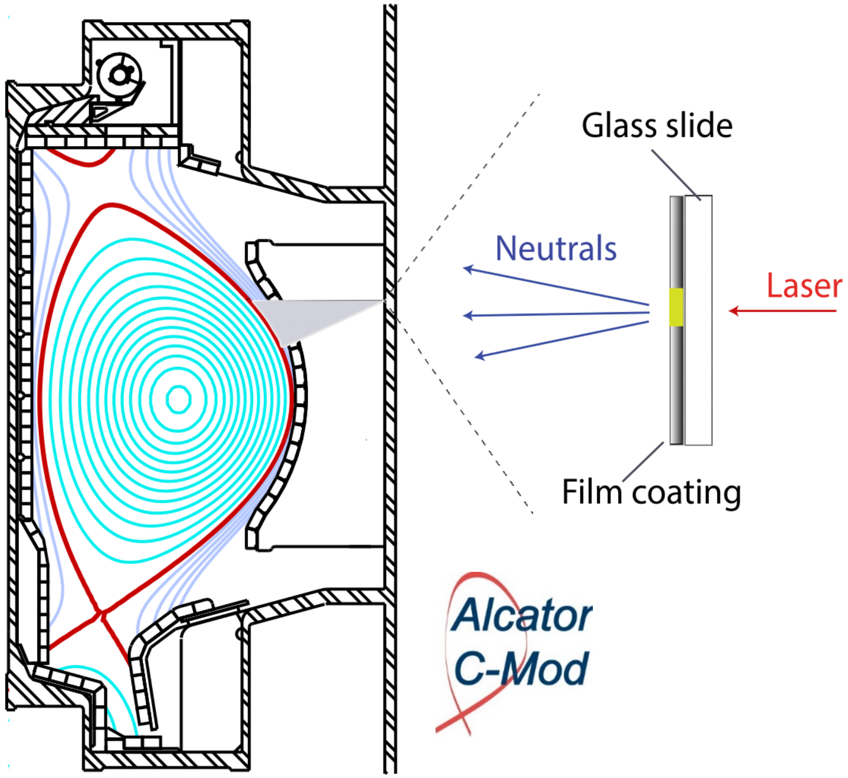


unfiltered fast camera in DIII-D $\delta < 0$ experiment

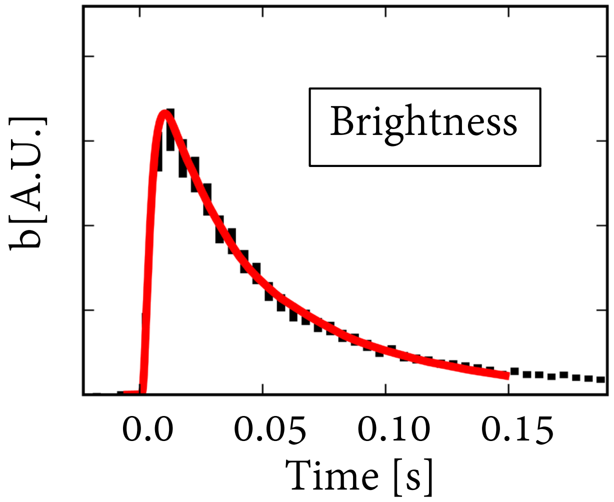
Non-perturbative *trace* amounts of *non-recycling*, *non-intrinsic* ions (Ca for C-Mod; F and Al for DIII-D)

- **Spectroscopic diagnostics** used to track ion spatio-temporal dynamics

Inferring particle transport from Laser Blow-Off (LBO) injections



Expt. data ⟷ Synth. data



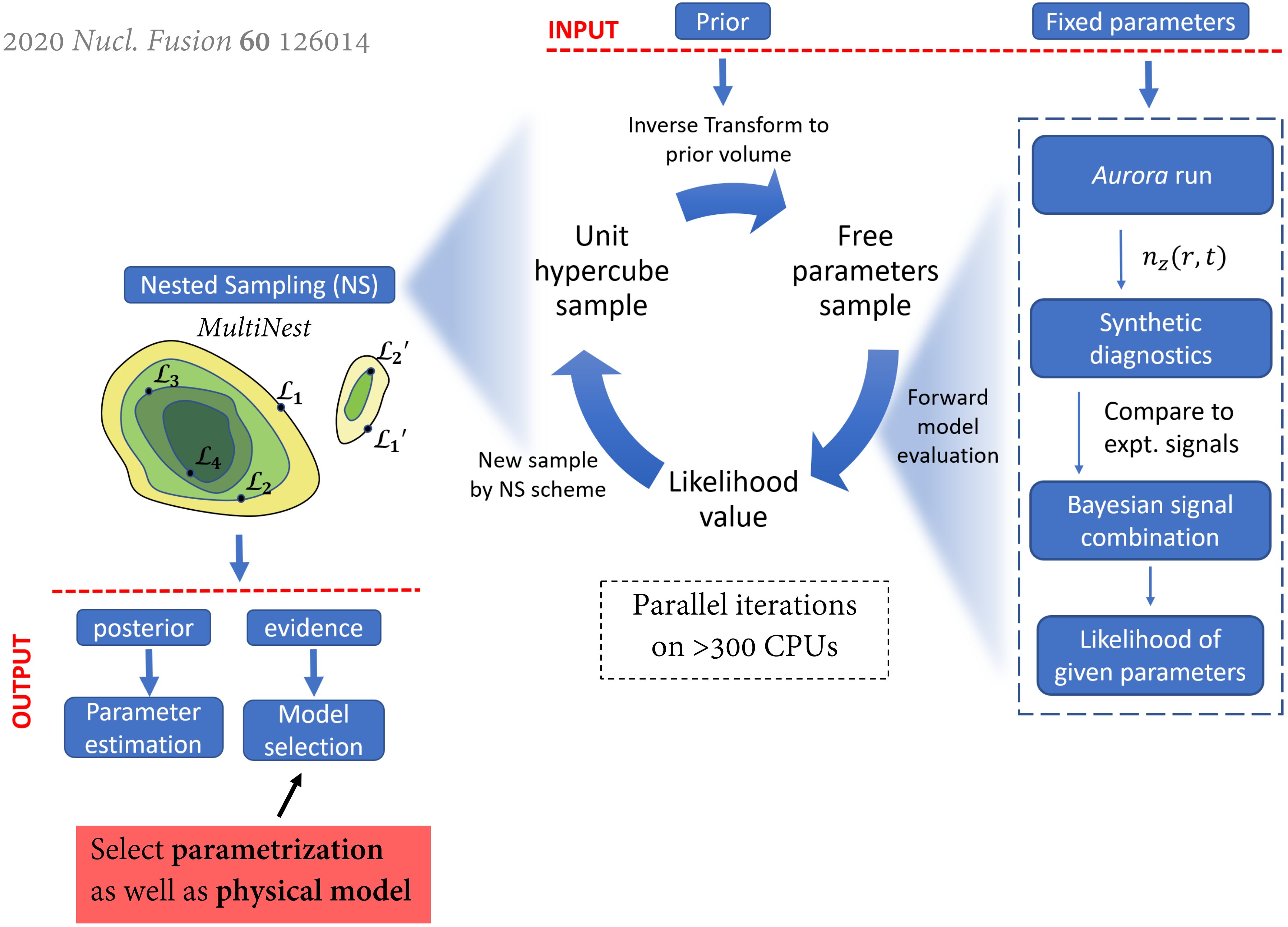
Aurora simulation (forward model)

Plasma geometry, kinetic profiles, …
D & v (free parameters)

Non-perturbative *trace* amounts of *non-recycling*, *non-intrinsic* ions (Ca for C-Mod; F and Al for DIII-D)

- **Spectroscopic diagnostics** used to track ion spatio-temporal dynamics

Sciortino *et al* 2020 *Nucl. Fusion* **60** 126014



Research highlights from Alcator C-Mod

Modeling the full K_α spectrum of He-like Ca and Li-like satellites

- On C-Mod, the **X**-ray **I**maging **C**rystal **S**pectroscopy (**XICS**) diagnostic measures **the entire Ca K_α (n=2-1) spectrum**

- New atomic data compilation from the atomDB database enables forward modeling of the **entire spectral range**

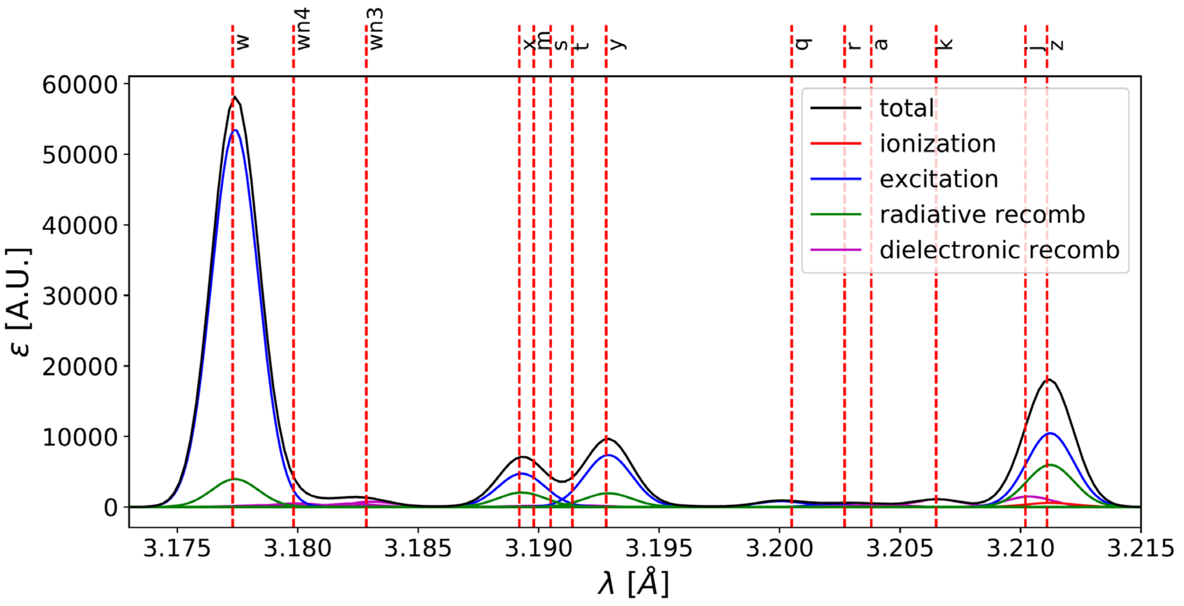
Includes hundreds of satellite lines from Li-like Ca

- Local spectra use *Doppler broadening and shifting from measured Ar data* using the Bayesian Spectral Fitting Code

  Sciortino & Cao 2020, *IEEE Trans. on Plasma Science*, 48, 1

- Line-integrated spectra can now be used to infer D & v

  Sciortino et al., *submitted to Nuclear Fusion*, 2021



$n_e = 10^{14}\ cm^{-3}; T_e = 1\ keV$

Stronger constraints on particle transport

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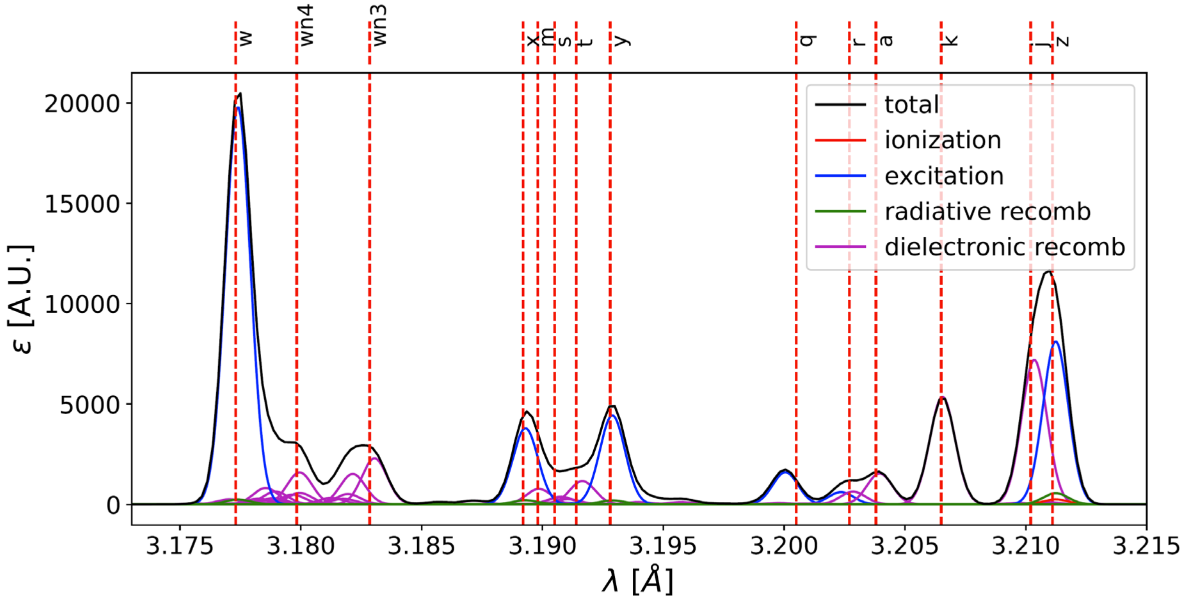

$n_e = 10^{14}\ cm^{-3}; T_e = 3.5\ keV$

Stronger constraints on particle transport

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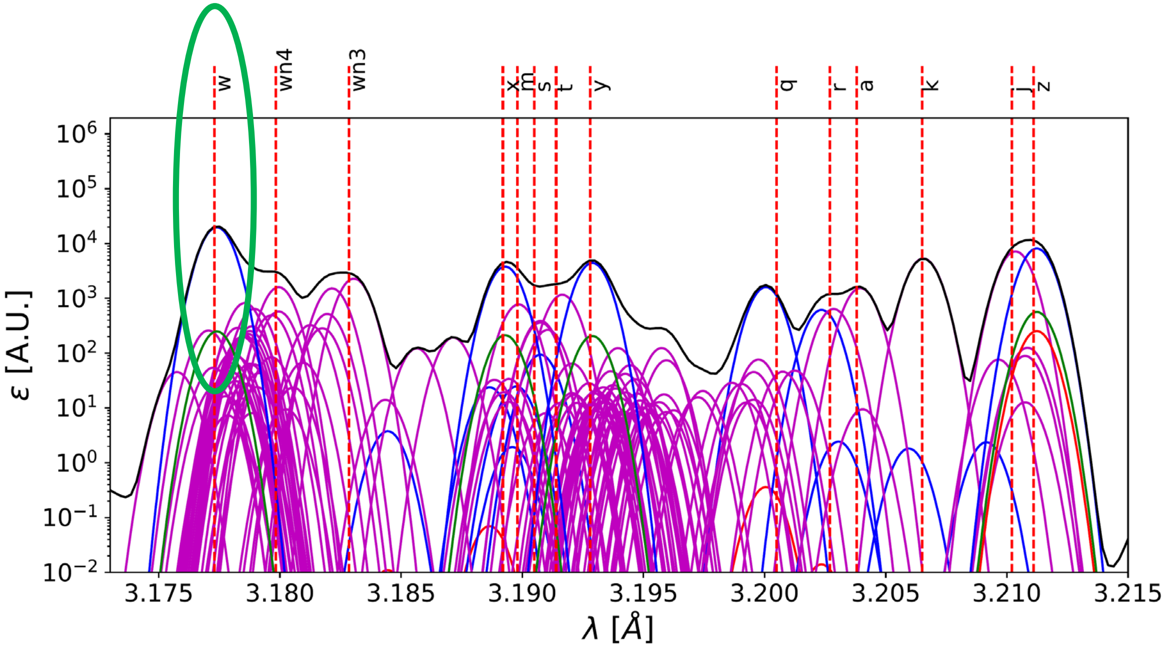


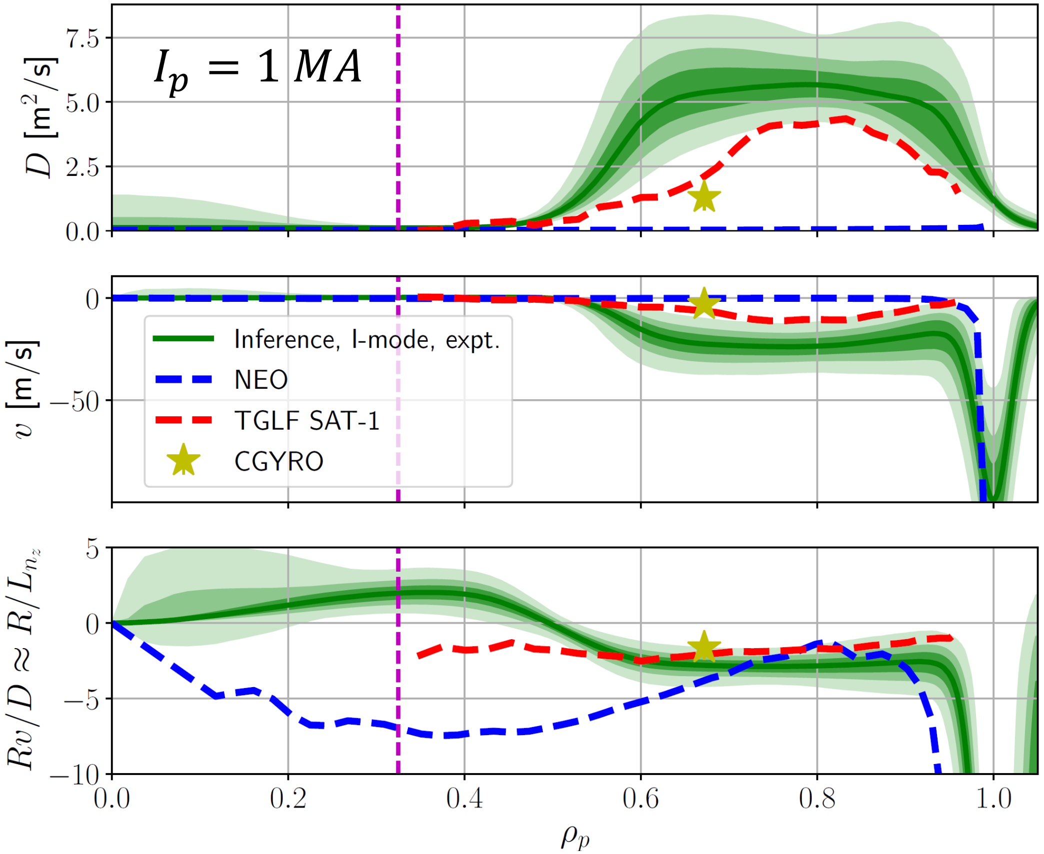
$n_e = 10^{14}\ cm^{-3}; T_e = 1\ keV$

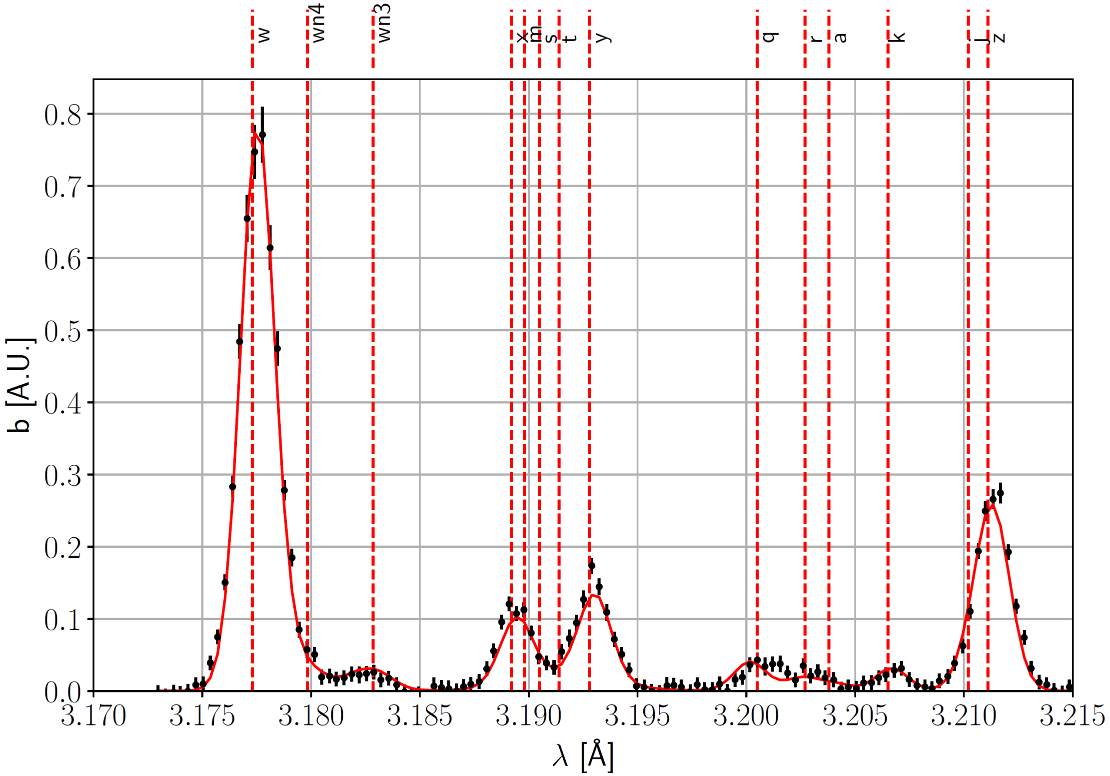
Stronger constraints on particle transport

Alcator C-Mod

Experimental inferences in multiple ELM-free regimes: I-mode

- In I-mode shot, we have relatively good matches in D and v
  - TGLF scans within inputs' uncertainties suggest that D and v predictions are accurate to 50% at best

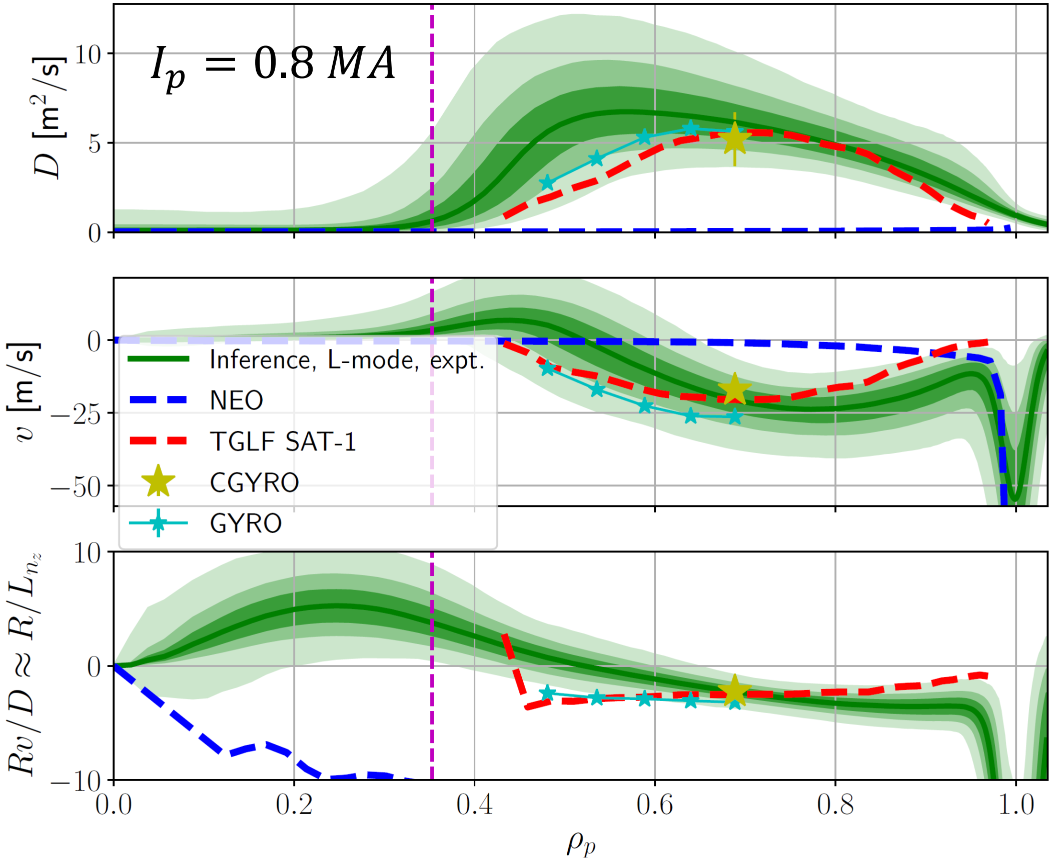


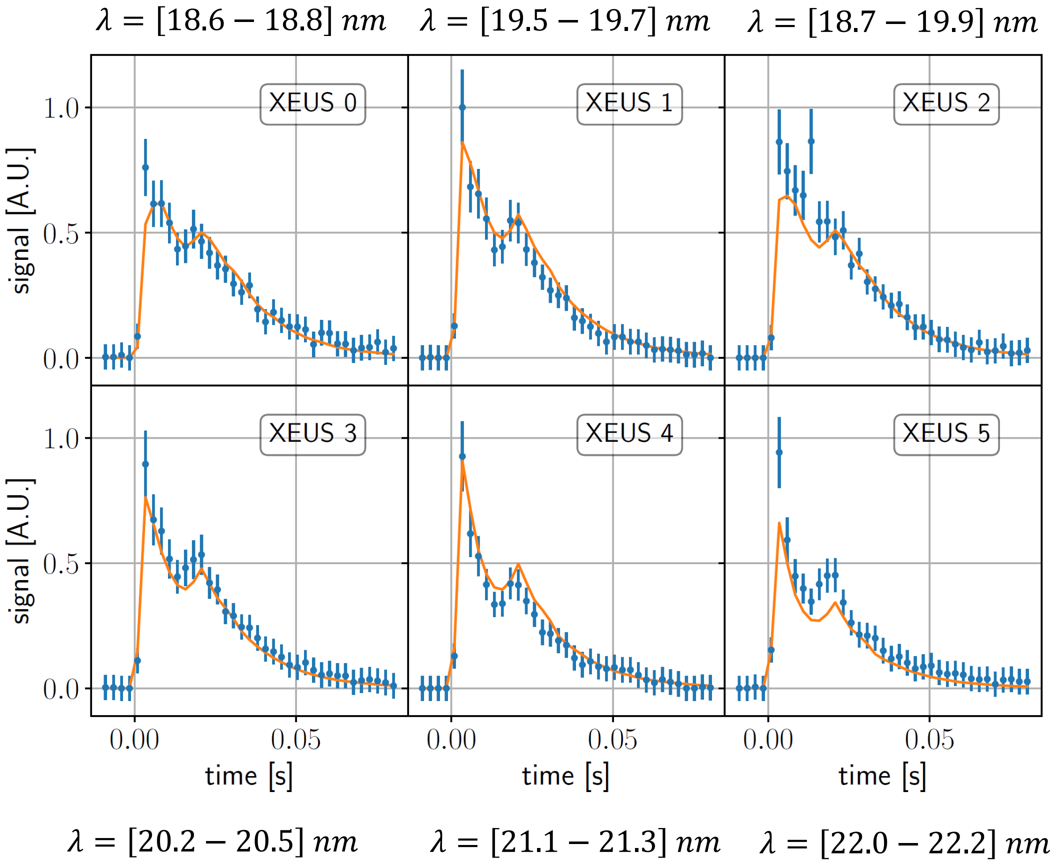


Alcator C-Mod

Experimental inferences in multiple ELM-free regimes: L-mode

- L-mode condition shows good agreement with theory
  - Relative amplitudes of EUV lines offer important constraints in outer part of the plasma (using ADAS rates)

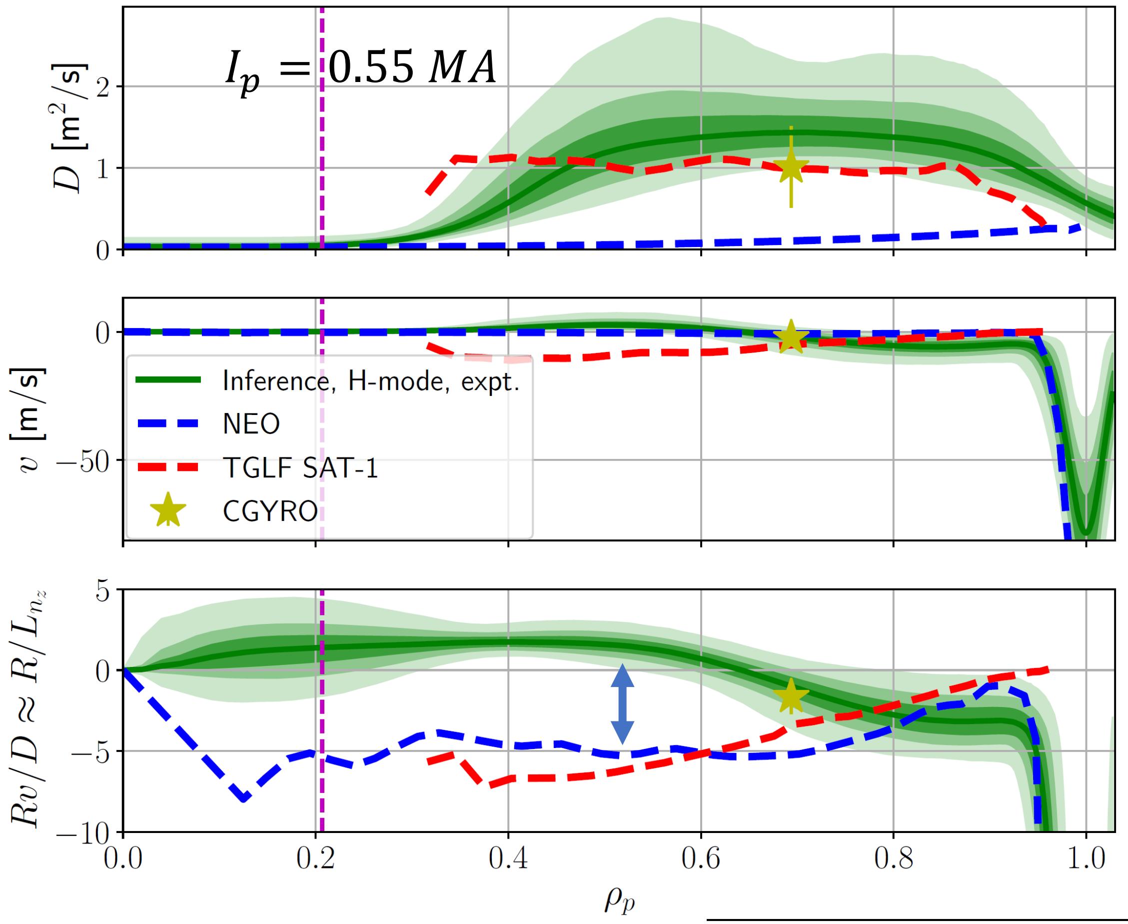


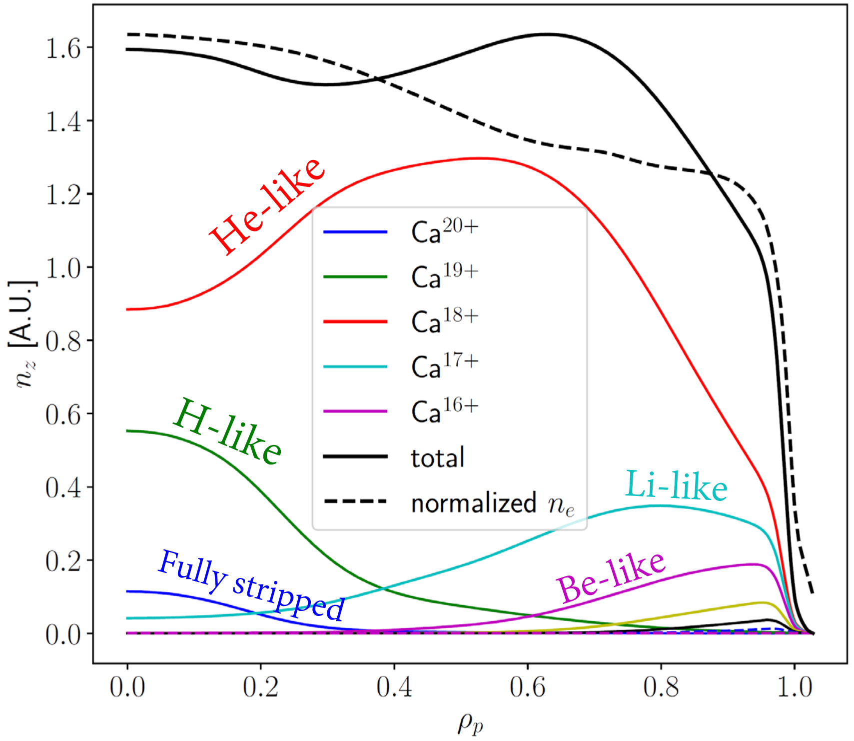


GYRO runs by N.T. Howard (~2012)

Experimental inferences in multiple ELM-free regimes: EDA H-mode

- EDA H-mode case has much smaller transport coefficients
  - Good agreement with theory models in D, but clear disagreement in v direction – hollow rather than peaked profiles





Research highlights from DIII-D

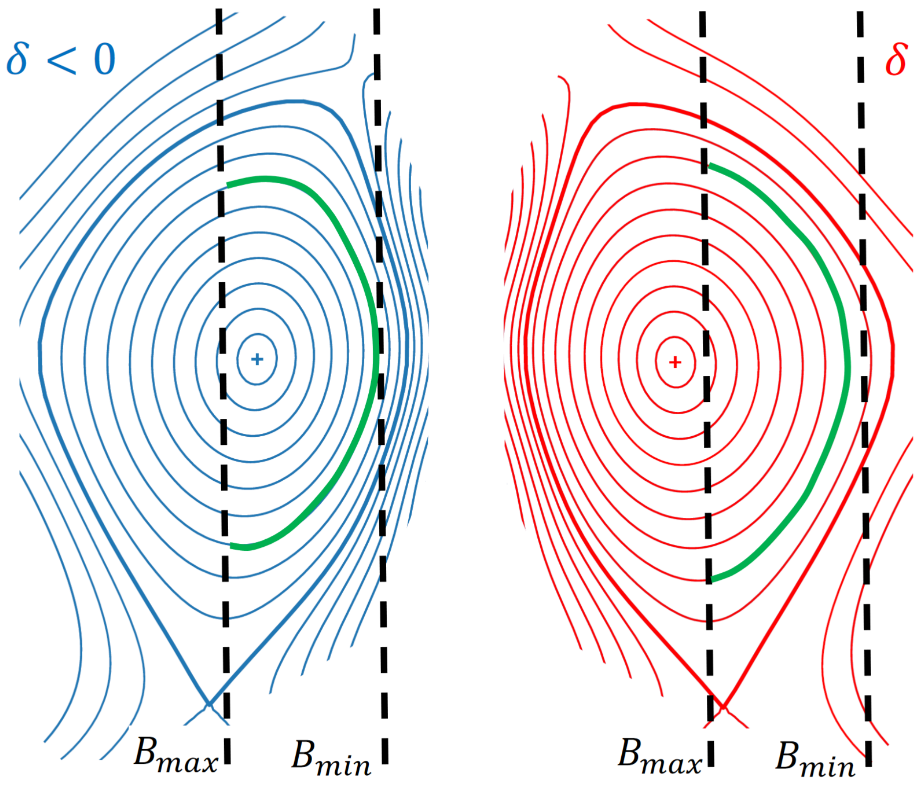
Diverted negative triangularity at DIII-D

- First **diverted $\boldsymbol{\delta < 0}$** experiments on DIII-D performed in 2019
  - H-mode performance with L-mode edge (no pedestal)
  - Advantageous "edge-first" approach to scenario development

  Marinoni et al. 2021, submitted to NF

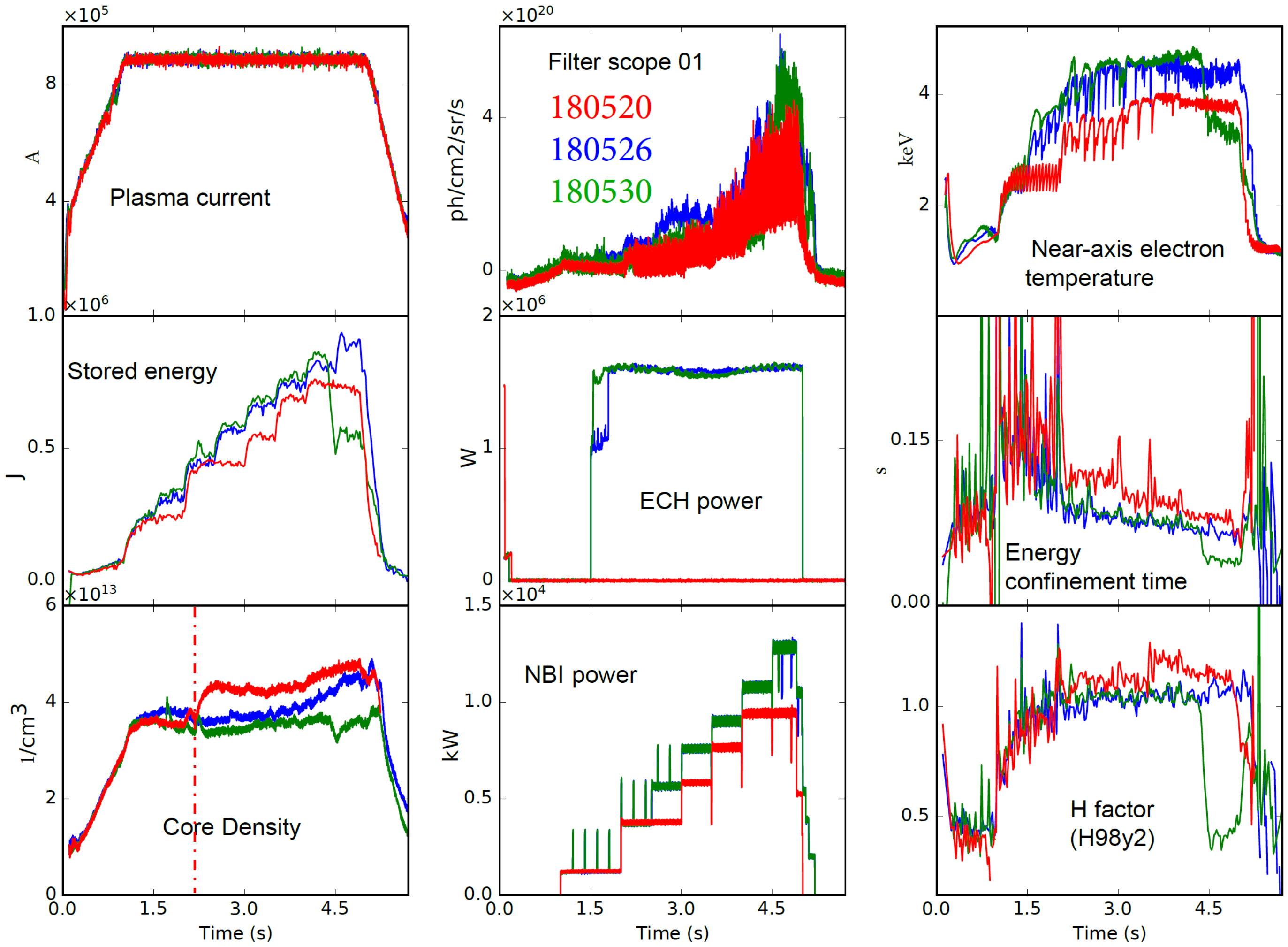
- **Previous $\boldsymbol{\delta < 0}$ research, with inner-wall limited plasmas, suggested shape effect on trapped particle orbits**

  Marinoni 2009 PPCF 51 055016
  Austin PRL 122, 115001 (2019)
  Fontana 2018 NF 58 024002
  …



Impurity transport generally observed to be "favorable" at $\delta < 0$, but not yet analyzed in detail

Examined 3 diverted negative triangularity discharges



Laser Blow-Off (LBO) injections of F and Al at different times for the chosen discharges:

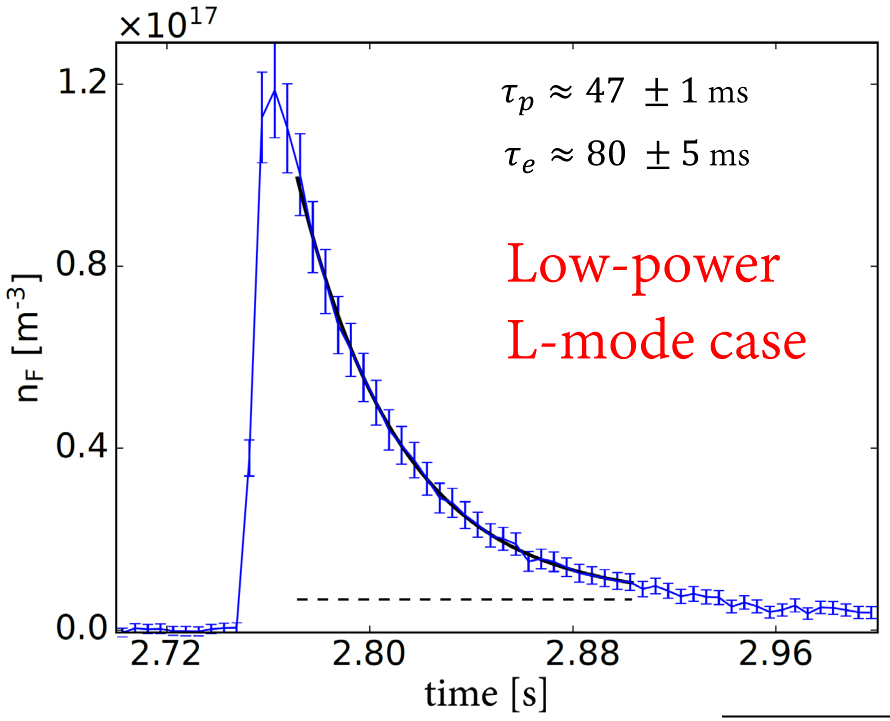
- $t = 2.5s$ in #180520: low-power H-mode
- $t = 2.75s$ in #180526: low-power L-mode
- $t = 3.8s$ in #180530: high-power L-mode

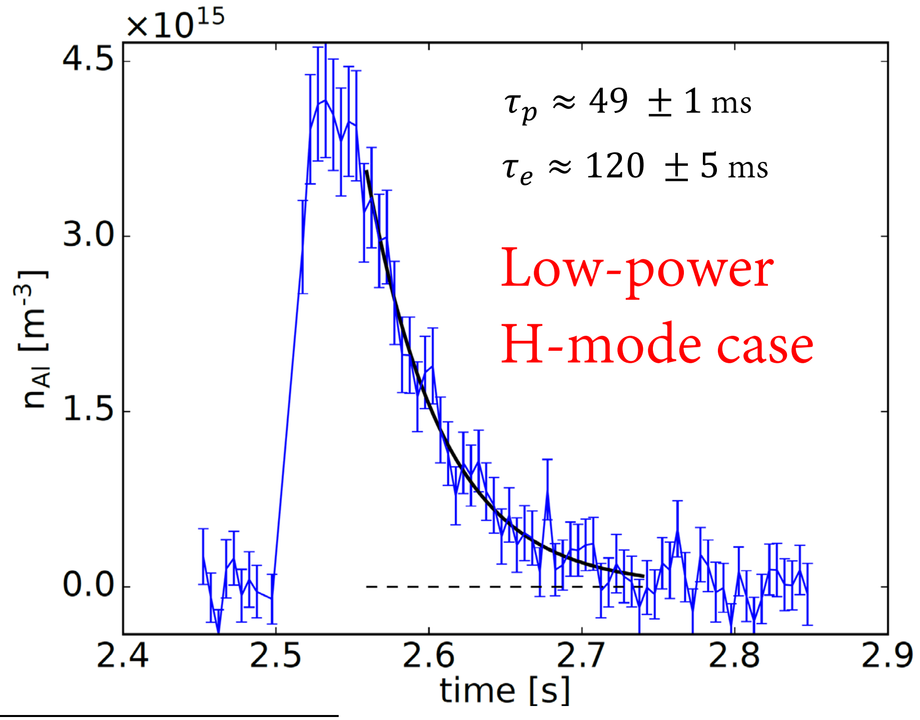
Confinement times indicate favorable impurity transport

Impurity confinement times are consistently observed to be short

- $\tau_p < 50$ ms ← also in H-mode!
- $\tau_p/\tau_e < 1$ ← compare to $\tau_p/\tau_e \approx 2-4$ of typical $\delta > 0$ H-mode plasmas on DIII-D

Suggests edge heat transport barrier, no particle transport barrier – <u>as in I-mode</u>





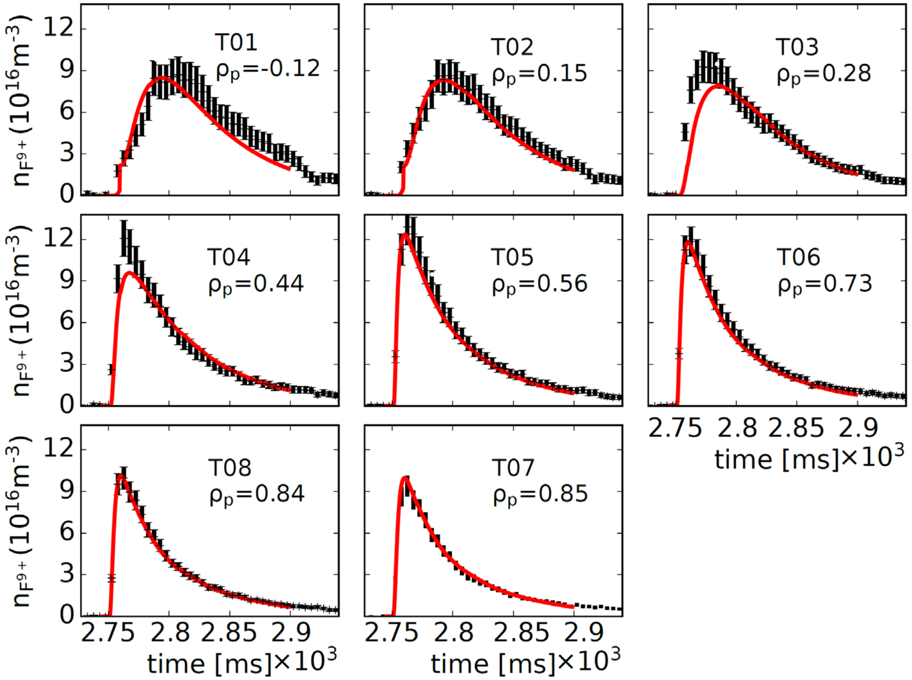
Multi-species inferences are a major new step for impurity transport model validation

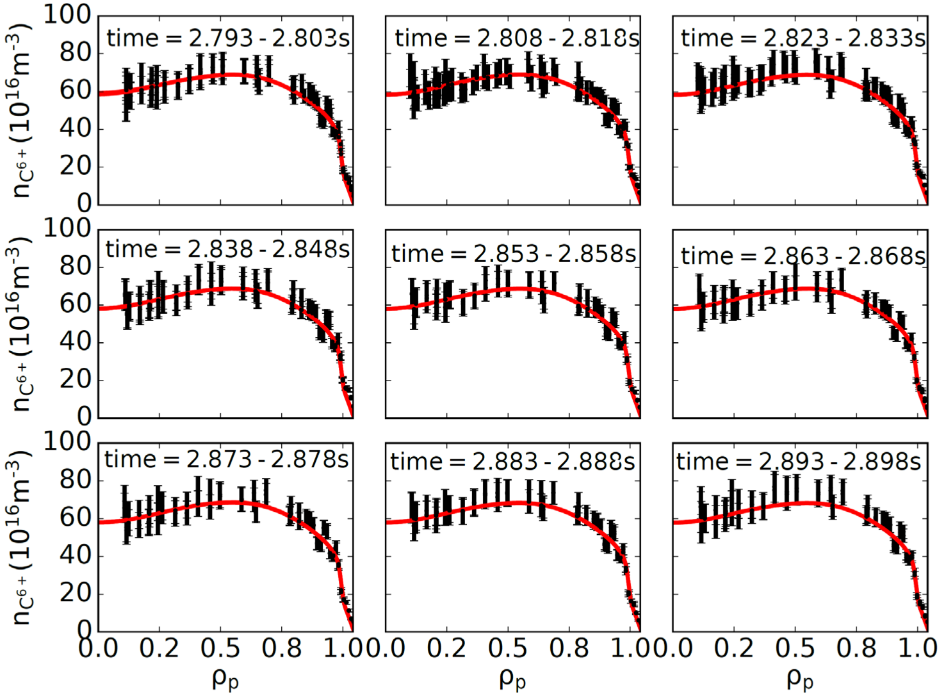
- **New ImpRad module in OMFIT is now generalized to handle an arbitrary number of species**
  - Same plasma background -- different sources, atomic rates and (possibly) D and v

Meneghini, Smith et al. 2015 NF 55 083008

We constrain transport using both intrinsic (quasi-steady) C and (rapidly-evolving) LBO-injected ions

t = 2.75*s* in #180526: low-power L-mode





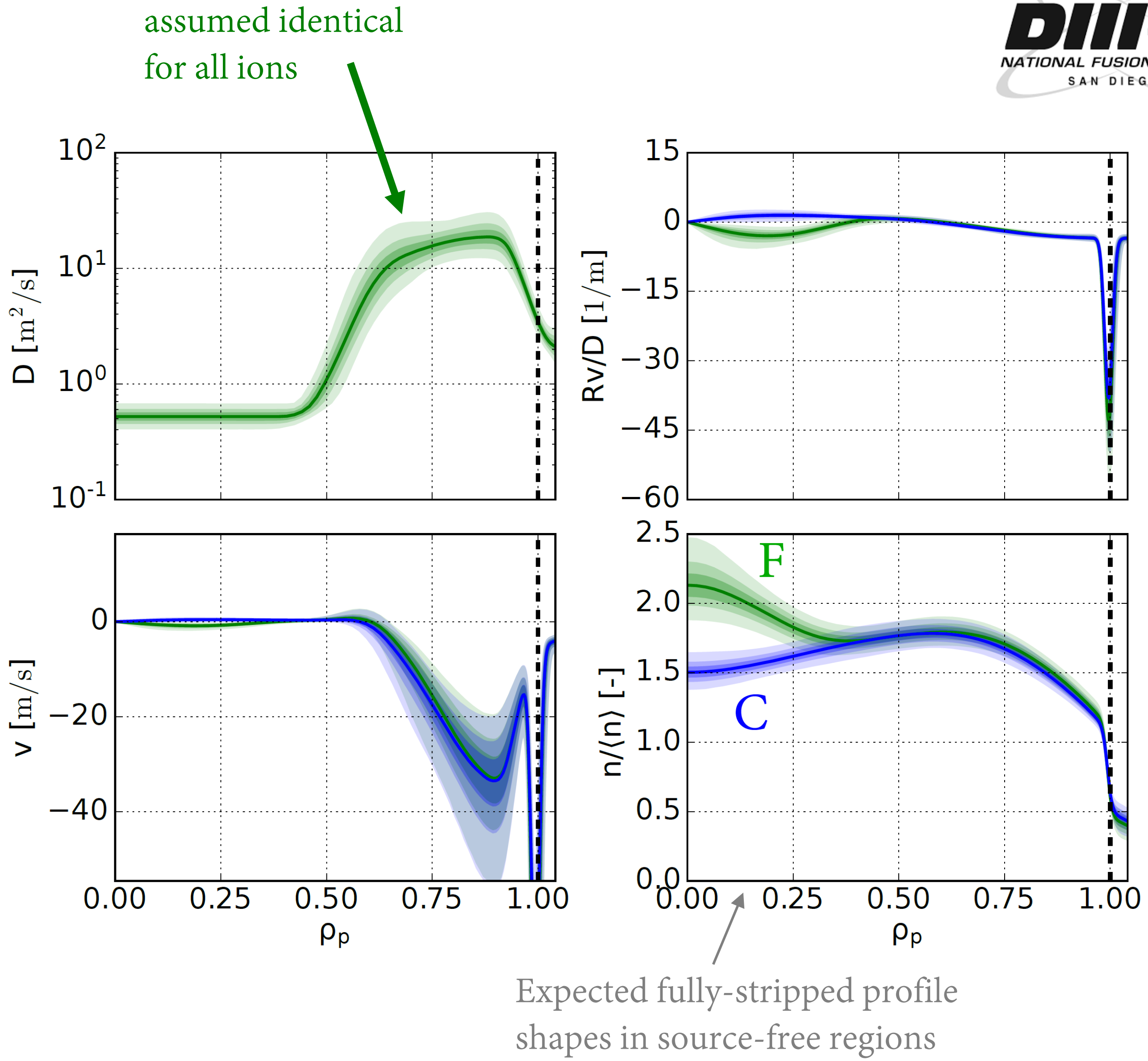
Further constraints on impurity transport from SXR and core-SPRED (additional slides)

Impurity transport inference in $\delta < 0$ low-power L-mode

- **Multi-species impurity transport inference in low-power L-mode**
  - F (LBO) and C (intrinsic)

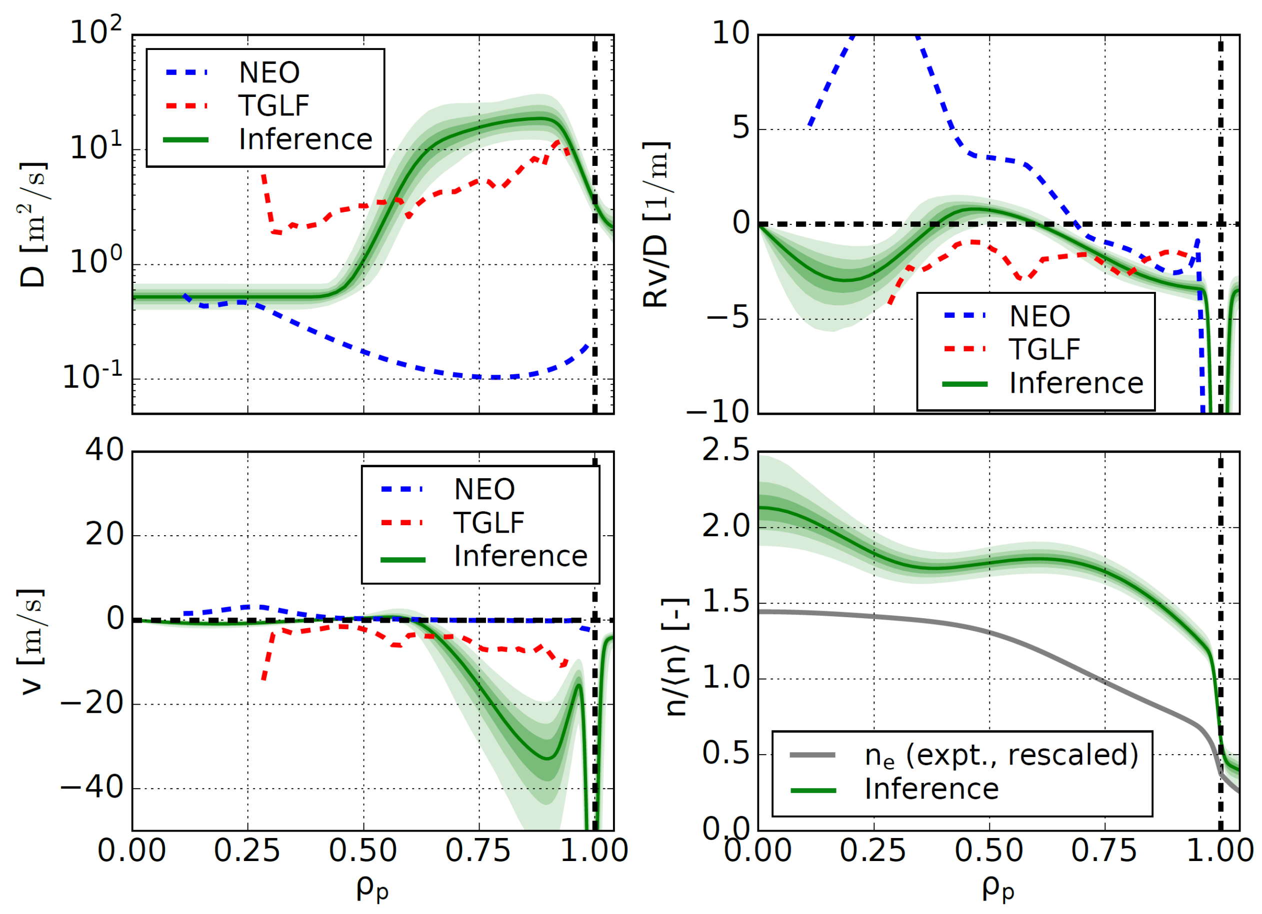
- **Near-axis peaking inverted between species**
  - Difference is outside of uncertainties
  - Z-scaling of transport?

Next: comparison to theory models for the species injected via LBO



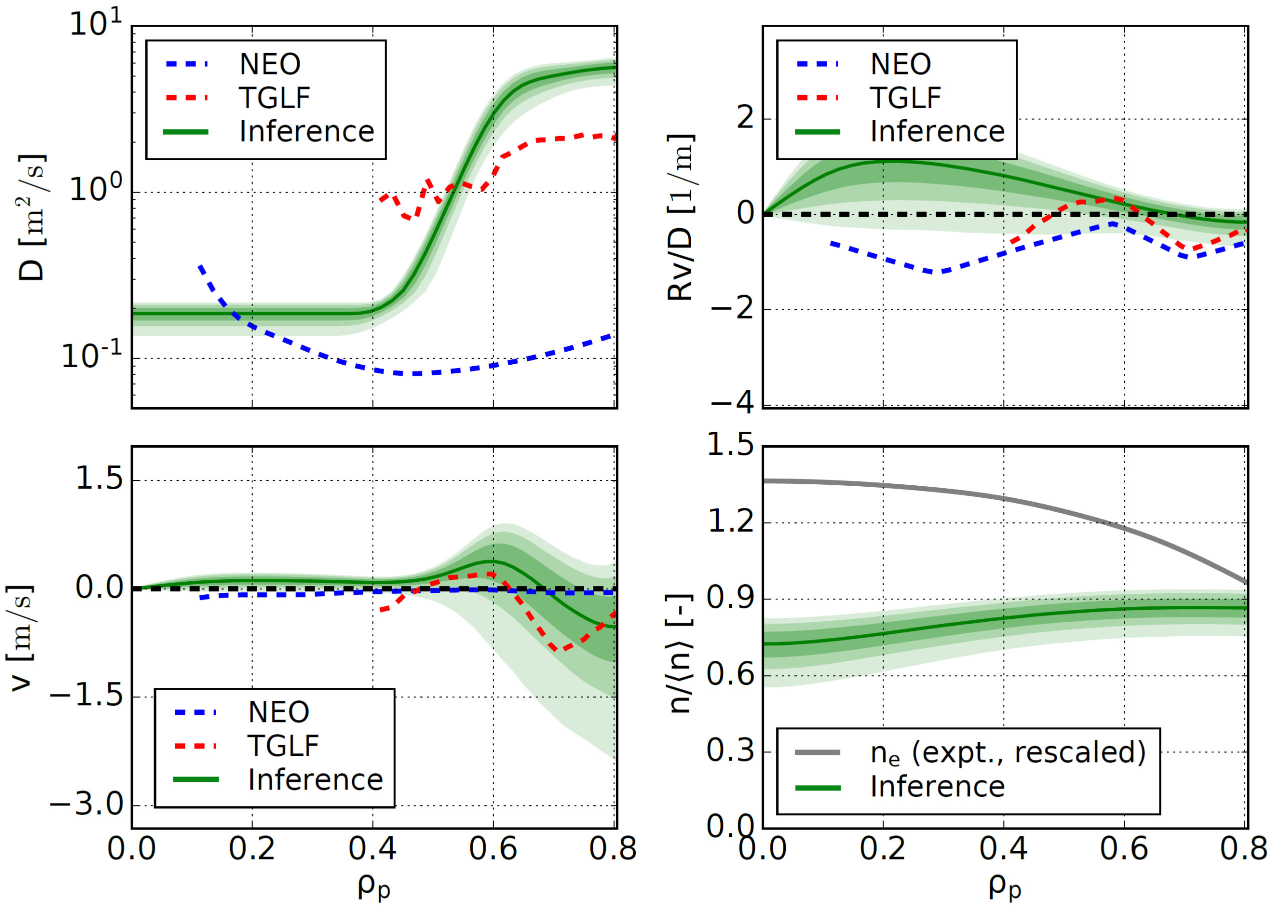
Qualitative (but not quantitative) agreement with theory in $\delta < 0$ low-power L-mode

- **Multi-species impurity transport inference in low-power L-mode**
  - F (LBO) and C (intrinsic)
- **Near-axis peaking inverted between species**
  - Difference is outside of uncertainties
  - Z-scaling of transport?
- D and v magnitudes match NEO near axis
- D at midradius is underestimated by ~2-3x
- $\boldsymbol{Rv/D}$ **prediction suggests peaked profiles, but actually ≈flat**



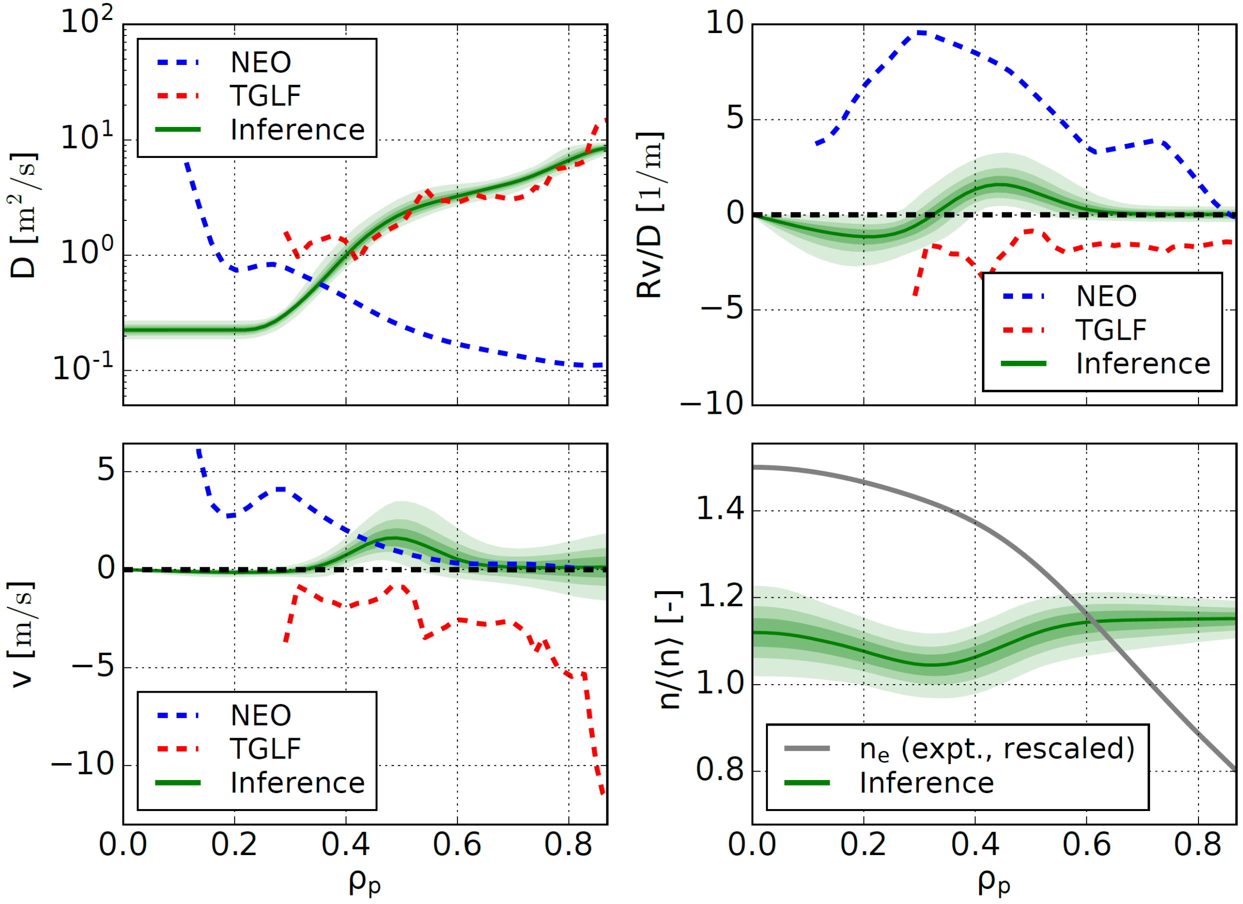
Qualitative (but not quantitative) agreement with theory in $\delta < 0$ low-power H-mode

- **Multi-species impurity transport inference in low-power H-mode**
  - Al (LBO) and C (intrinsic)
- Unclear LBO source prevents us from making statements about pedestal transport…
- **Significant discrepancy in *D* at midradius**
- **Flat (or hollow) impurity profiles**
  - Relatively good agreement between theory and experiment on Rv/D



Qualitative (but not quantitative) agreement with theory in $\delta < 0$ high-power L-mode

- **Multi-species impurity transport inference in high-power L-mode**
  - Al (LBO) and C (intrinsic)
- Unclear LBO source prevents us from making statements about pedestal transport…
- **Close agreement in *D* at midradius, but discrepancy with NEO near axis**
  - Sharp features related to rotation profile
- **Flat (or hollow) impurity profiles**
  - TGLF suggests a peaked profile; unvaried within reasonable uncertainties of inputs



Contents

1. *Aurora*
2. *Charge exchange between neutrals and impurities*
3. *Bayesian Inference of Experimental Particle Transport Coefficients*
4. *Highlights from research on*
   a) *Alcator C-Mod*
   b) *DIII-D*
5. *Conclusions*

Main thesis contributions

1. Development of the open-source **Aurora** package for particle transport and radiation[4]
2. Quantification of the impact of **charge exchange** with background neutrals on pedestal impurity studies[4,5]
3. Comparisons of particle transport coefficients between **theory and experiment** for both C-Mod[1,2,3,5] and DIII-D[6]
   a) Creation of **HPC** frameworks for **Bayesian** inference[2]
   b) On C-Mod, forward model for the **entire K_α spectrum** and analysis of extreme-UV **line ratios**[5]
   c) On DIII-D, co-development of **ImpRad**[4] tools for inferences using **multiple atomic species**[6]

1. F. Sciortino and N. M. Cao, "Bayesian spectral moment estimation and uncertainty quantification", *IEEE Transactions on Plasma Science*, vol. 48, no. 1, pp. 22-30, Jan. 2020, https://ieeexplore.ieee.org/document/8879689
2. F. Sciortino et al., "Inference of experimental radial impurity transport on Alcator C-Mod: Bayesian parameter estimation and model selection", *Nuclear Fusion*, vol. 60, no. 12, Sept. 2020, https://doi.org/10.1088/1741-4326/abae85
3. F. Sciortino et al., "Particle transport constraints via Bayesian spectral fitting of multiple atomic lines", *Review of Scientific Instruments (invited)*, 92, 053508, 2021, https://doi.org/10.1063/5.0043765
4. F. Sciortino et al., "Modeling of particle transport, neutrals and radiation in magnetically-confined plasmas with Aurora", submitted to *Plasma Physics & Controlled Fusion*, 2021 - https://arxiv.org/abs/2106.04528
5. F. Sciortino et al., "Experimental inference of neutral and impurity transport in Alcator C-Mod using high-resolution x-ray and ultra-violet spectra", submitted to *Nuclear Fusion*, 2021 - https://arxiv.org/abs/2107.13471
6. F. Sciortino et al., "Experimental inference of radial impurity transport in DIII-D diverted negative triangularity plasmas", 2021, *in preparation*