

Experimental Inference of Particle Transport in Tokamak Plasmas

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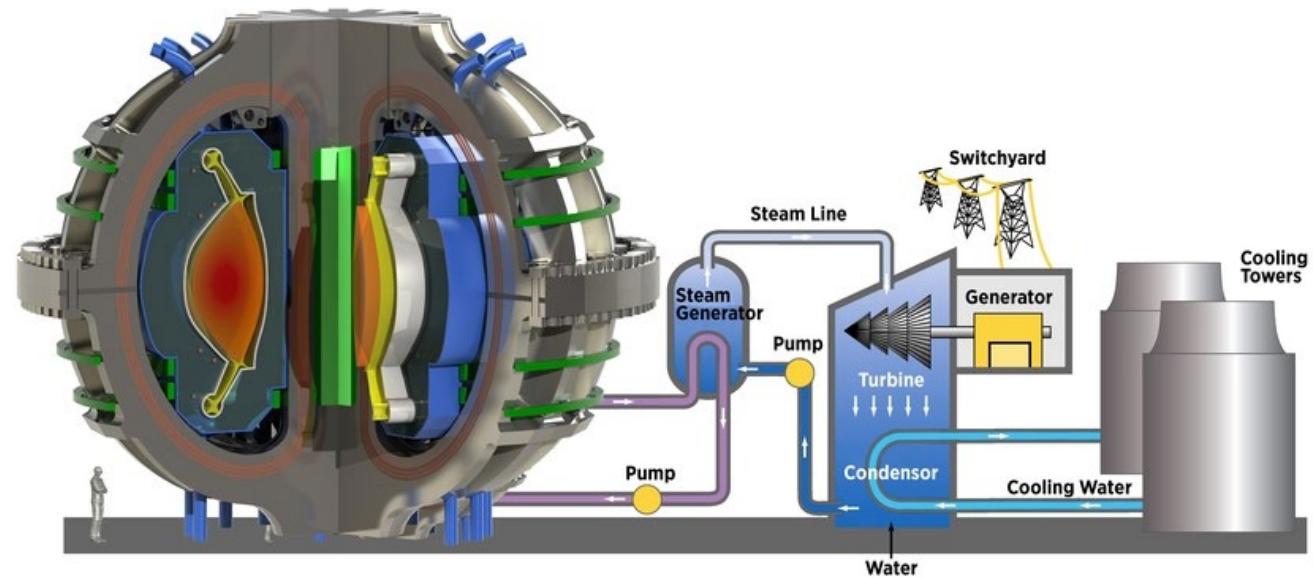
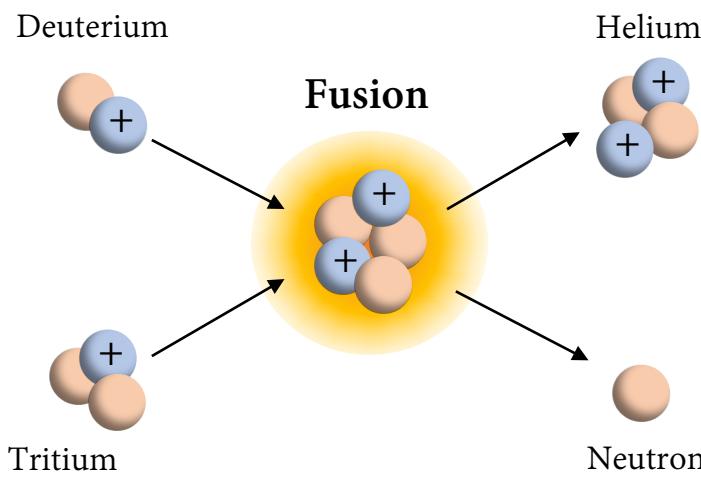


August 4, 2021



Fusion energy and plasma physics

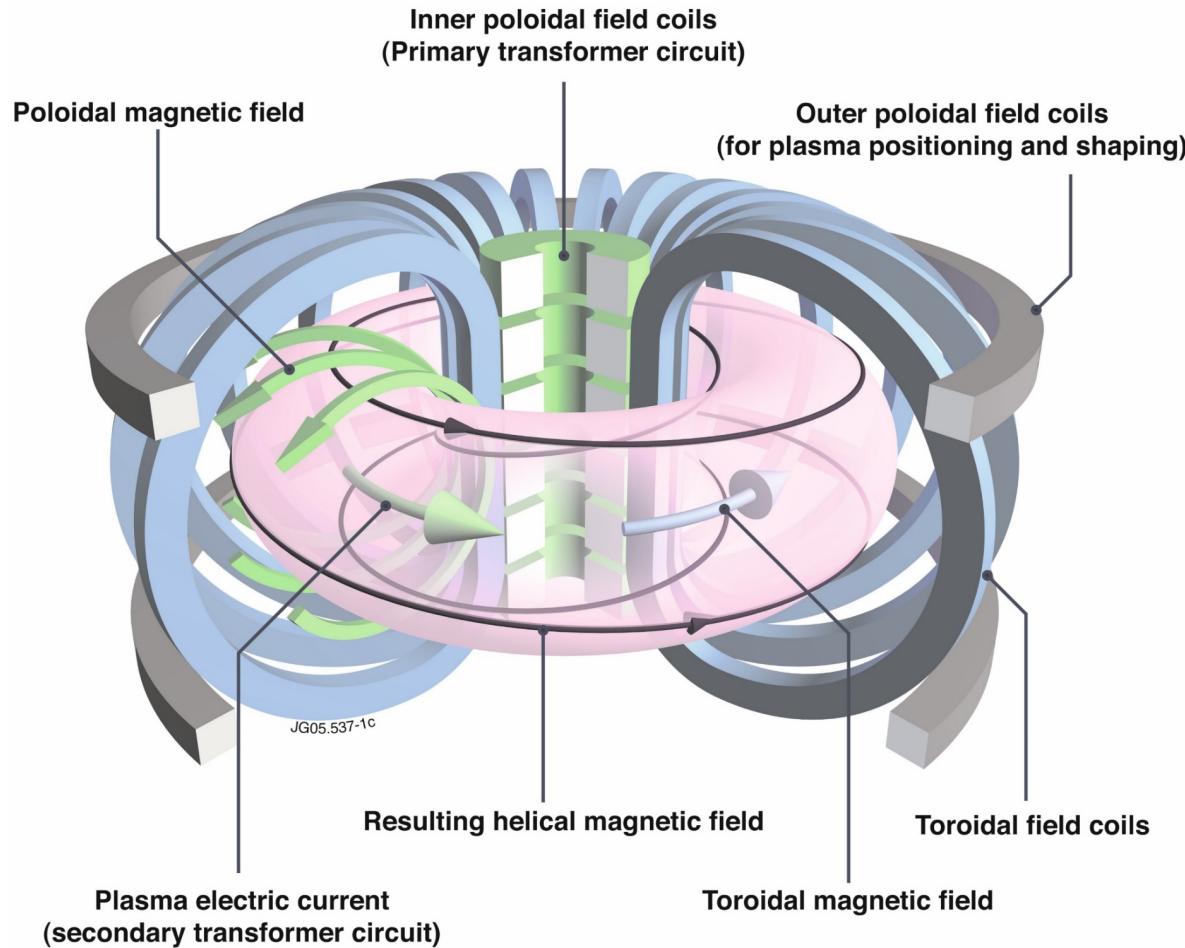
- Fusion energy could be key to fulfilling energy demands in a sustainable way
 - “Burns” light nuclei, releasing large amounts of energy
 - Enabling technologies must be **safe, clean, economical**



Source: Courtesy of PSFC, adapted from Wikimedia Commons

Magnetic confinement fusion & the tokamak

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

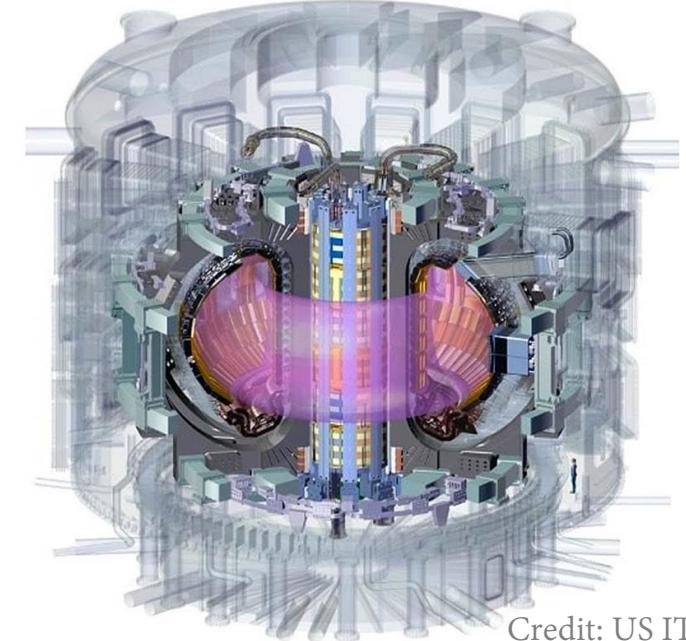


The future: *technology* and *scale* are leading us to breakthroughs

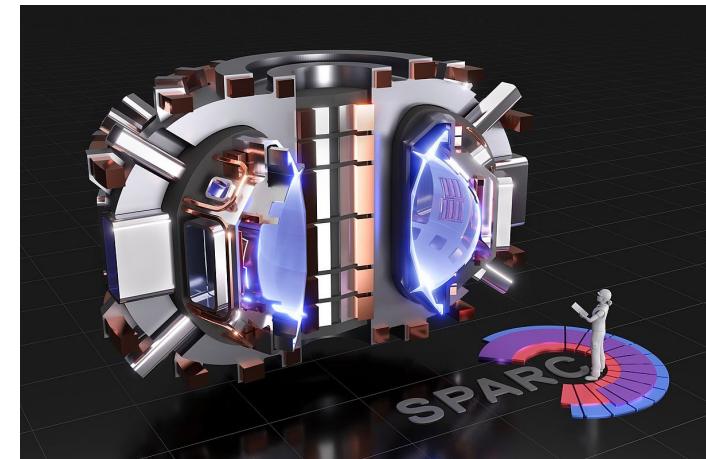
ITER & SPARC are now on their way to break-even:

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

- 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



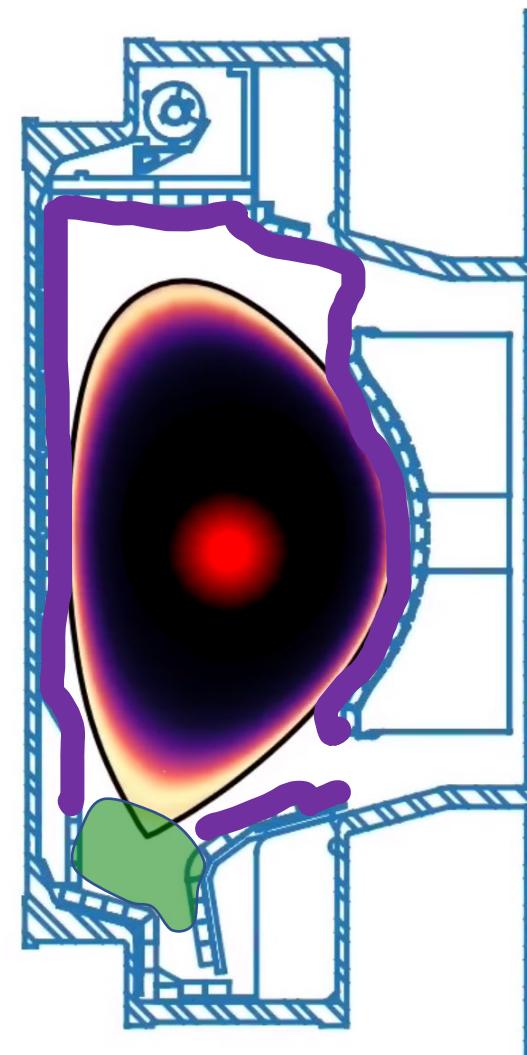
Credit: T. Henderson, CFS/MIT-PSFC

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 radiation⁴
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-D⁶

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

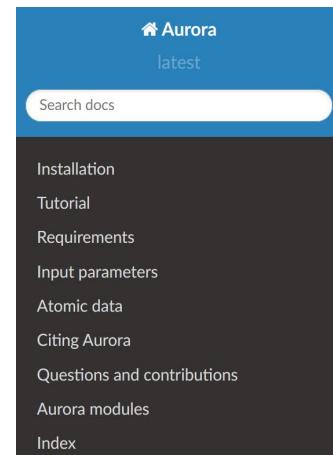
1. [F. Sciortino](#) and N. M. Cao, *IEEE Trans. Plasma Science*, vol. 48, no. 1, 2020
2. [F. Sciortino](#) et al., *Nuclear Fusion*, vol. 60, no. 12, 2020
3. [F. Sciortino](#) et al., *Review of Scientific Instruments* (invited), 92, 053508, 2021
4. [F. Sciortino](#) et al., *submitted to Plasma Physics & 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*
3. *Bayesian Inference of Experimental Particle Transport Coefficients*
4. *Highlights from research on*
 - a) *Alcator C-Mod*
 - b) *DIII-D*
5. *Conclusions*

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>
- 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: a modern toolbox for particle transport and radiation modeling [Edit on GitHub](#)

Aurora: a modern toolbox for particle transport and radiation modeling

Github repo: <https://github.com/fsciortino/Aurora>

Paper/presentation on the arXiv: <https://arxiv.org/abs/2106.04528>

Overview

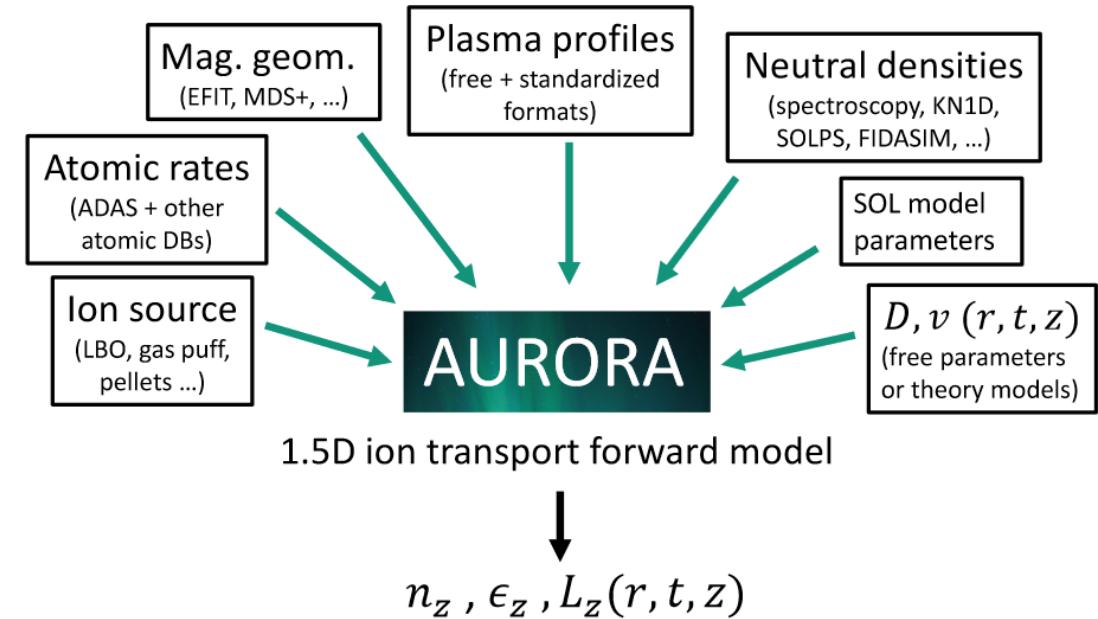
Aurora is a package to simulate heavy-ion transport and radiation in magnetically-confined plasmas. It includes a 1.5D impurity transport forward model which inherits many of the methods from the historical STRAHL code and has been thoroughly benchmarked with it. It also offers routines to analyze neutral states of hydrogen isotopes, both from the edge of fusion plasmas and from neutral beam injection. Aurora's code is mostly written in Python 3 and Fortran 90. A Julia interface has also recently been added. The package enables radiation calculations using ADAS atomic rates, which can easily be applied to the output of Aurora's own forward model, or coupled with other 1D, 2D or 3D transport codes.



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

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



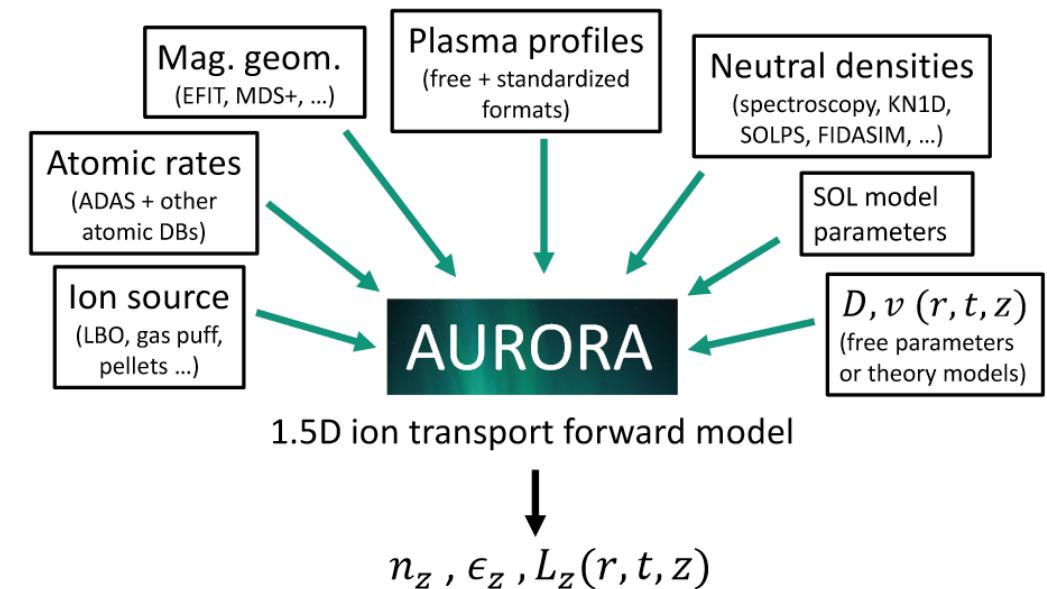
n_z : charge state densities

ϵ_z : spectral line emissivities

L_z : radiated power coefficients

Aurora's forward model of particle transport

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



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

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

$$Q_{I,Z} = - (n_e S_{I,Z} + n_e \alpha_{I,Z} + n_n \alpha_{I,Z}^{cx}) n_{I,Z} \\ + n_e S_{I,Z-1} n_{I,Z-1} \\ + (n_e \alpha_{I,Z+1} + n_n \alpha_{I,Z+1}^{cx}) n_{I,Z+1}$$

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

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

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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

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

$$Q_{I,Z} = -(n_e S_{I,Z} + n_e \alpha_{I,Z} + n_n \alpha_{I,Z}^{cx}) n_{I,Z} \\ + n_e S_{I,Z-1} n_{I,Z-1} \\ + (n_e \alpha_{I,Z+1} + n_n \alpha_{I,Z+1}^{cx}) n_{I,Z+1}$$

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

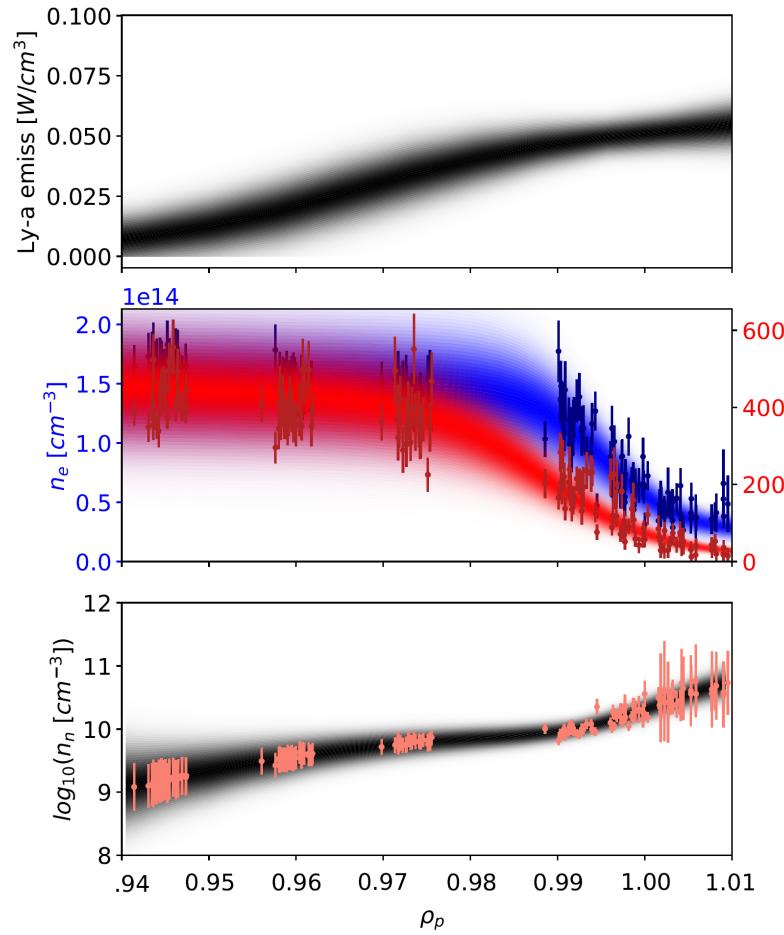
On C-Mod, all D neutrals are typically from the tokamak edge

measured via a Ly_a midplane array
(H-like ion $n = 2 \rightarrow 1$ transition)

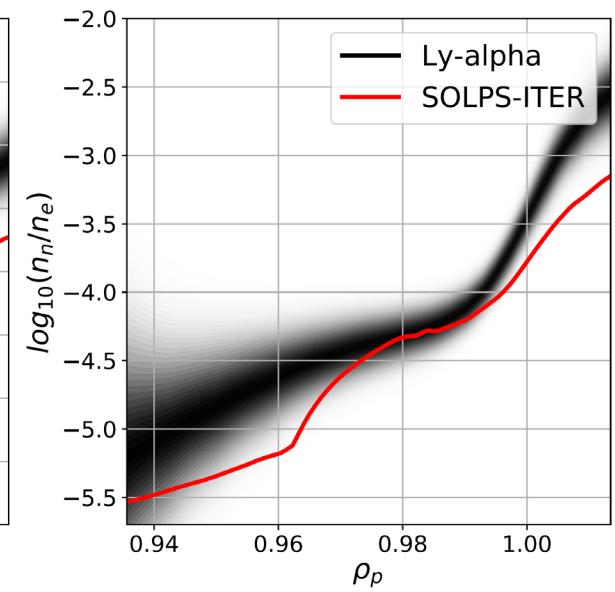
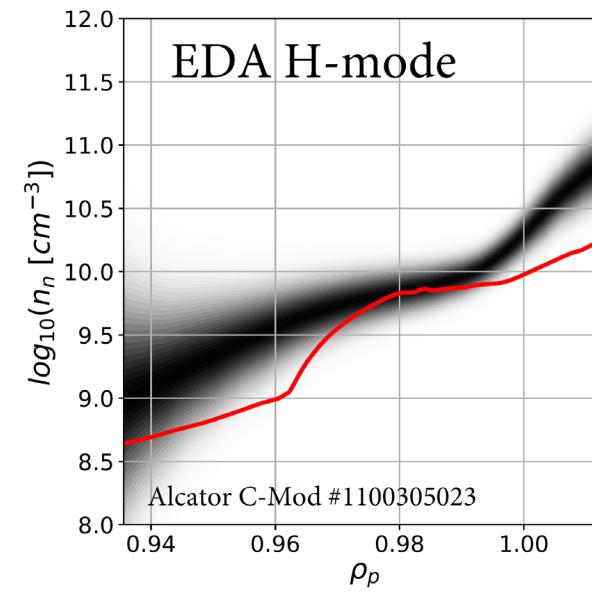
On C-Mod, we compare experimental $Ly\alpha$ outer midplane signals with SOLPS-ITER

- D $Ly\alpha$ brightness is Abel-inverted to obtain local emissivity

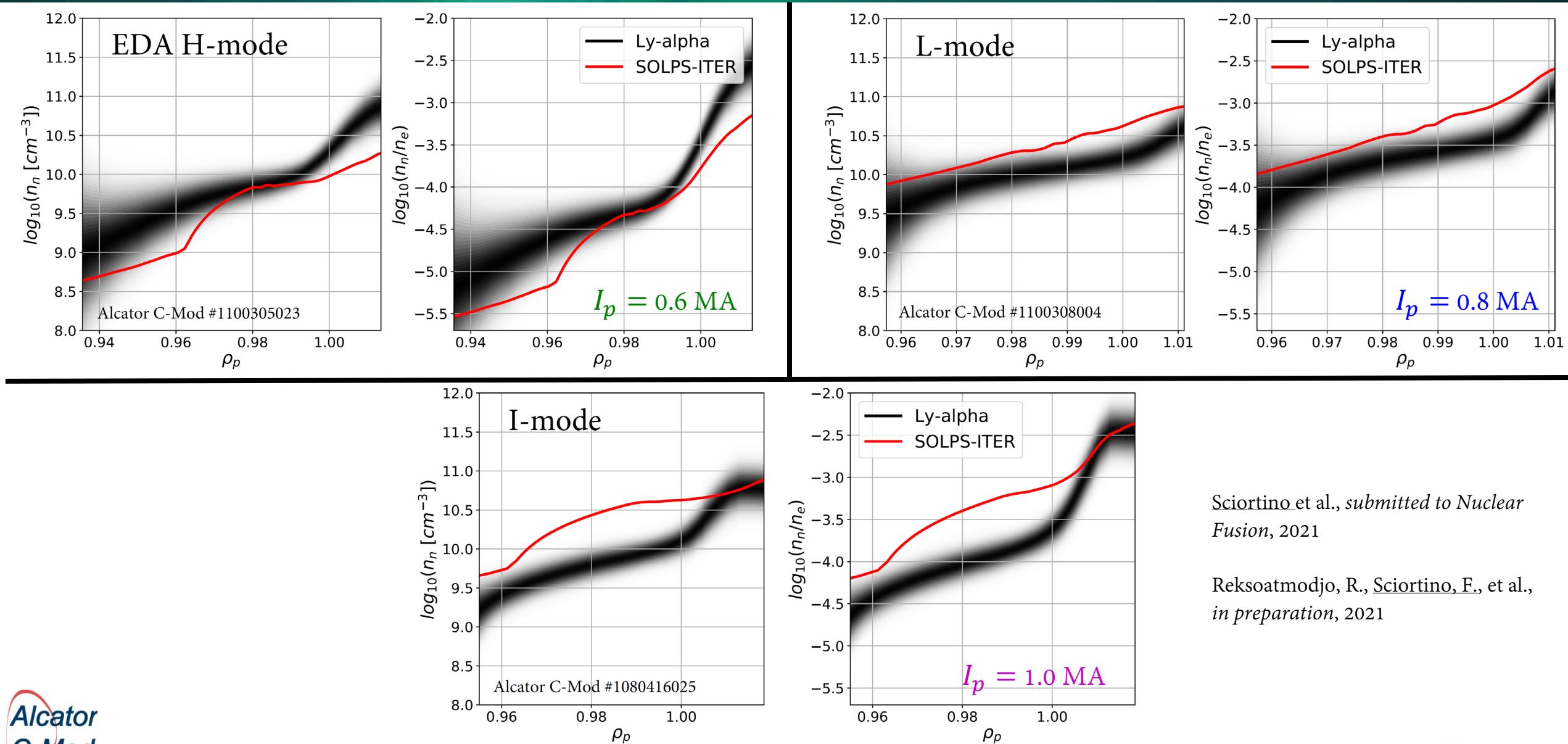
$$n_n = \frac{\varepsilon_{Ly\alpha}}{\Delta E_{Ly\alpha} \ n_e \ PEC_{Ly\alpha}(n_e, T_e)}$$



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



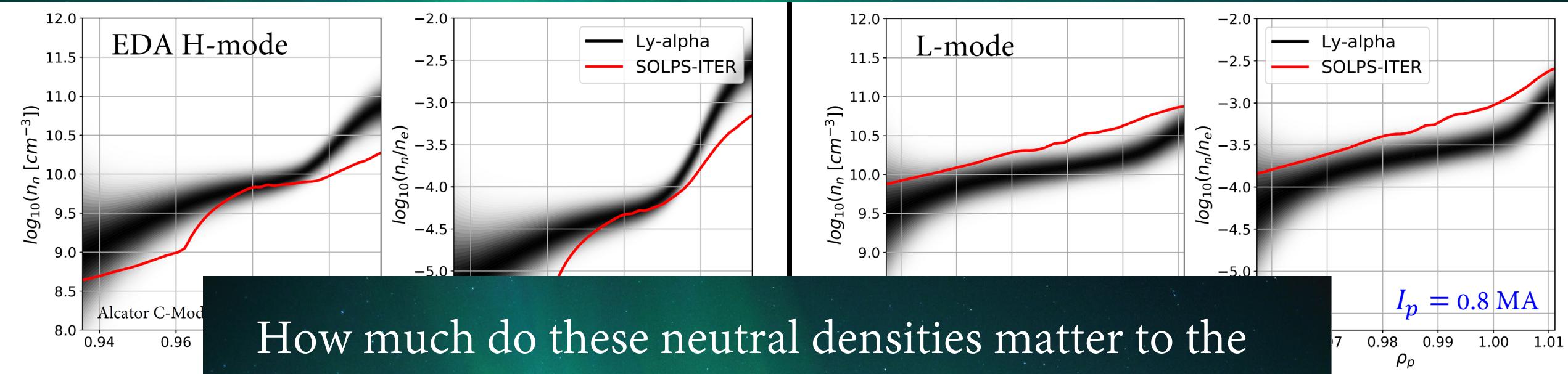
Good agreement between SOLPS-ITER and outer midplane $Ly\alpha$ measurements



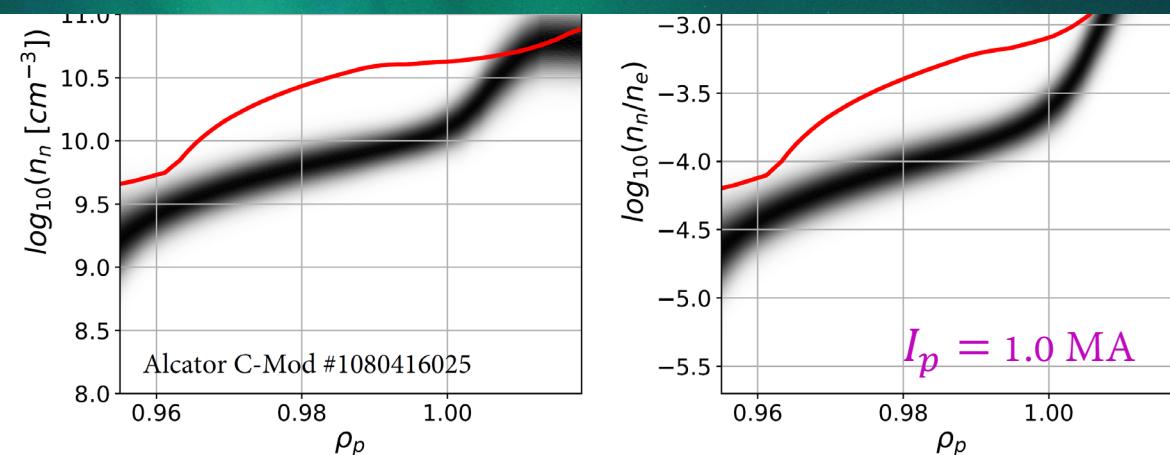
[Sciortino et al., submitted to Nuclear Fusion, 2021](#)

Reksoatmodjo, R., [Sciortino, F.](#), et al.,
in preparation, 2021

Good agreement between SOLPS-ITER and outer midplane $Ly\alpha$ measurements



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



[Sciortino et al., submitted to Nuclear Fusion, 2021](#)

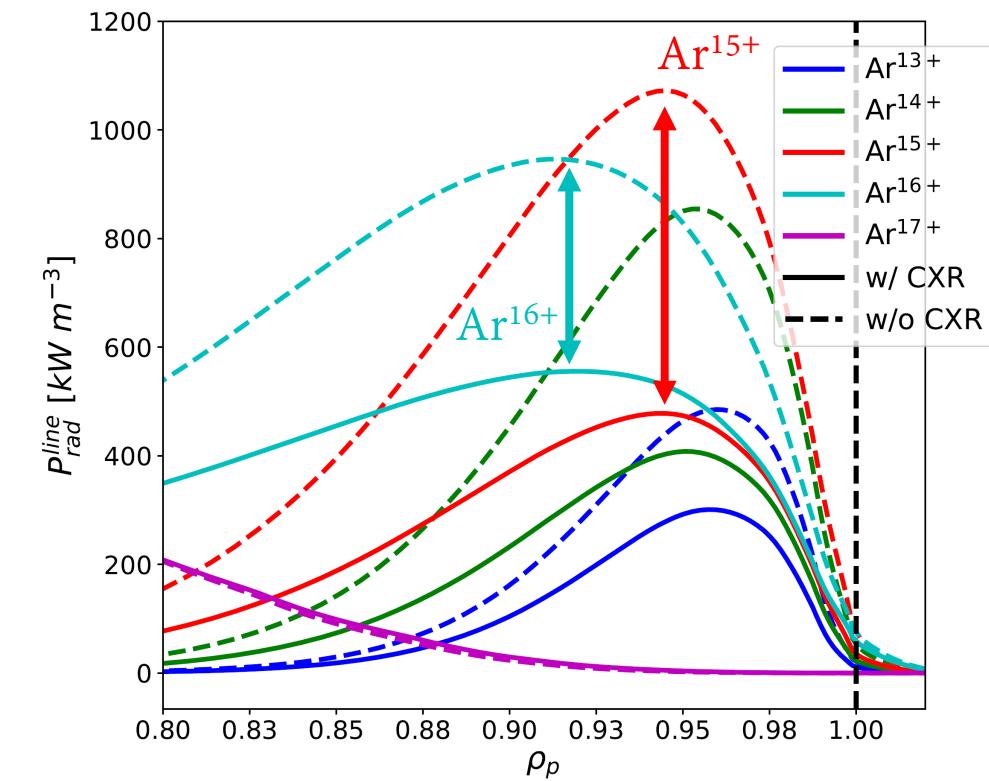
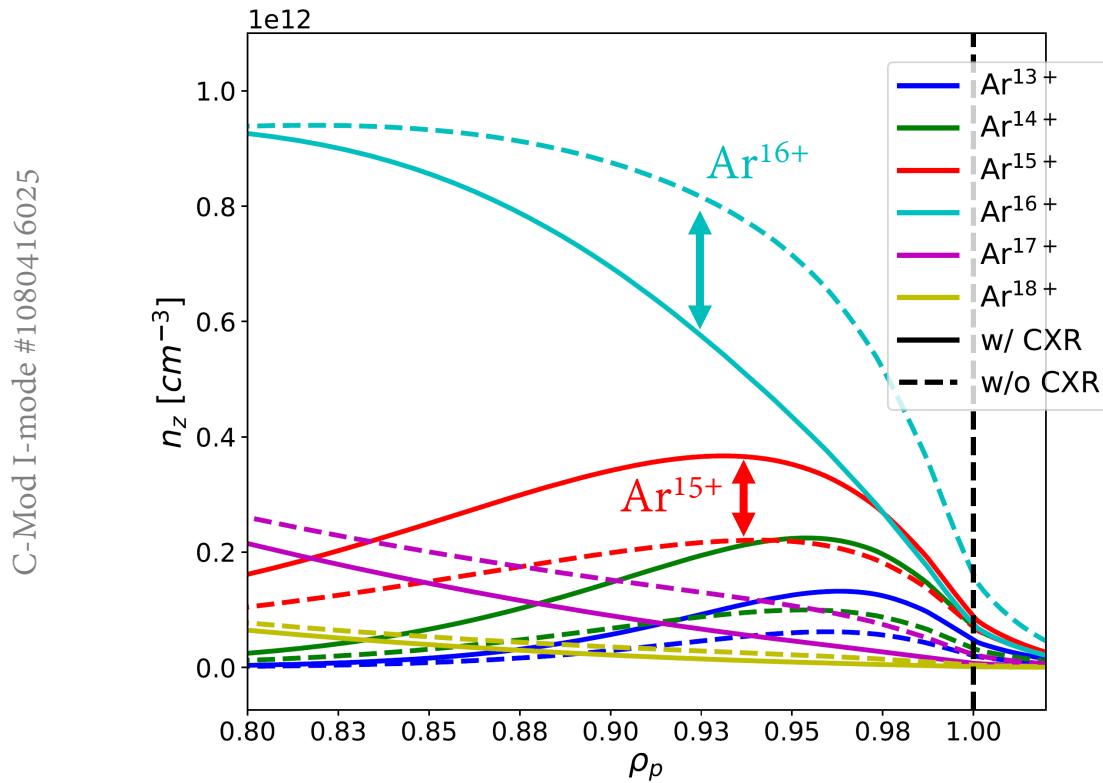
[Reksoatmodjo, R., Sciortino, F., et al., in preparation, 2021](#)

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

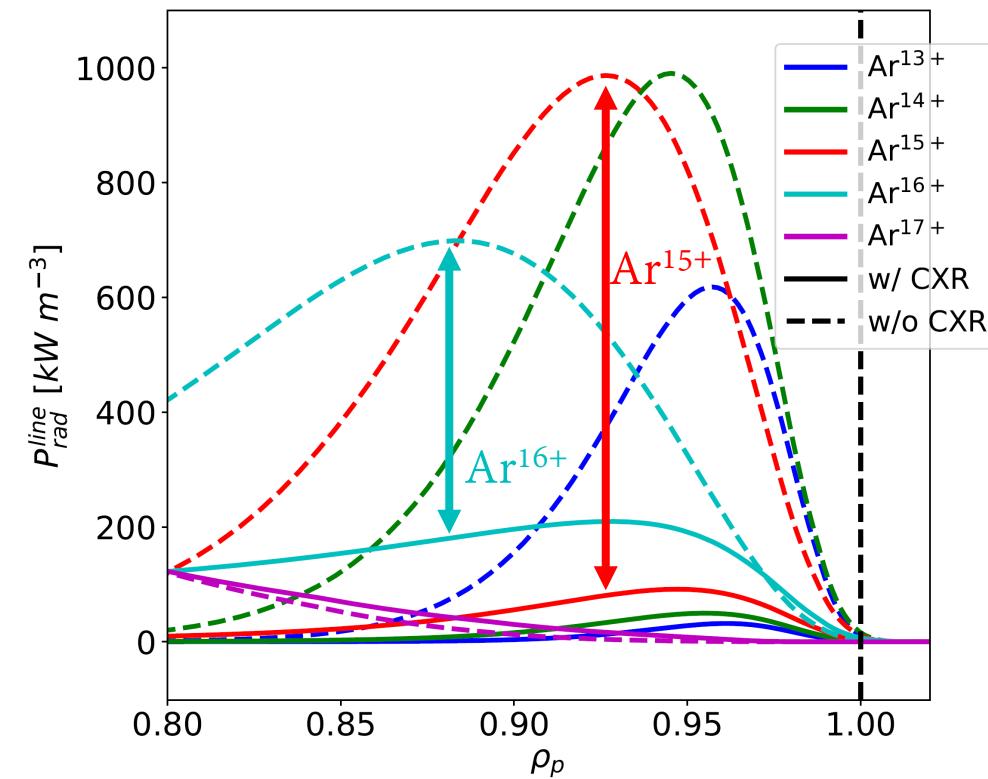
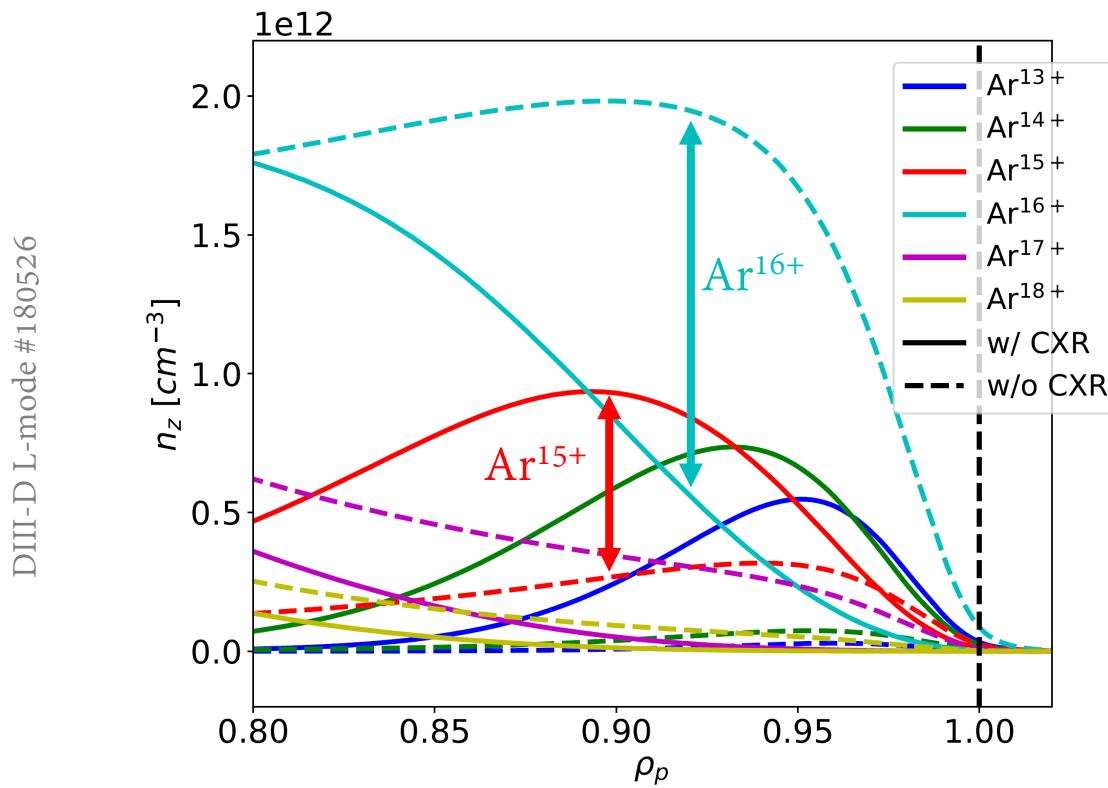
- Neutral densities from SOLPS-ITER/EIRENE (I-mode case)



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)



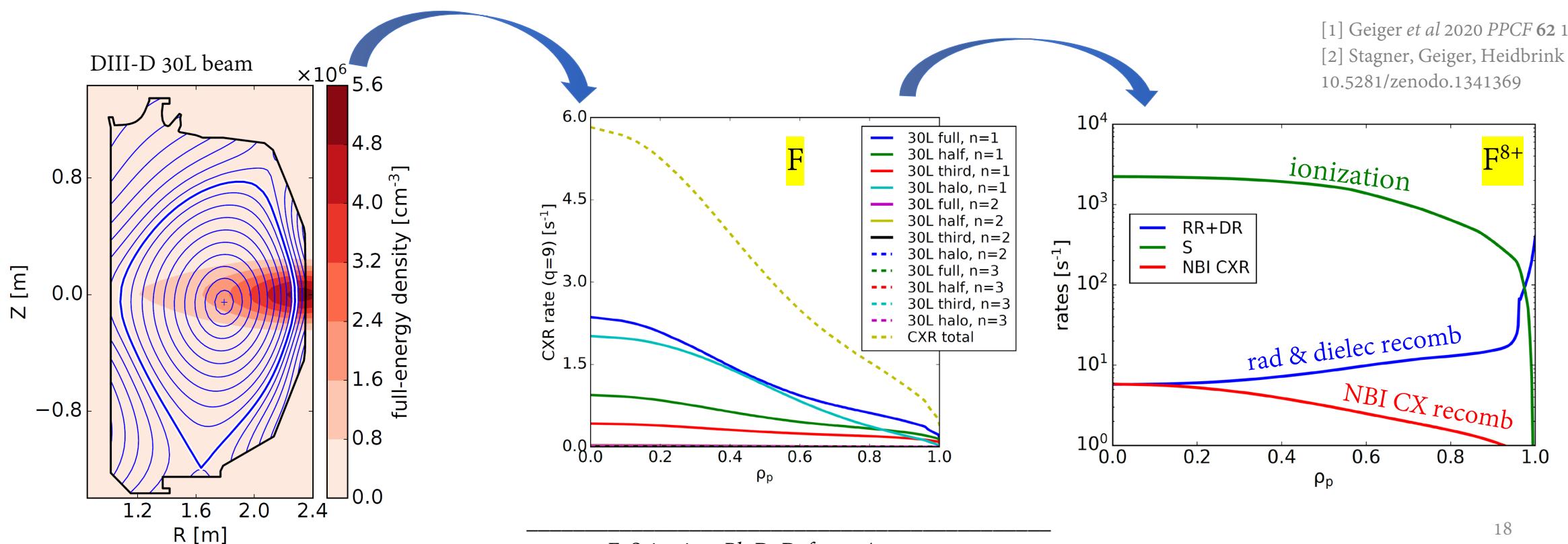
See also Dux et al 2020 *Nucl. Fusion* 60 126039

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

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



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



Neutral Beam Injection produces neutral populations at different energies (max \sim 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

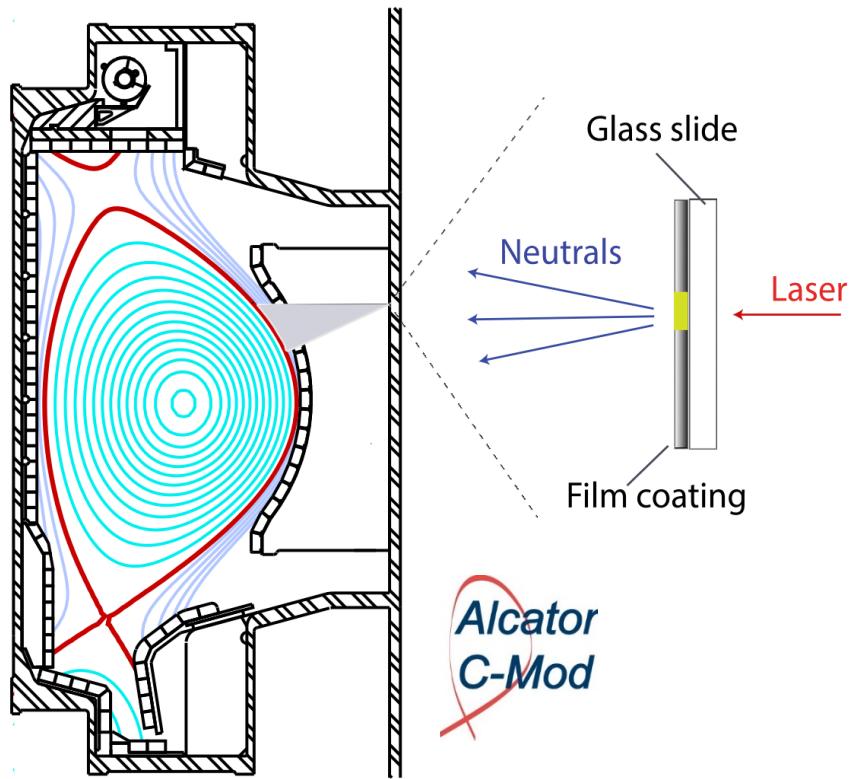
[2] Stagner, Geiger, Heidbrink -
10.5281/zenodo.1341369

**NBI CXR never as important as edge neutrals for
particle transport simulations**

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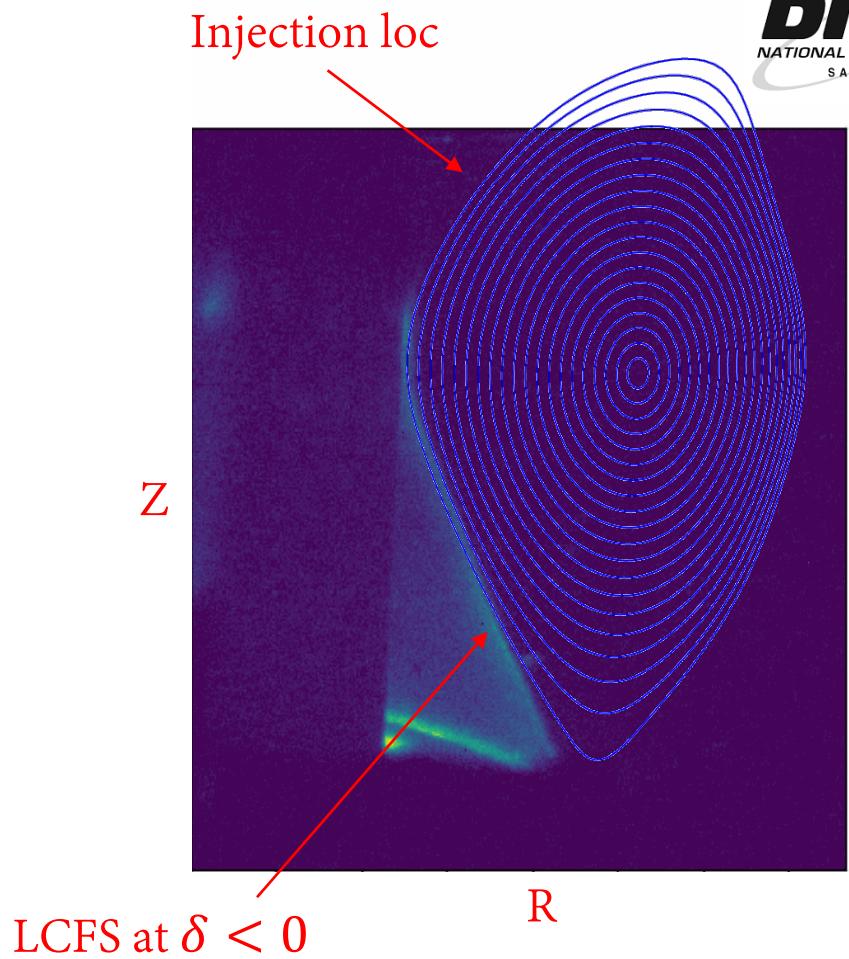
Inferring particle transport from Laser Blow-Off (LBO) injections



*Alcator
C-Mod*

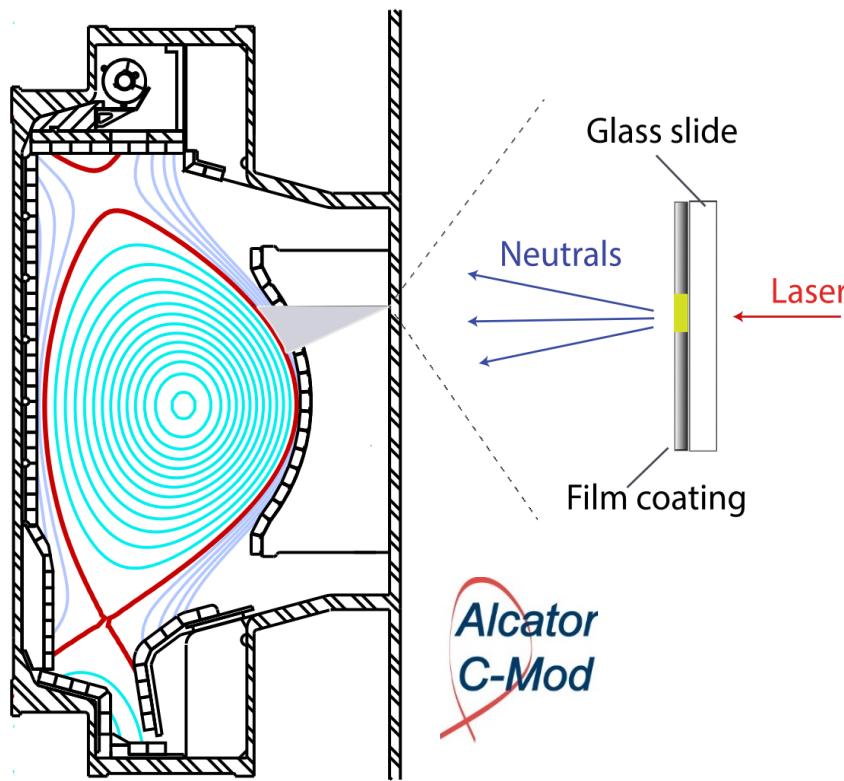
Non-perturbative *trace* amounts of *non-recycling, non-intrinsic* ions
(Ca for C-Mod; F and Al for DIII-D)

- Spectroscopic diagnostics used to track ion spatio-temporal dynamics



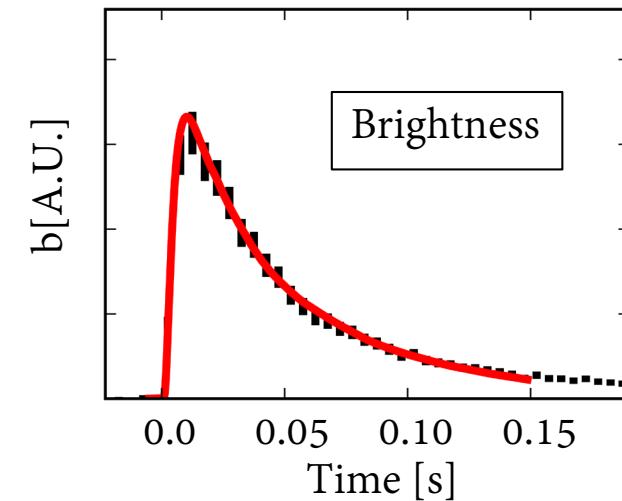
unfiltered fast camera in DIII-D $\delta < 0$ experiment

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



Expt. data

Synth. data



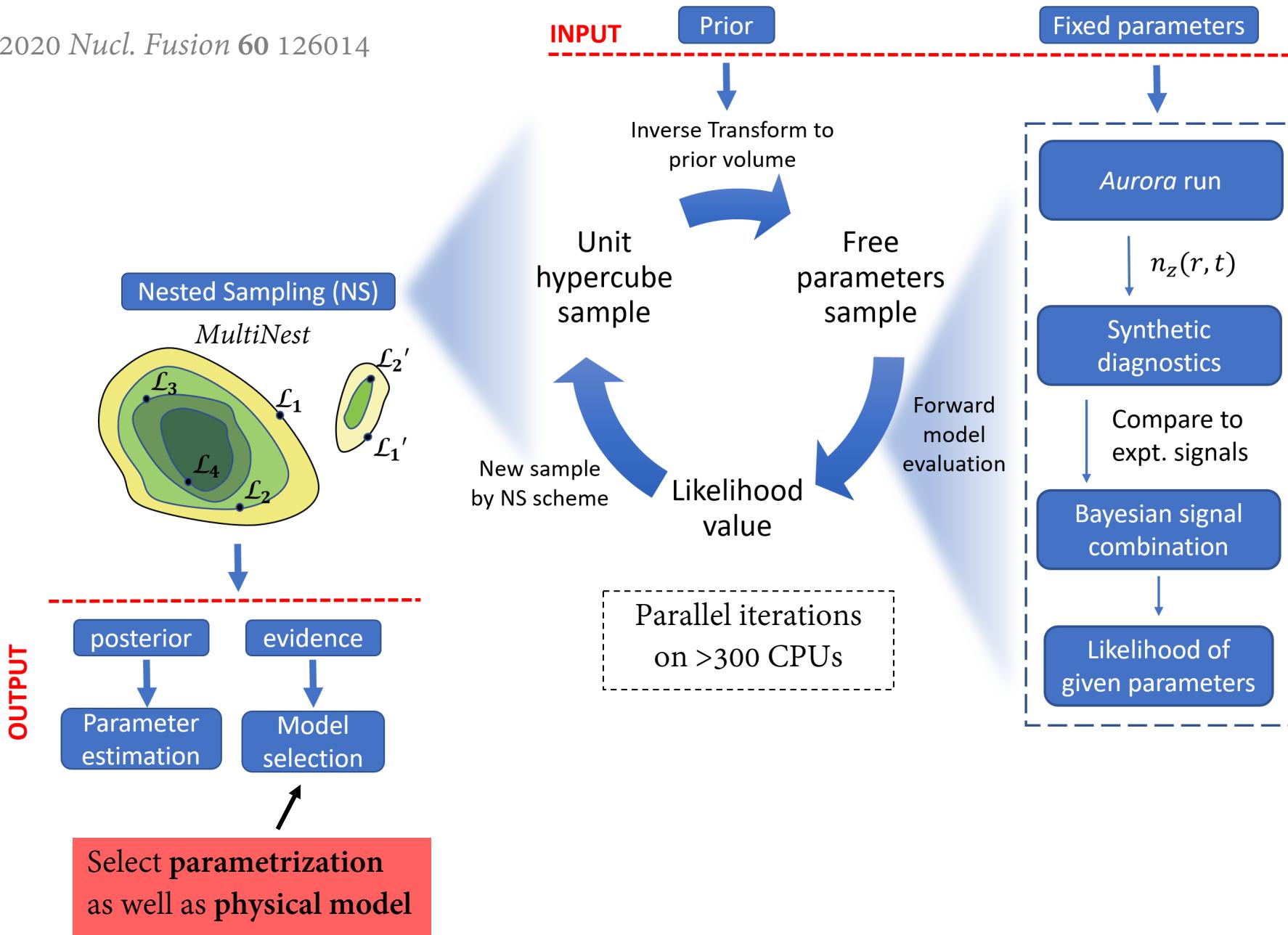
Aurora simulation
(forward model)

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

Plasma geometry, kinetic profiles, ...

D & v (free parameters)



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 Imaging Crystal Spectroscopy (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

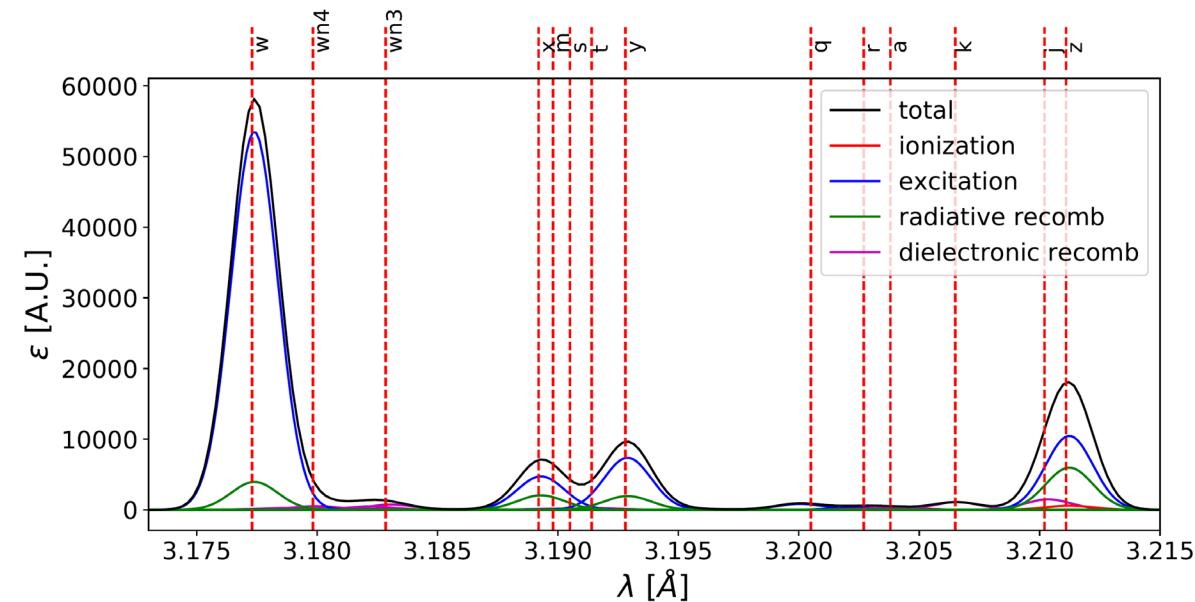
Includes hundreds of satellite lines from Li-like Ca

- 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



Stronger constraints on particle transport

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

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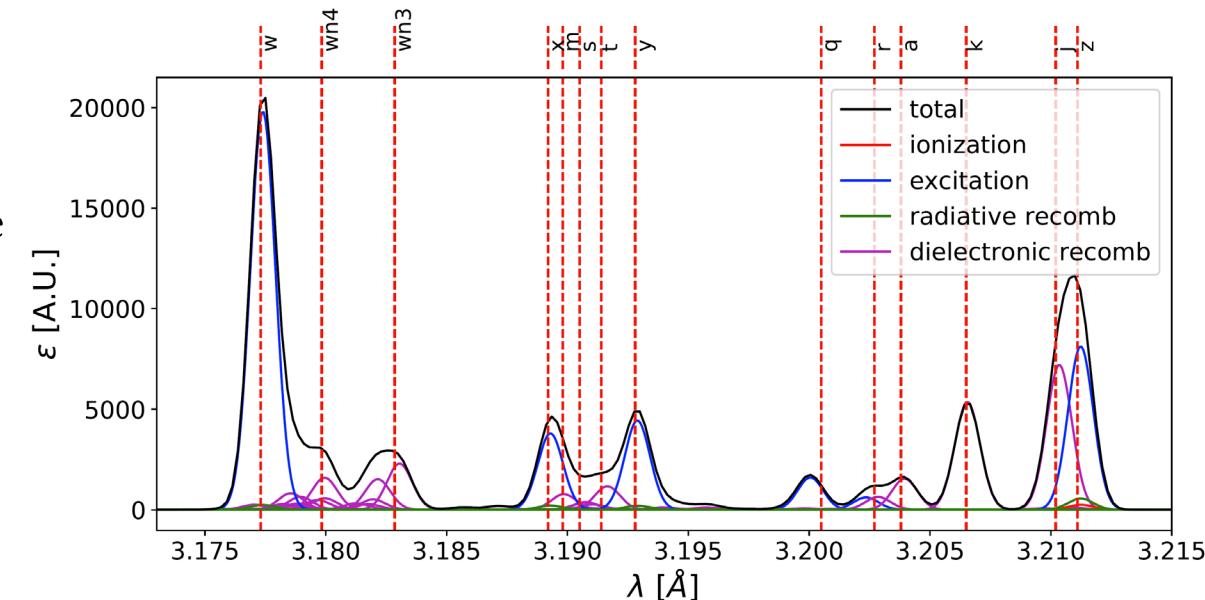
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Sciortino et al., *submitted to Nuclear Fusion*, 2021



Stronger constraints on particle transport

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

Modeling the full K_{α} spectrum of He-like Ca and Li-like satellites

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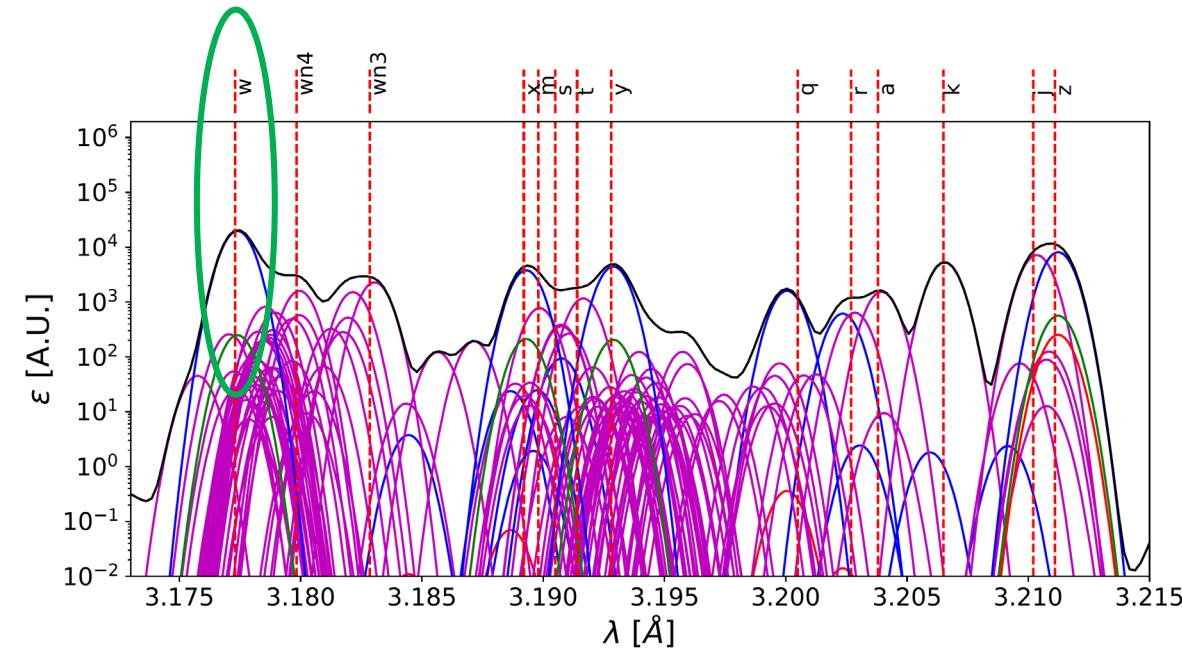
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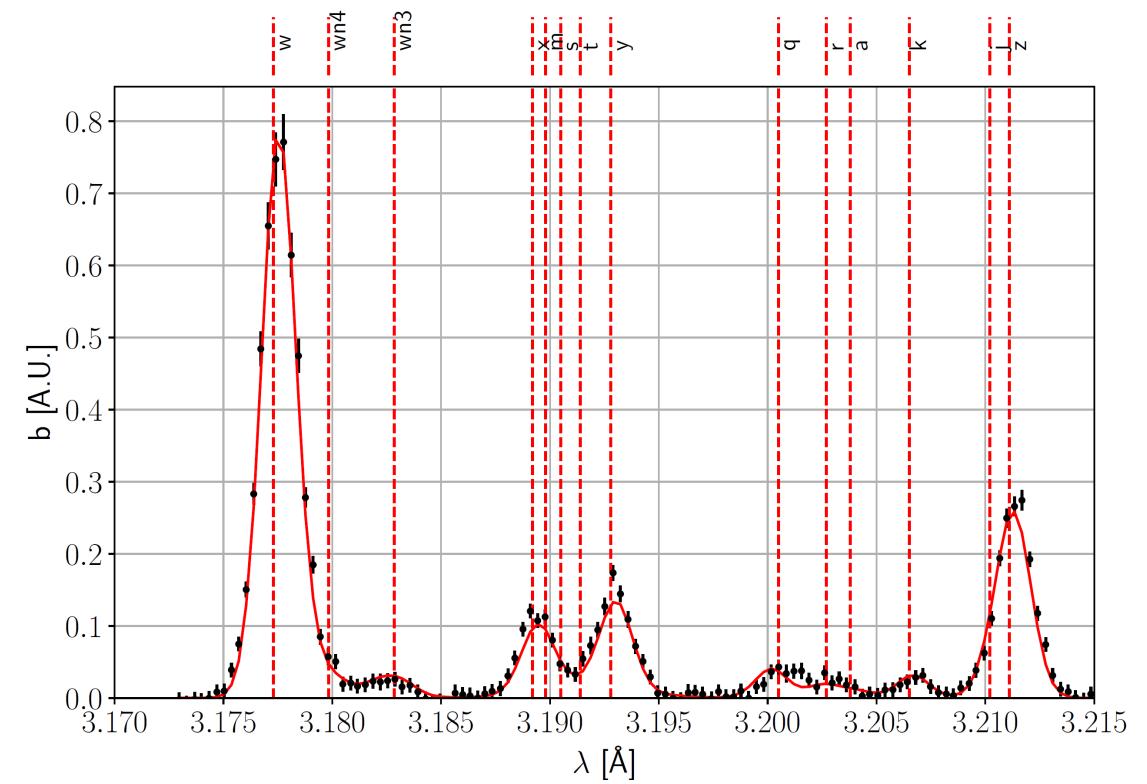
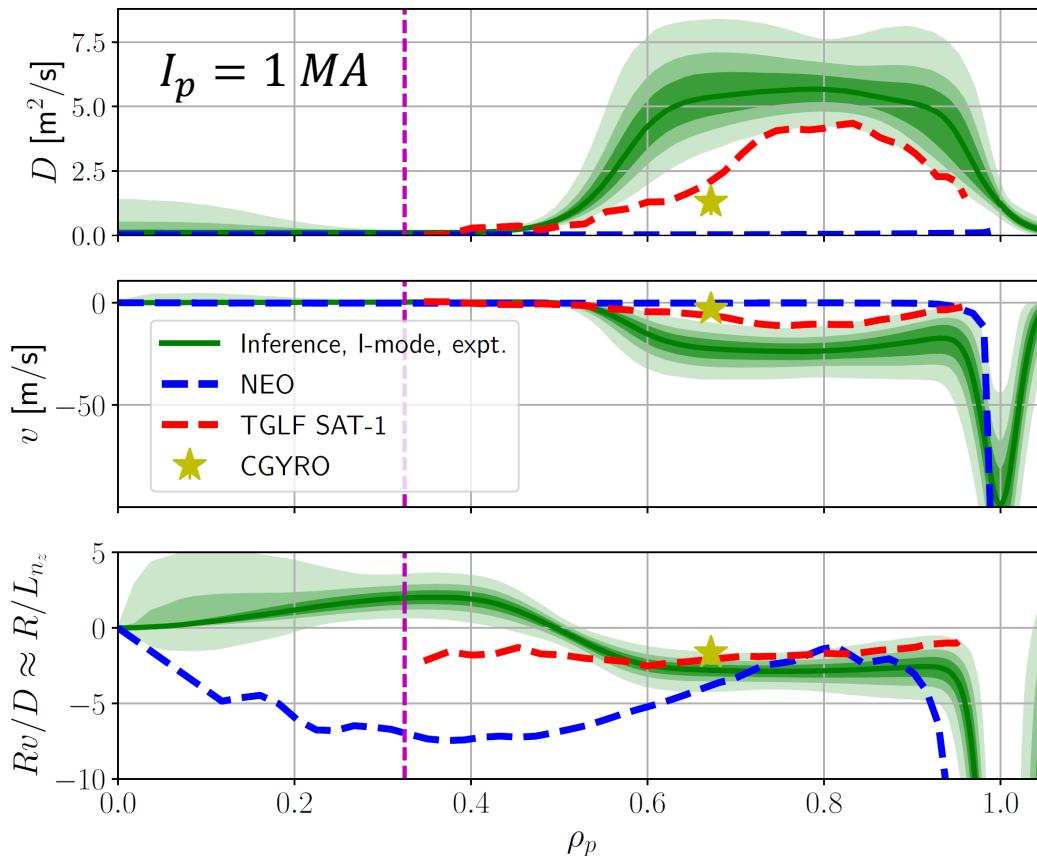


Stronger constraints on particle transport

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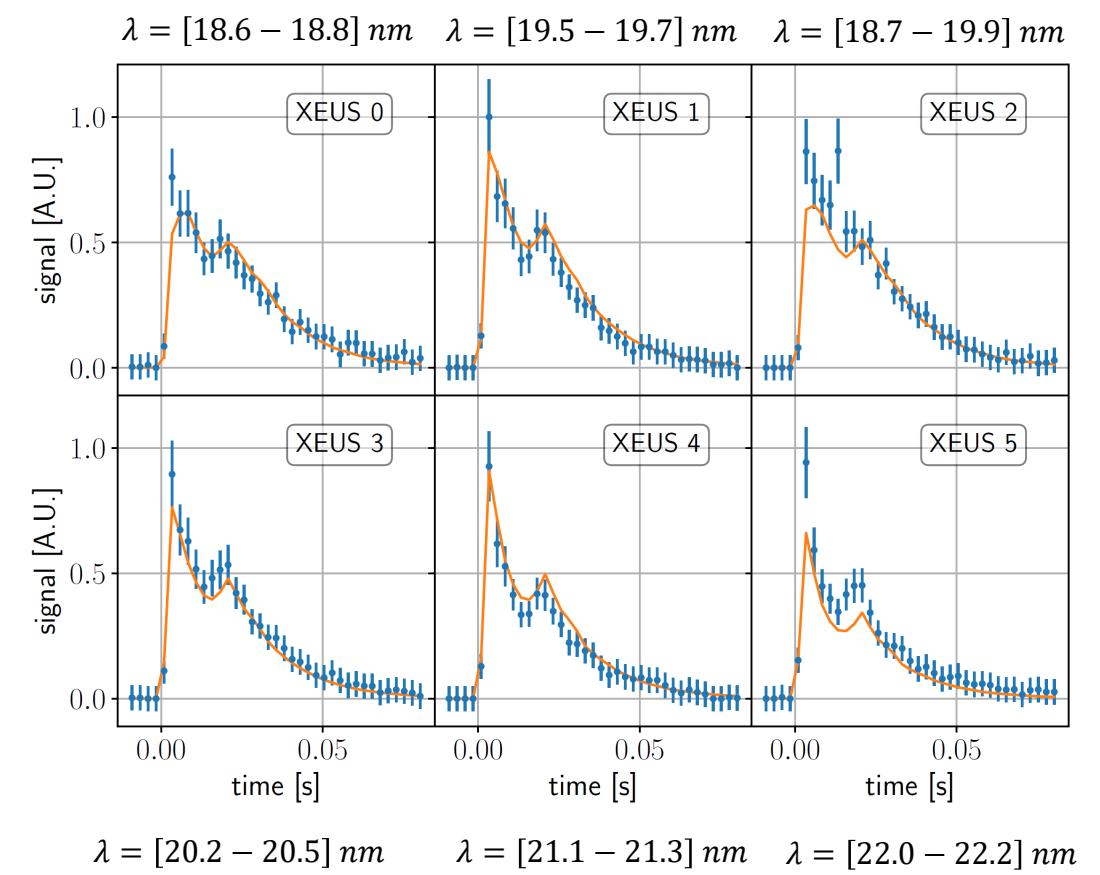
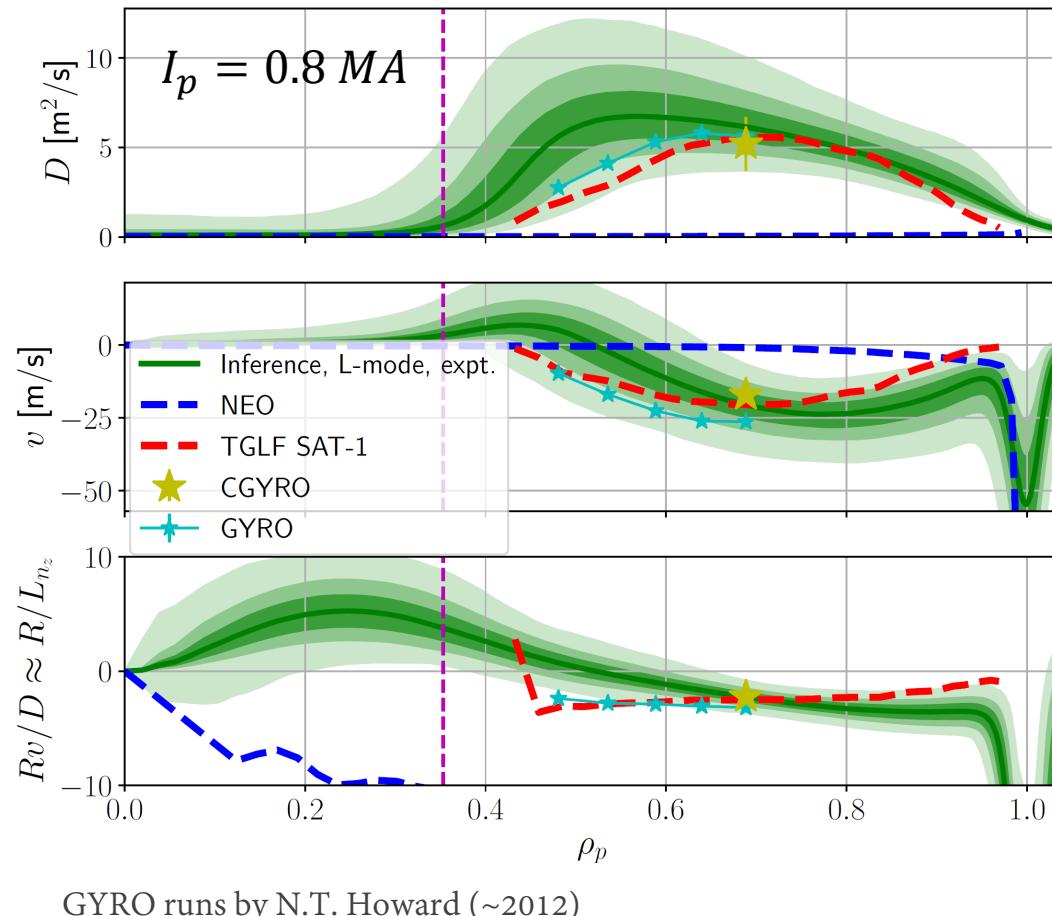
Experimental inferences in multiple ELM-free regimes: I-mode

- 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



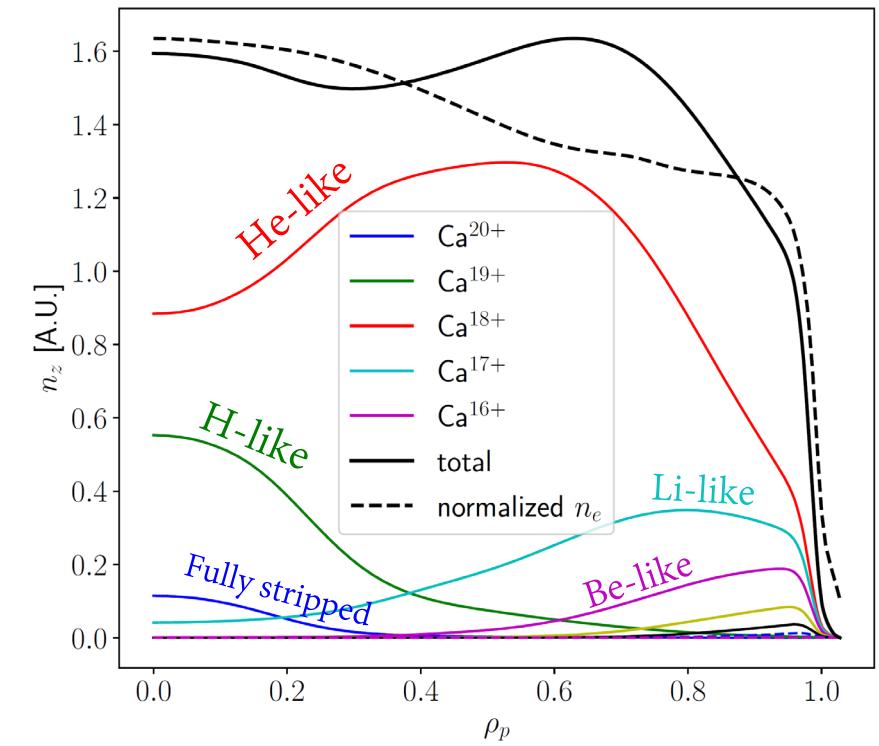
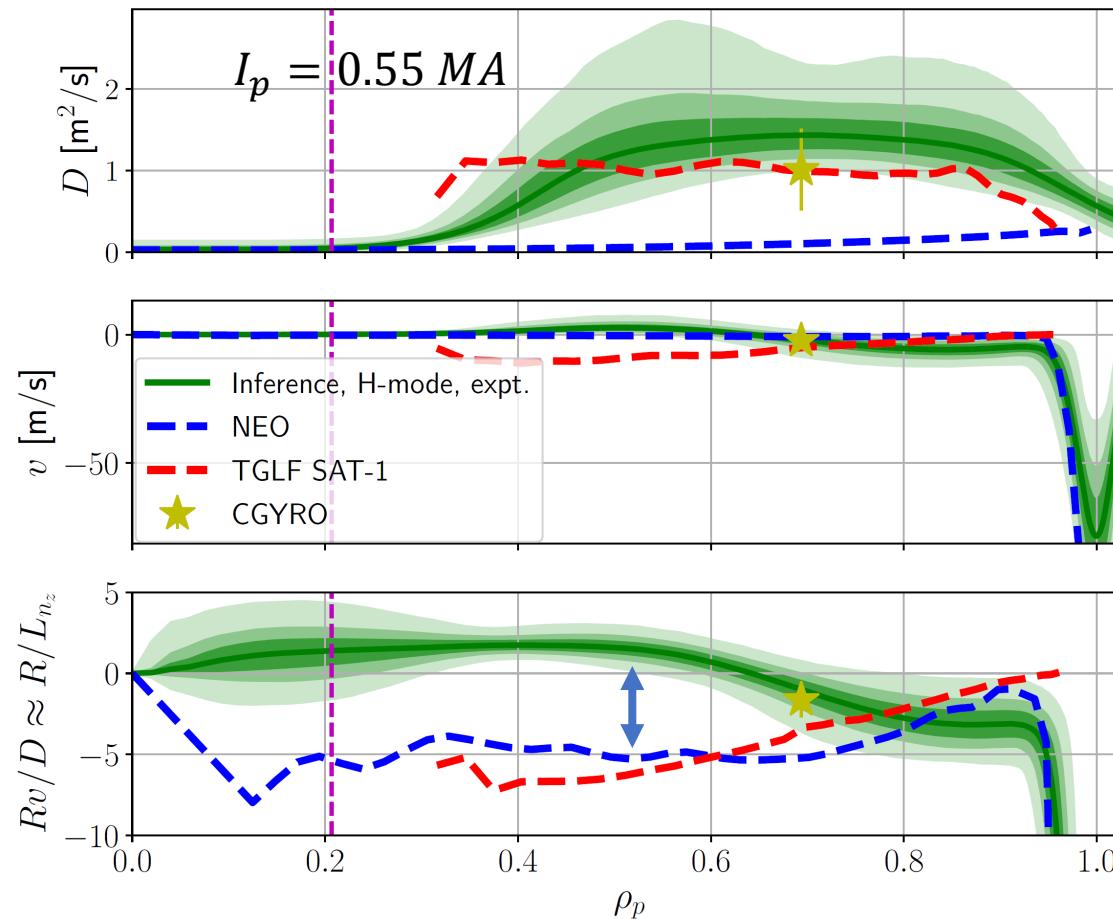
Experimental inferences in multiple ELM-free regimes: L-mode

- 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)



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 $\delta < 0$ 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

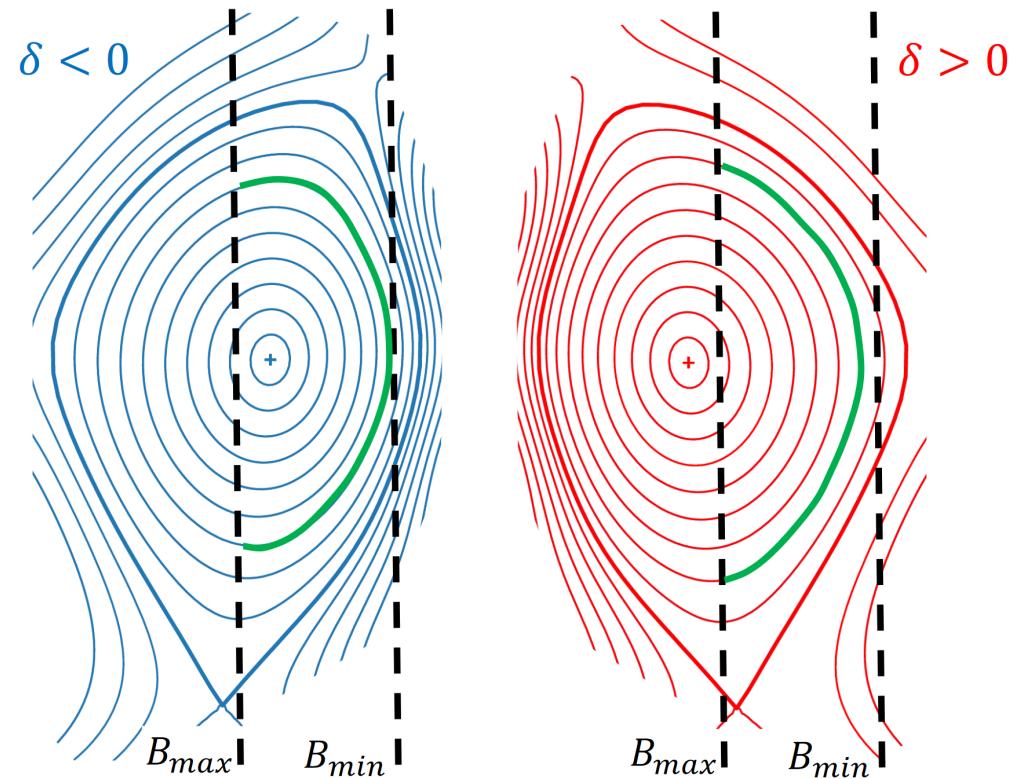
- Previous $\delta < 0$ research, with inner-wall limited plasmas, suggested shape effect on trapped particle orbits

Marinoni 2009 PPCF 51 055016

Austin PRL 122, 115001 (2019)

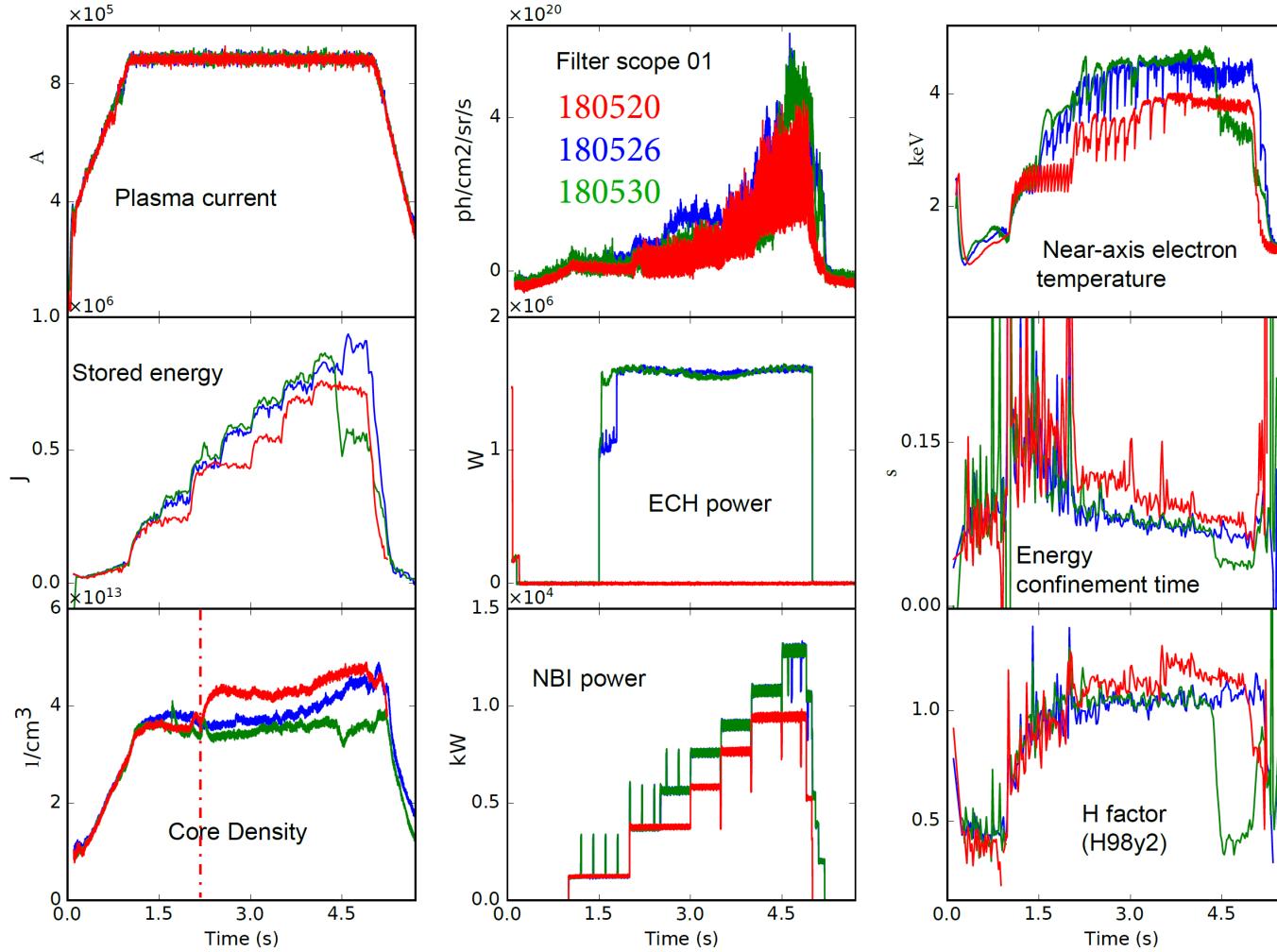
Fontana 2018 NF 58 024002

...



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:

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

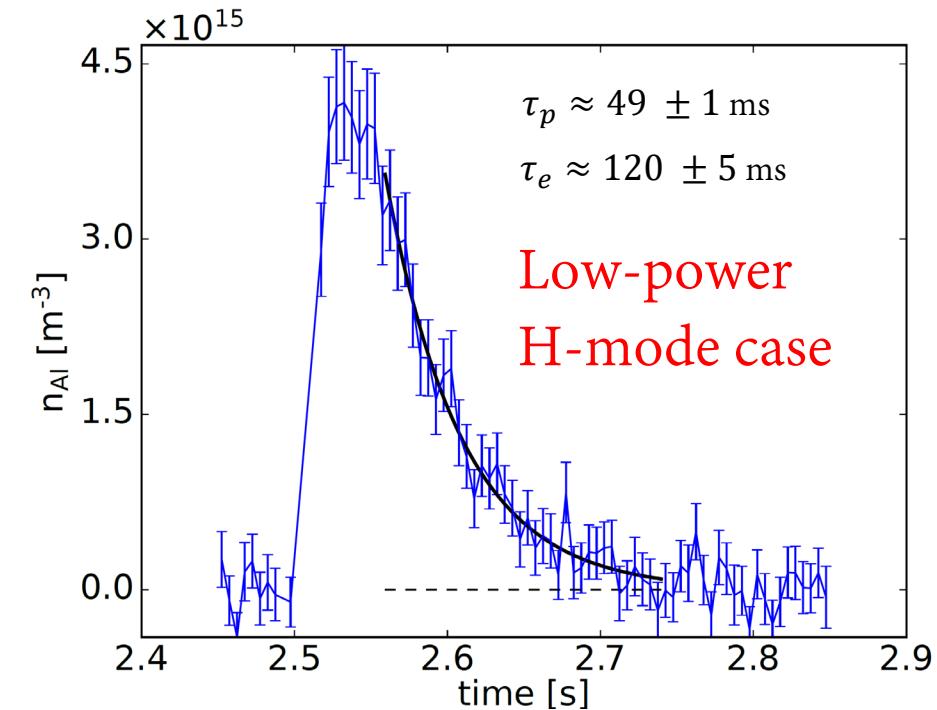
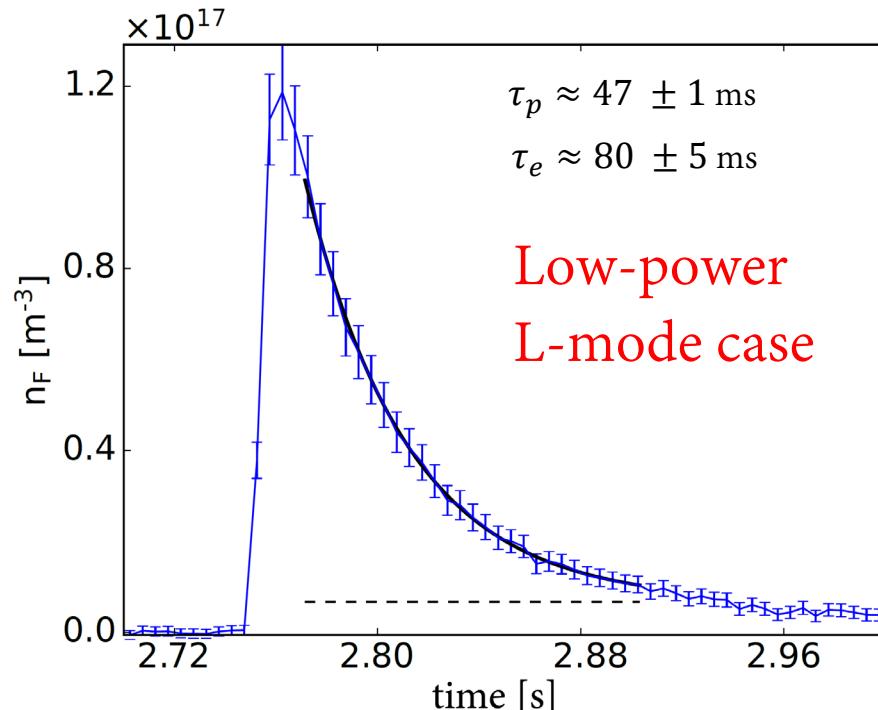
Confinement times indicate favorable impurity transport



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 – as in I-mode



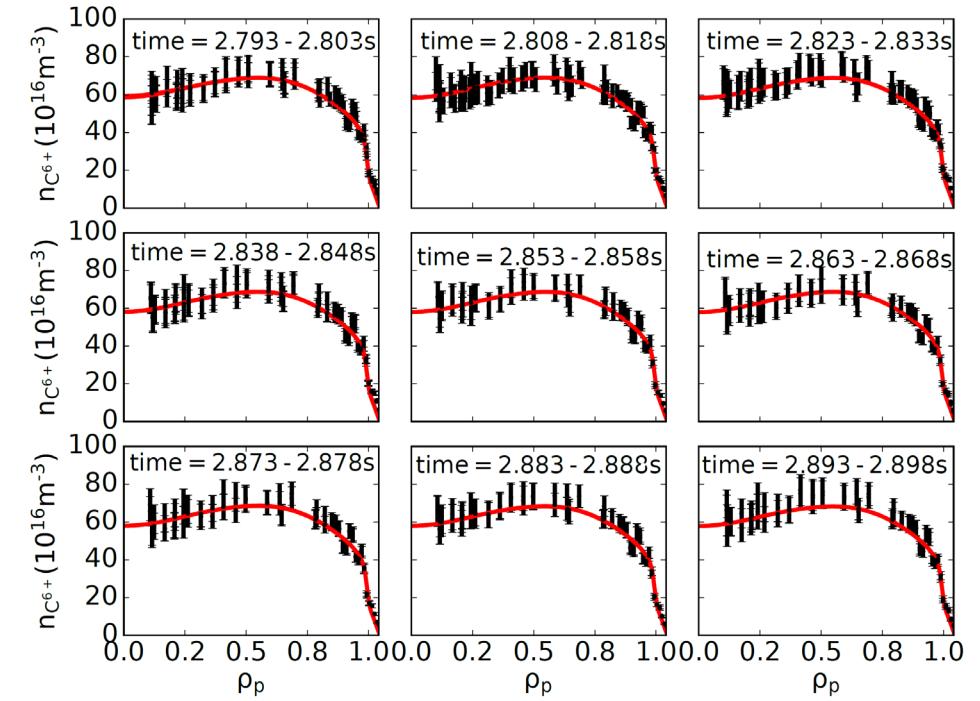
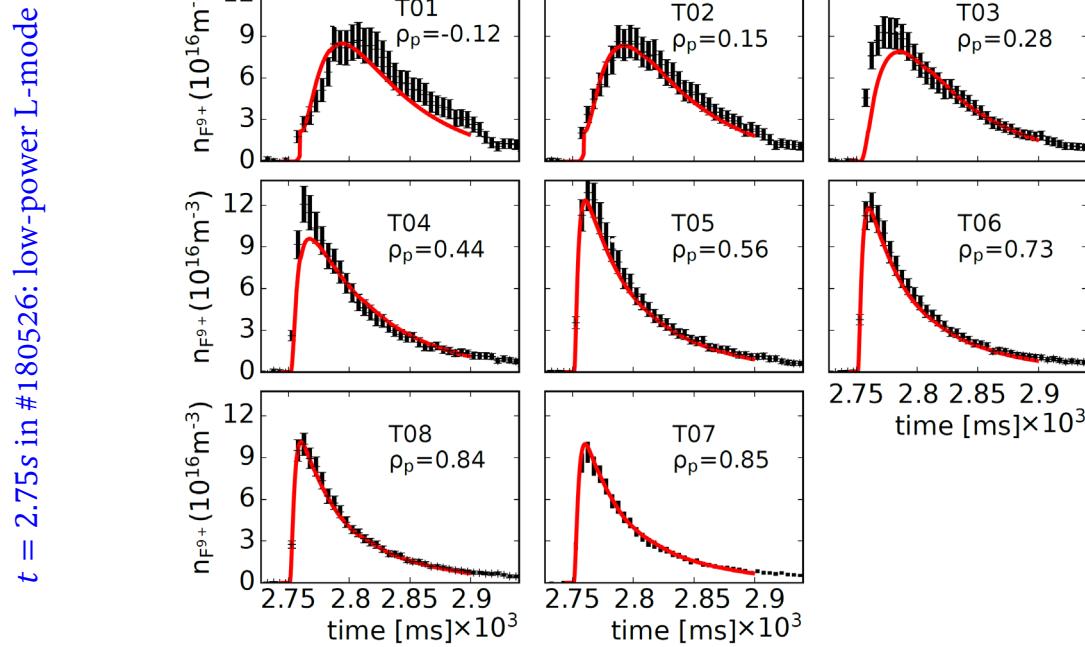
Multi-species inferences are a major new step for impurity transport model validation

- 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 ν



Meneghini, Smith et al.
2015 NF 55 083008

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



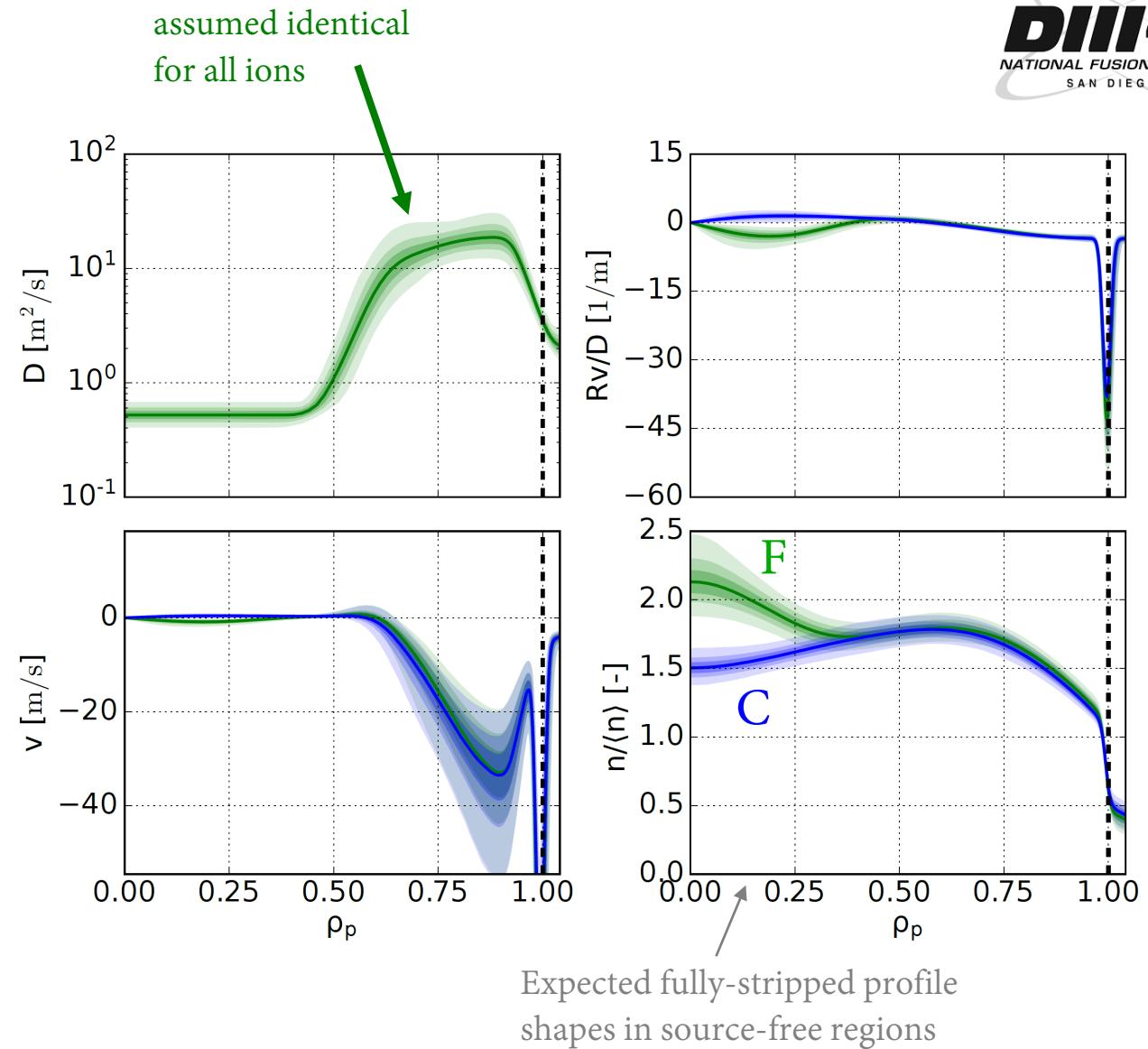
Further constraints on impurity transport from SXR and core-SPRED (additional slides)

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?

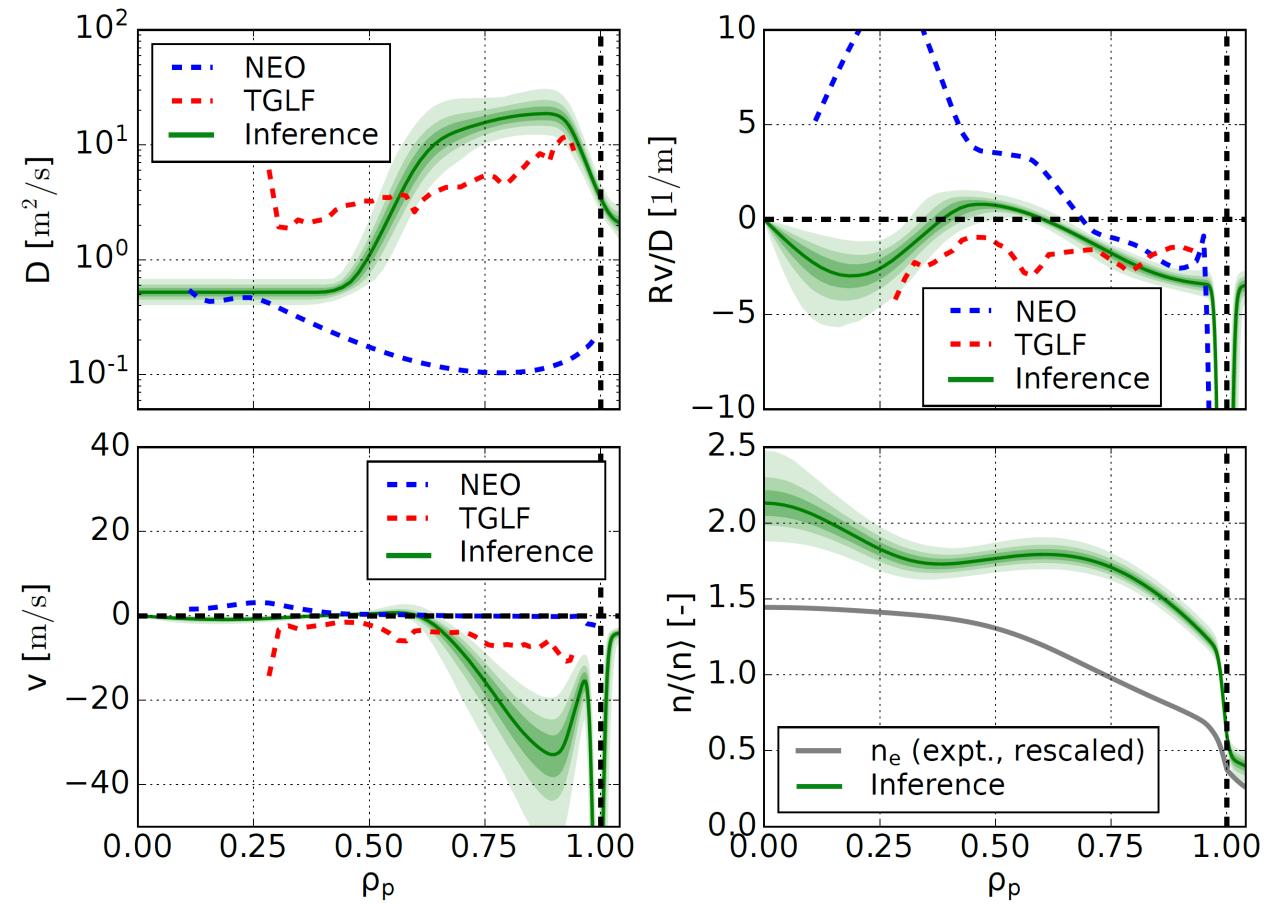
Next: comparison to theory models
for the species injected via LBO



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



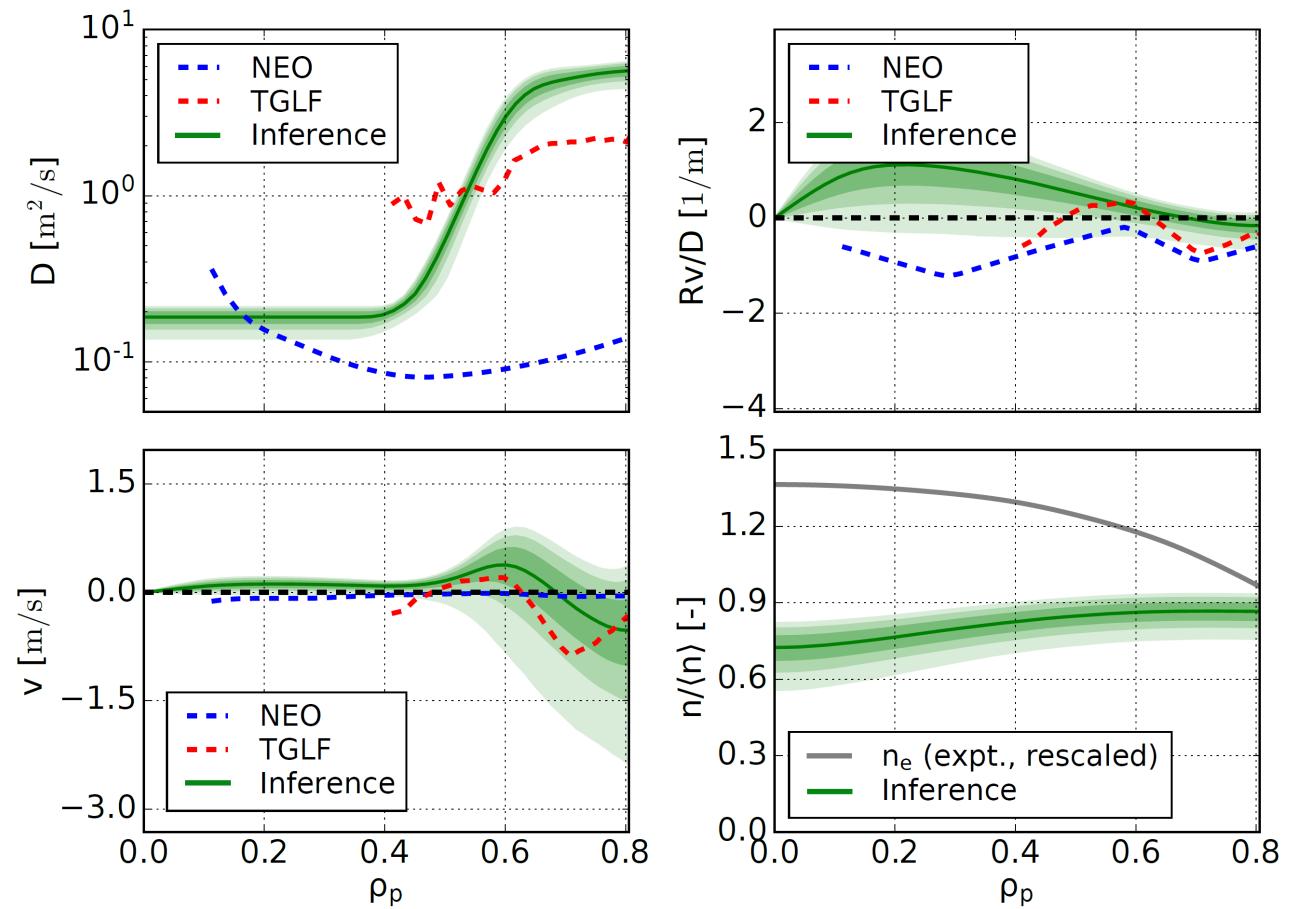
- Multi-species impurity transport inference in **low-power L-mode**
 - F (LBO) and C (intrinsic)
- Near-axis peaking inverted between species
 - Difference is outside of uncertainties
 - Z-scaling of transport?
- D and v magnitudes match NEO near axis
- D at midradius is underestimated by $\sim 2\text{-}3x$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



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



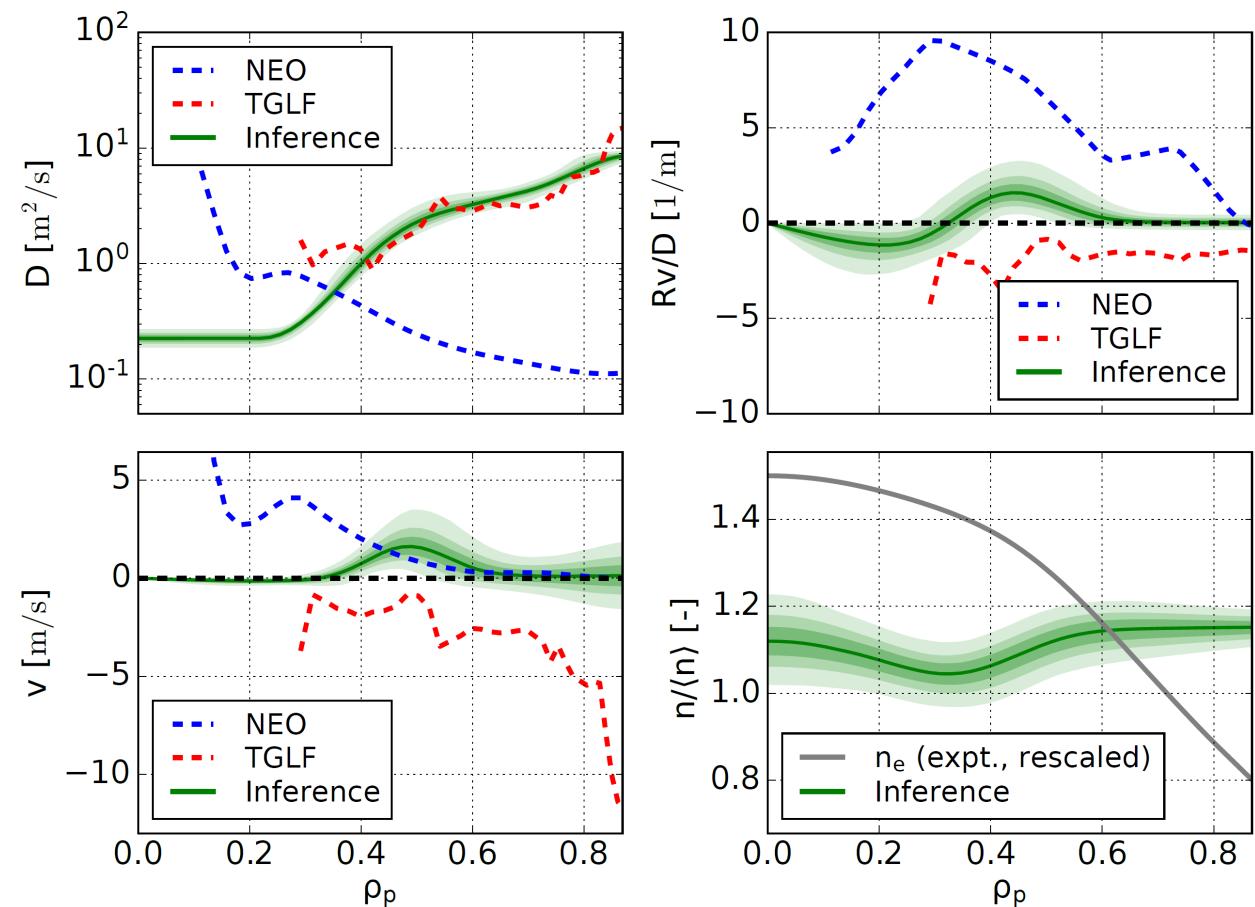
- Multi-species impurity transport inference in **low-power H-mode**
 - Al (LBO) and C (intrinsic)
- Unclear LBO source prevents us from making statements about pedestal transport...
- Significant discrepancy in D at midradius
- Flat (or hollow) impurity profiles
 - Relatively **good agreement between 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 radiation⁴
 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-D⁶
 - a) Creation of **HPC** frameworks for **Bayesian** inference²
 - 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
-
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 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*