# Bayesian inference of Experimental Particle Transport in Tokamak Plasmas

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Alcator C-Mod

MIT PSFC

# Impurities and neutrals are key to core-edge integration

This talk is about inference of D's and v's and comparison to theory models

Parameter Estimation
Uncertainty Quantification
Model Selection

Question: are any discrepancies due to inadequate **experimental analysis** or **wrong theory**?

Approach: enable models to disagree with theory
advance forward models
integrated analysis of multiple measurements

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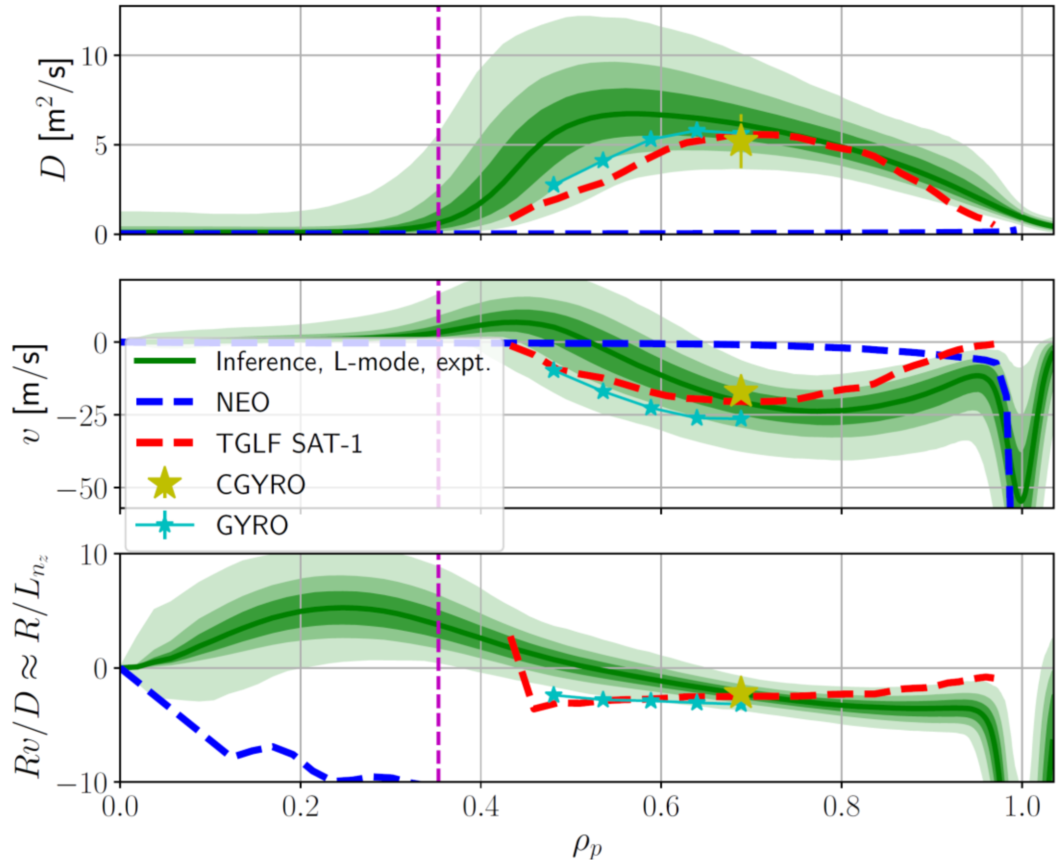
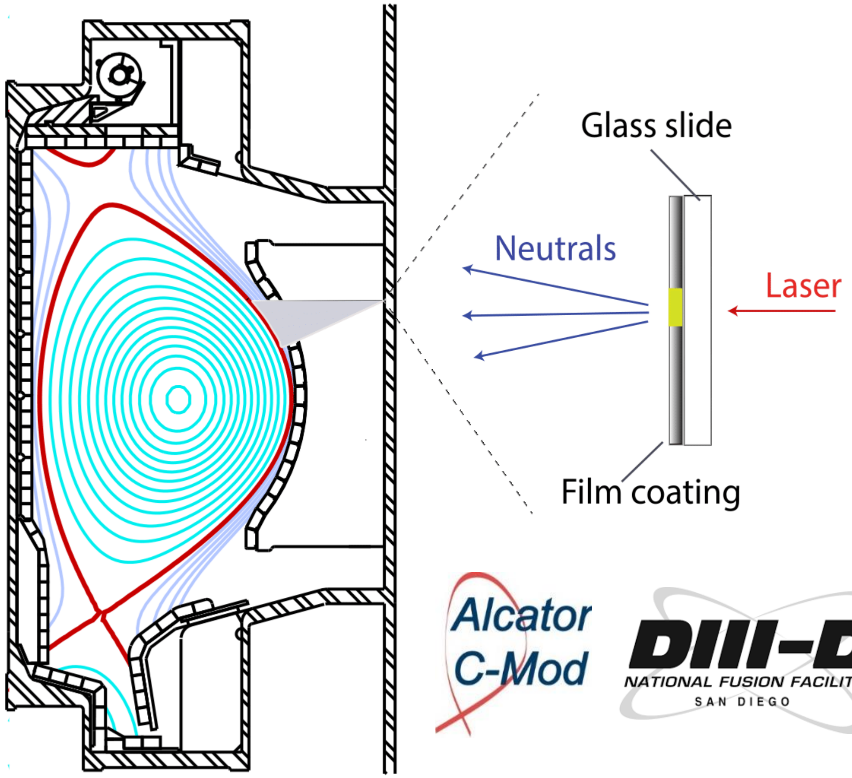
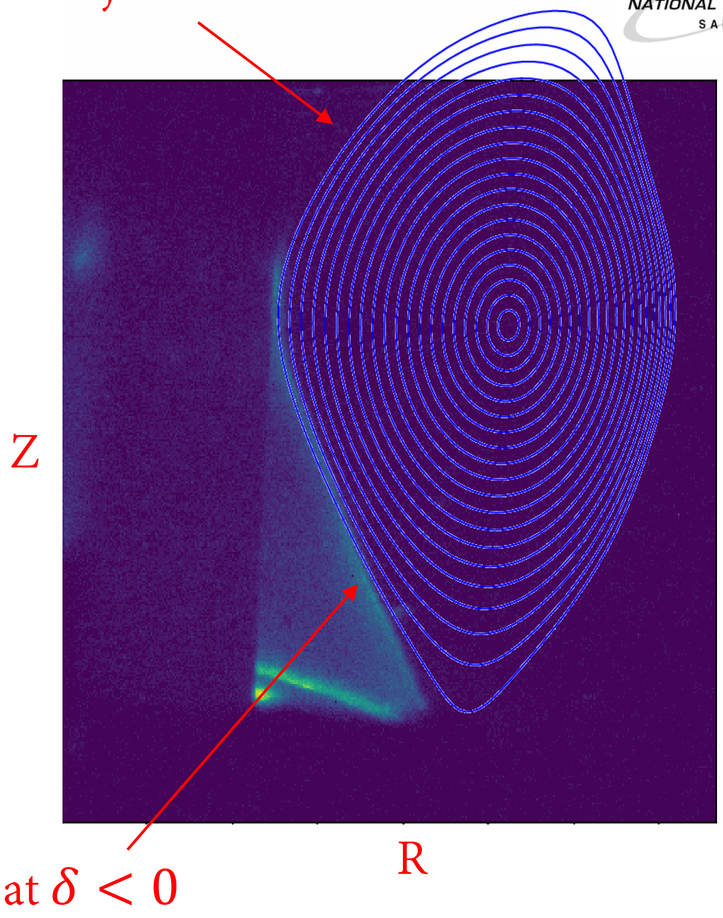



Fig: C-Mod example of D and v inference & comparison to theory models

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




Non-perturbative *trace* amounts of *non-recycling*, *non-intrinsic* ions




*Alternative method for core transport: boron modulation via ICRH [Bruhn PPCF 2018, McDermott NF 2021]*

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

I. Forward models for spectroscopy

II. Bayesian inference of particle transport coefficients

# I. Forward models for spectroscopy

- Simulation capabilities: modeling with Aurora
- Physics fidelity: Charge Exchange (CX) with background neutrals
- Synthetic diagnostics: high-resolution spectral analysis

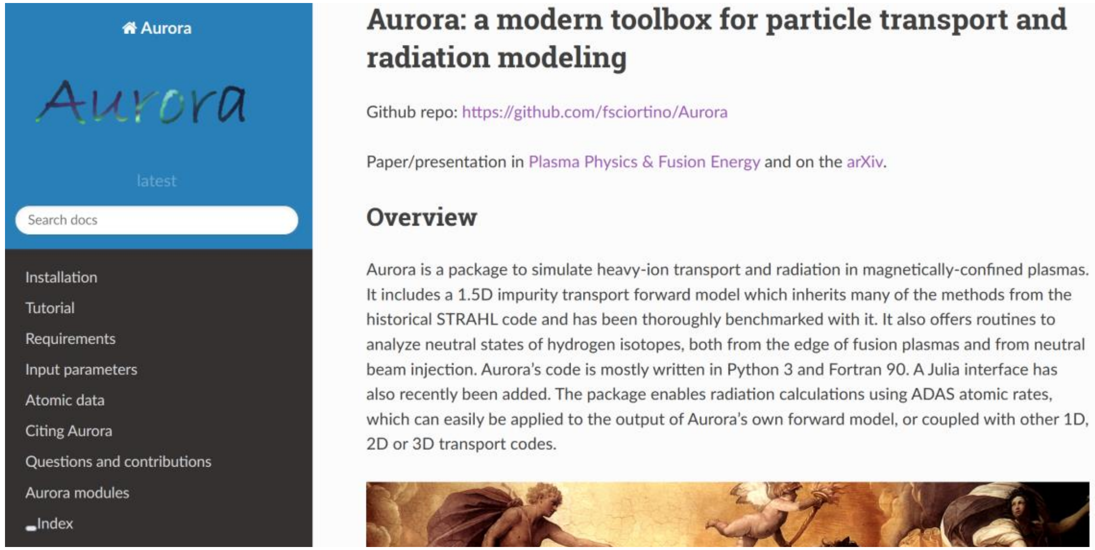
# *Aurora*: a toolbox for particle transport and radiation modeling

- Initially based on the STRAHL code, used for benchmarks

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

- User-friendly and flexible radiation modeling using ADAS rates
  [Summers *et al* 2006 PPCF **48** 263]

- 1.5D impurity transport simulations
  - Efficiently parallelized to infer transport coefficients
  - Options to model ion superstages, arbitrary Z dependences…


Aurora

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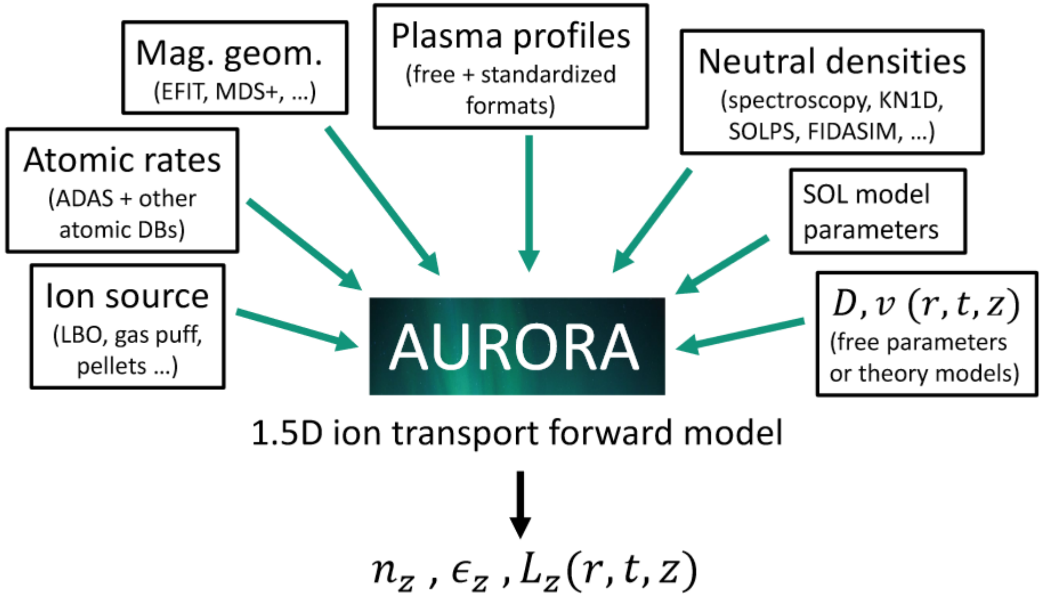
**Aurora: a modern toolbox for particle transport and radiation modeling**

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

Paper/presentation in Plasma Physics & Fusion Energy and on the arXiv.

**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.

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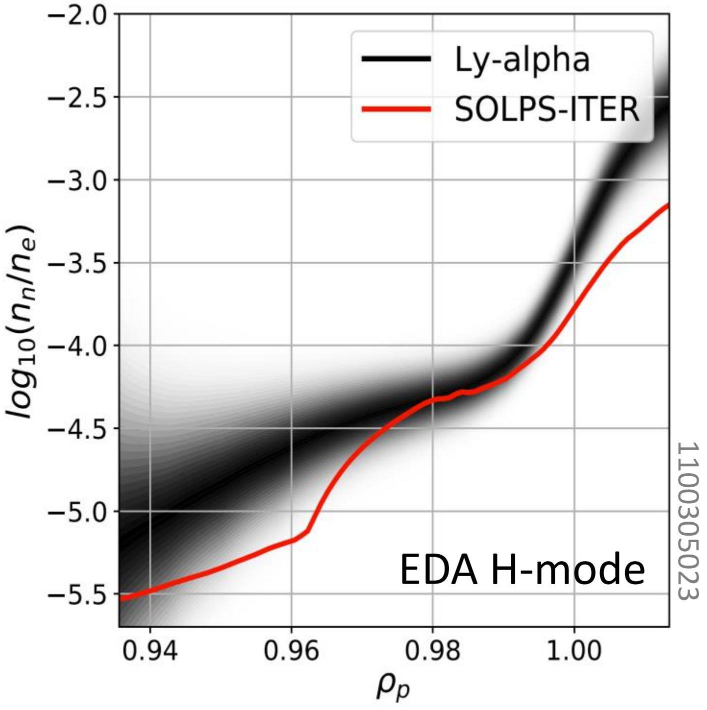
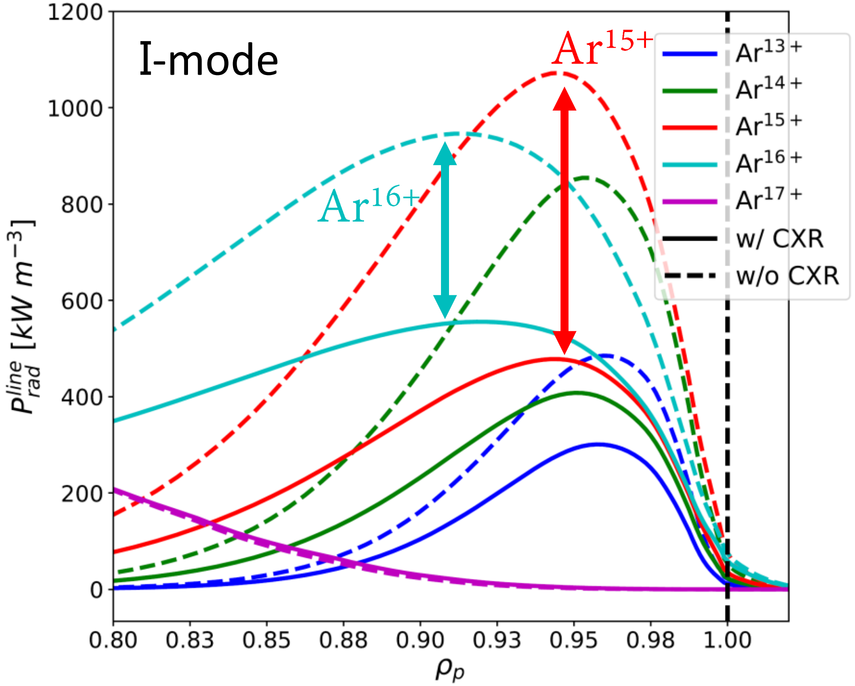
# Physics fidelity: Charge Exchange (CX) between impurities and neutrals

CX can strongly affect the ionization balance of impurities – must be considered for particle transport studies [Dux, NF 2020]

- Direct neutrals measurements are rare, but available on C-Mod via $\mathrm{Ly}_\alpha$ spectroscopy at the outer midplane

Favorable comparison to SOLPS-ITER [Wiesen JNM 2015] using the EIRENE [Reiter FST 2005] Monte Carlo neutral model




Aurora

Alcator C-Mod

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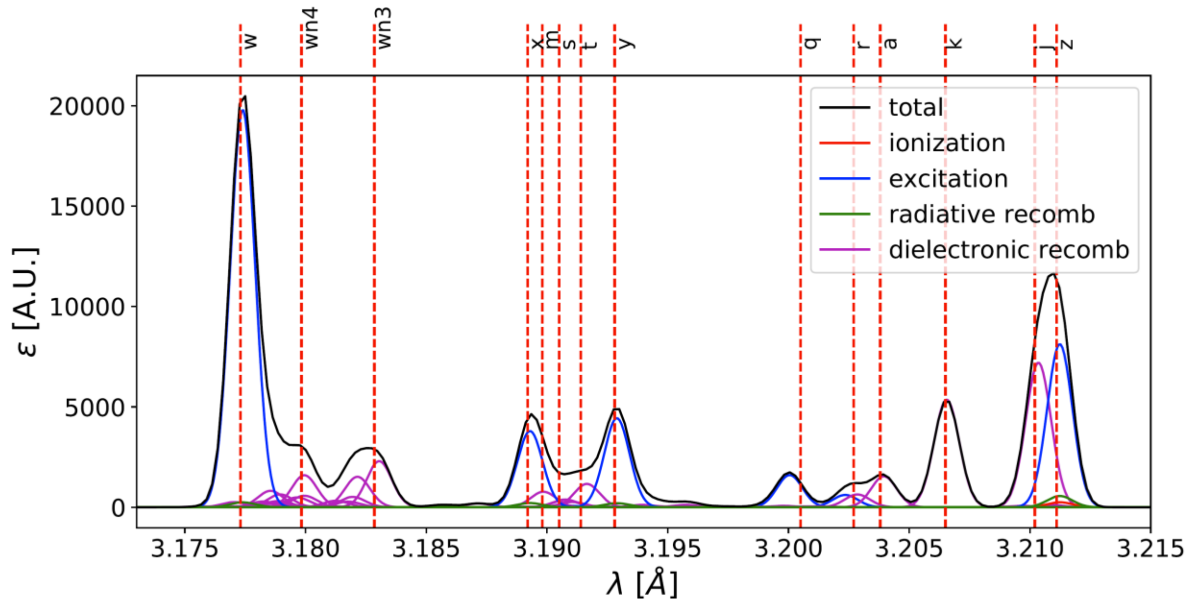
# Advanced synthetic diagnostics: Modeling the full Ca $K_\alpha$ spectrum of XICS

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

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




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

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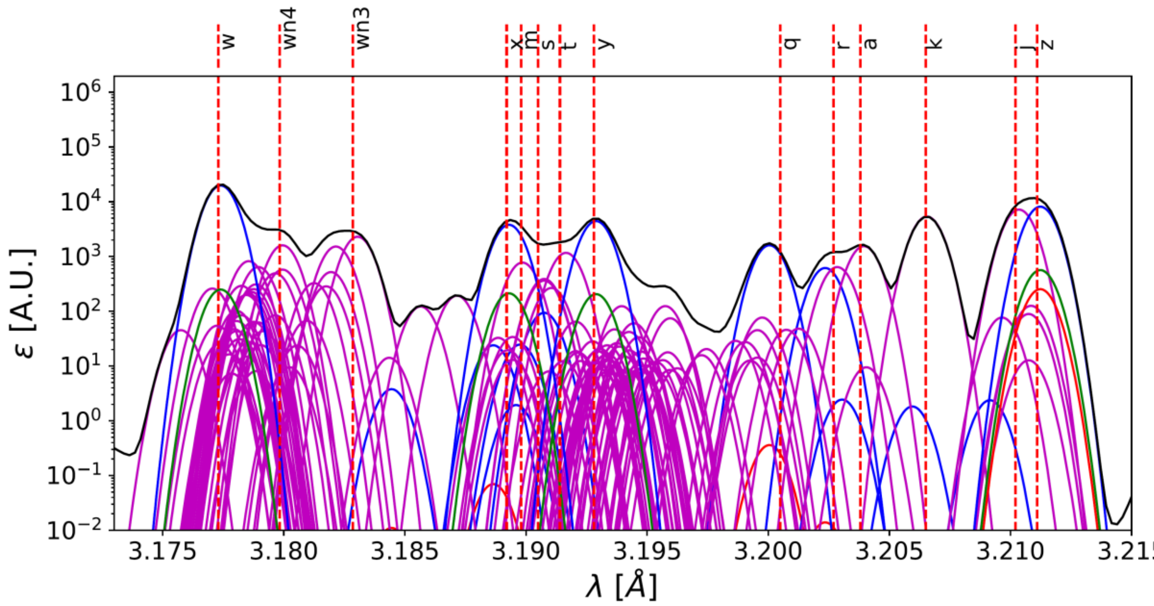
**Includes hundreds of satellite lines from Li-like Ca**

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

**Stronger constraints on particle transport**

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Alcator C-Mod

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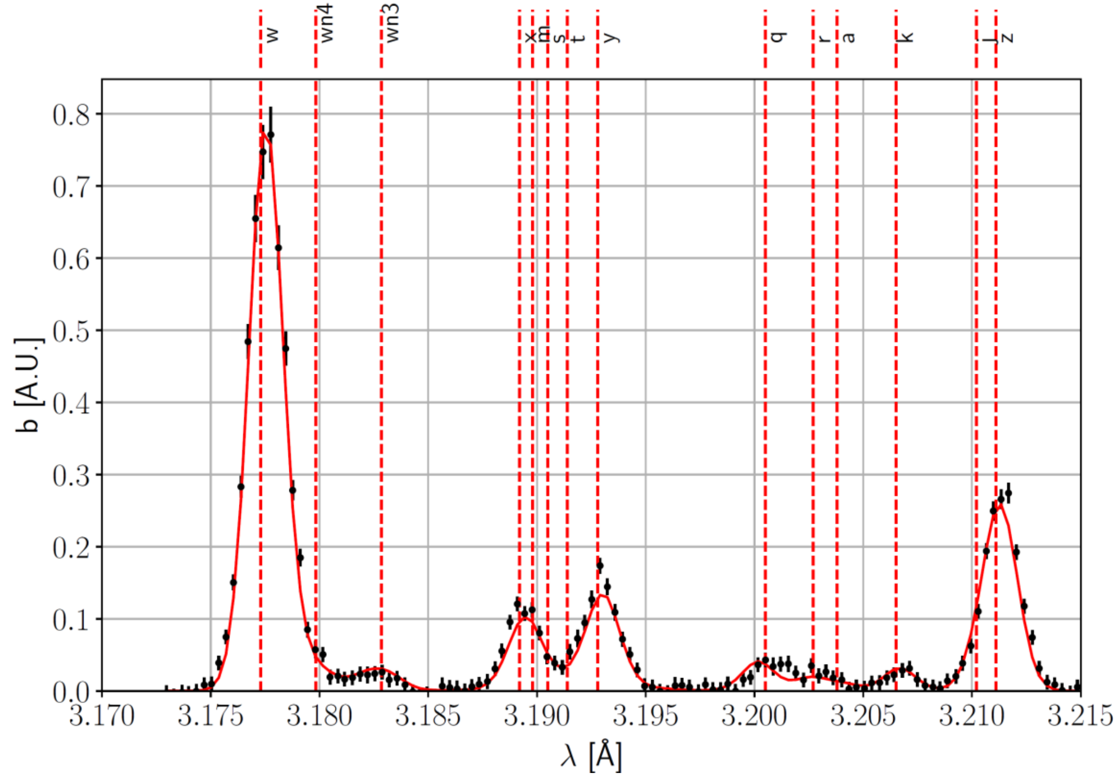


Experimental XICS Ca $K_\alpha$ spectrum matched by forward model

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I. Forward models for spectroscopy

II. Bayesian inference of particle transport coefficients

## II. Bayesian inference of particle transport coefficients

Methods:

- Model selection
- Physically-correlated priors
- Free spline knots
- Multi-species constraints

Applications:

- On C-Mod: L-, H-, and I-mode
- On DIII-D: RMP H-mode, $\delta < 0$

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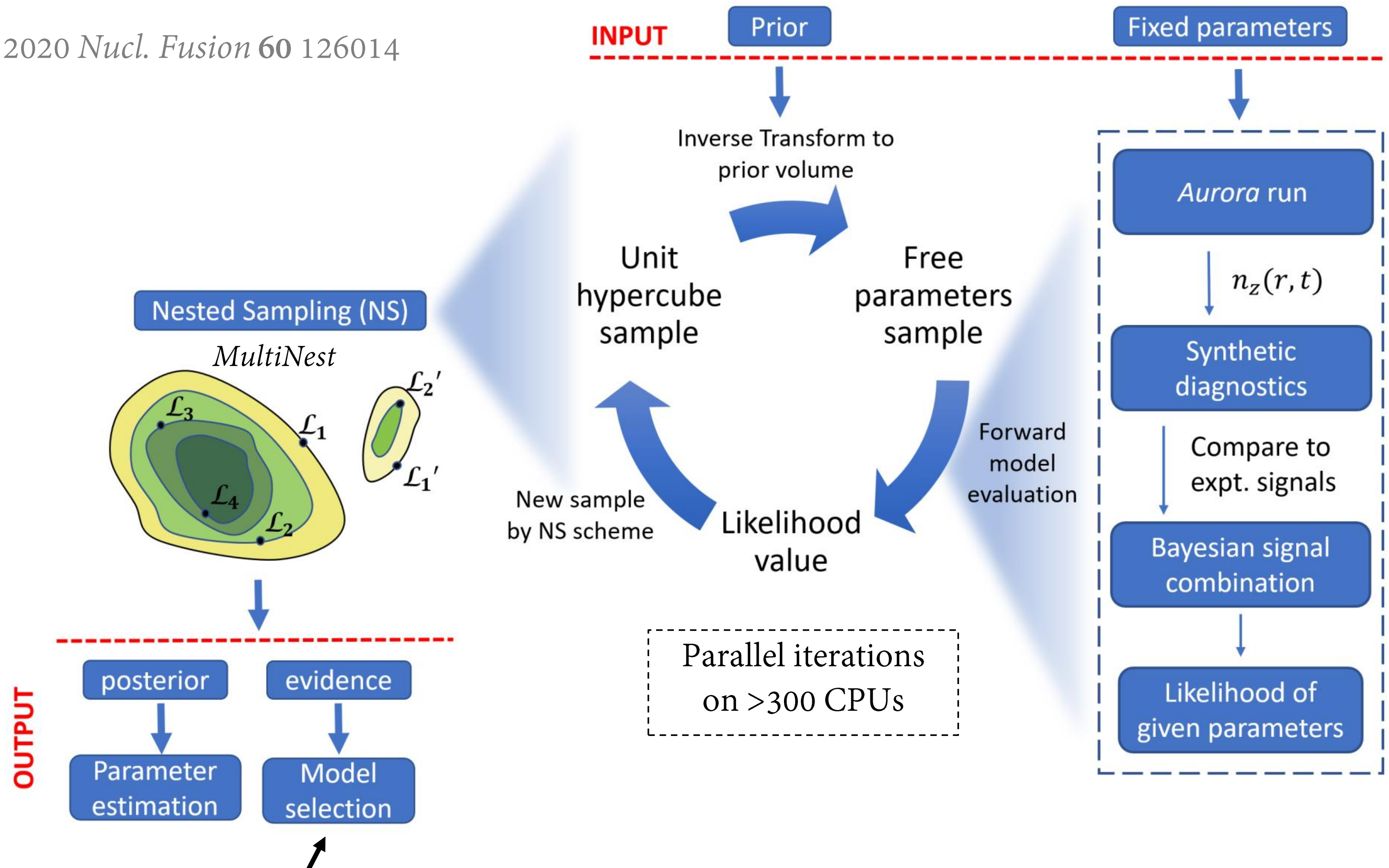


Select **parametrization** as well as **physical model**

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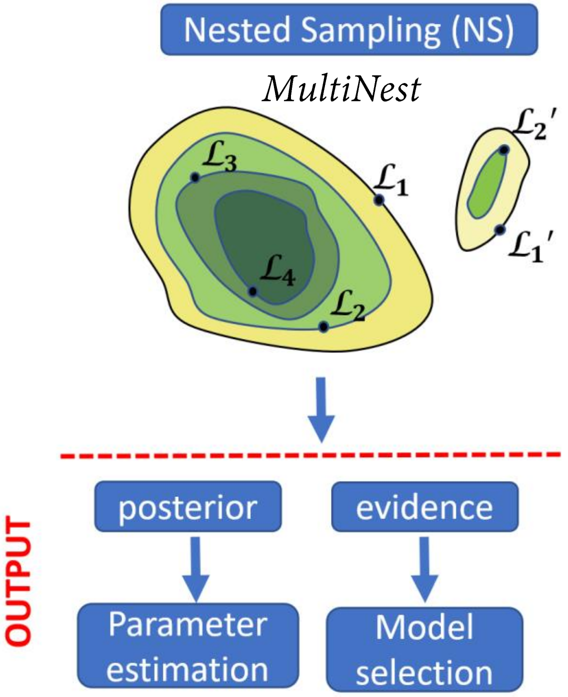
*Bayesian evidence normalized to best case*

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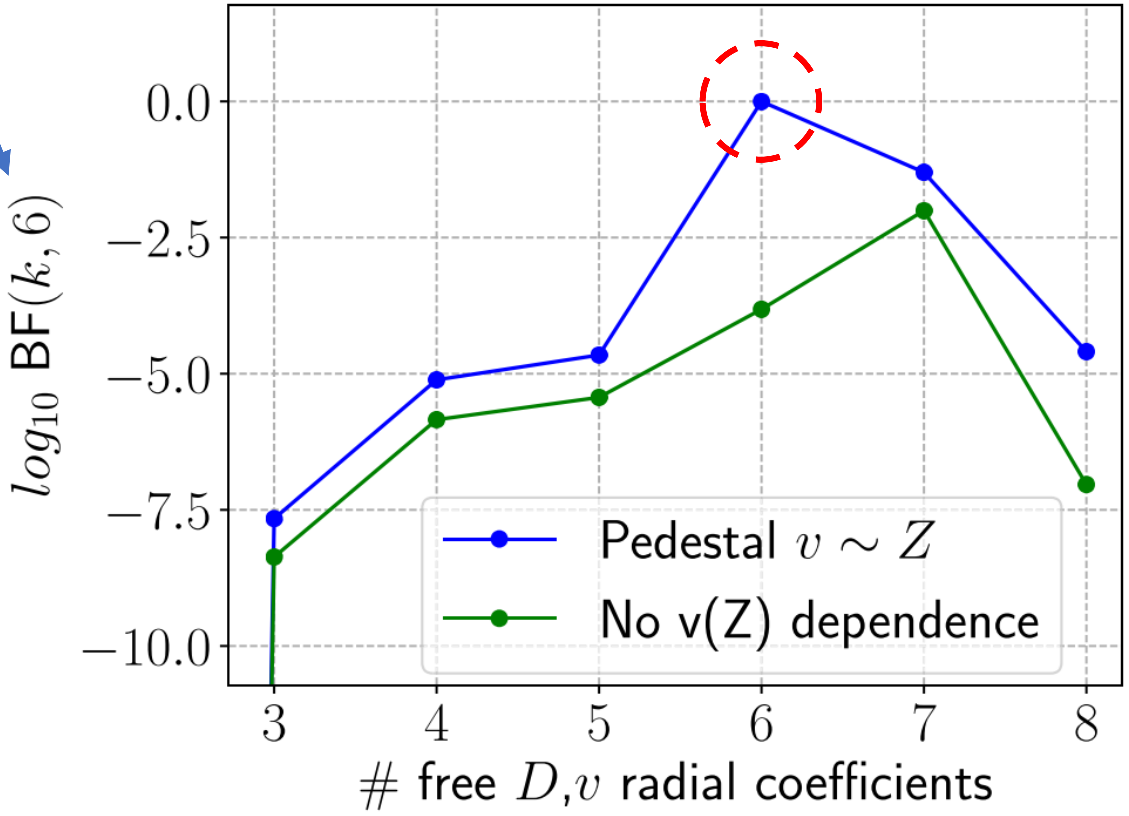


# Physical Bayesian Sampling of Transport Coefficients

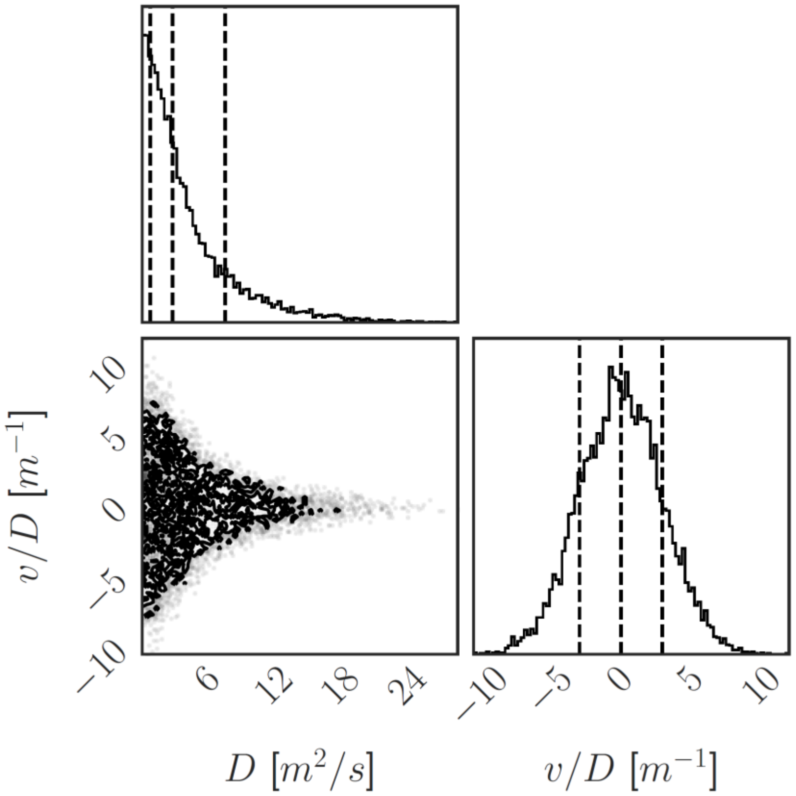
Problem:

How to ensure that sampling 2 parameters (e.g. $D$ and $v$) within priors gives physical ratios/products (e.g. $v/D$)?

Approach/solution:

Constrain ratios/products of parameters by sampling in the complex plane

- Simple idea: sample $\tan(\theta) = \chi\, v/D$ and $r = \sqrt{|\chi\, v|^2 + D^2}$ with $\chi$ a parameter that separates $D$ and $v$ scales

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# Free spline knots with forced identifiability

Problem:

Fixing spline knots can limit models & lead to under-/over-fitting if not combined with model selection

Approach #1:

Use non-parametric description of profiles (high-dim, hard time-dependent) – see *T. Nishizawa's earlier talk*

Approach #2:

Free spline knots sampled within a hyper-triangle, with prior $\pi(\theta) = \begin{cases} \frac{1}{n!(\theta_{\max}-\theta_{\min})^n} & \text{for } \theta_{\min} < \theta_1 < \cdots < \theta_n < \theta_{\max} \\ 0 & \text{otherwise.} \end{cases}$

After some algebra, one finds that

$$\theta_i = \theta_{i-1} + (\theta_{max} - \theta_{i-1}) x_i^{1/(n-i+1)}$$

unit-hypercube sample

transforms unit-hypercube samples into ordered, identifiable, free spline knots

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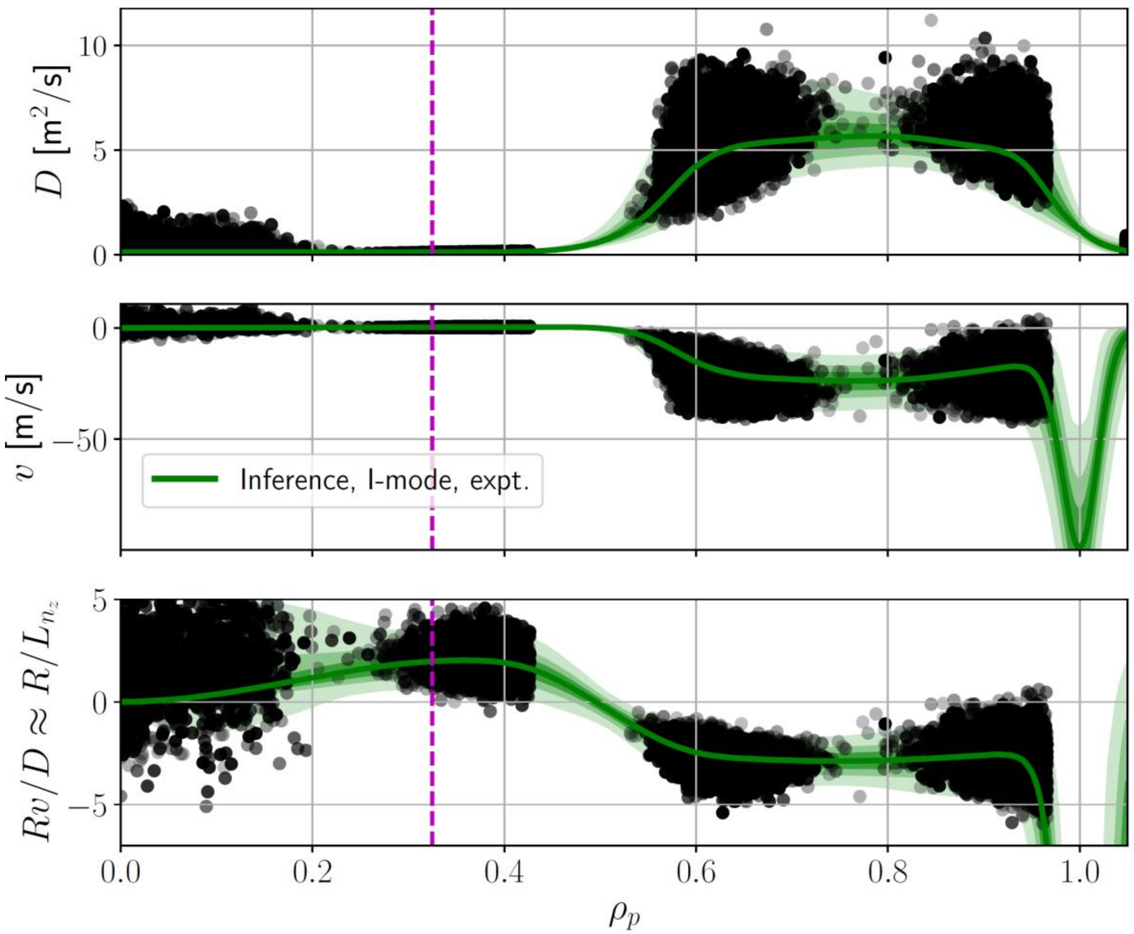
# Free spline knots with forced identifiability

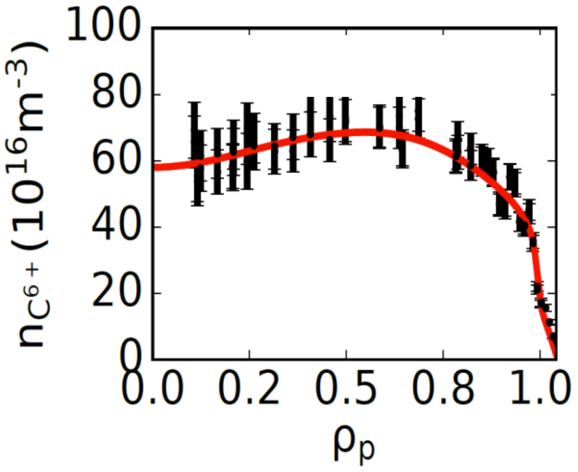


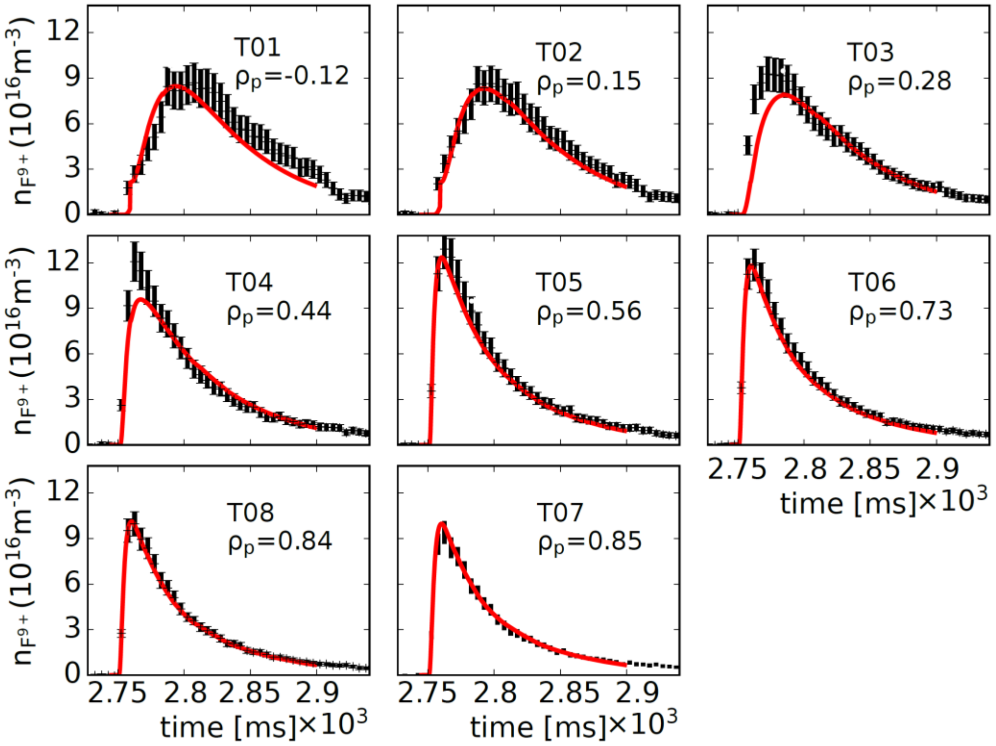

$$\theta_i = \theta_{i-1} + (\theta_{max} - \theta_{i-1}) x_i^{1/(n-i+1)}$$

# Constraints from multiple diagnostics + species: new important tools for validation

**New OMFIT ImpRad module is now generalized to handle an arbitrary number of species**

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



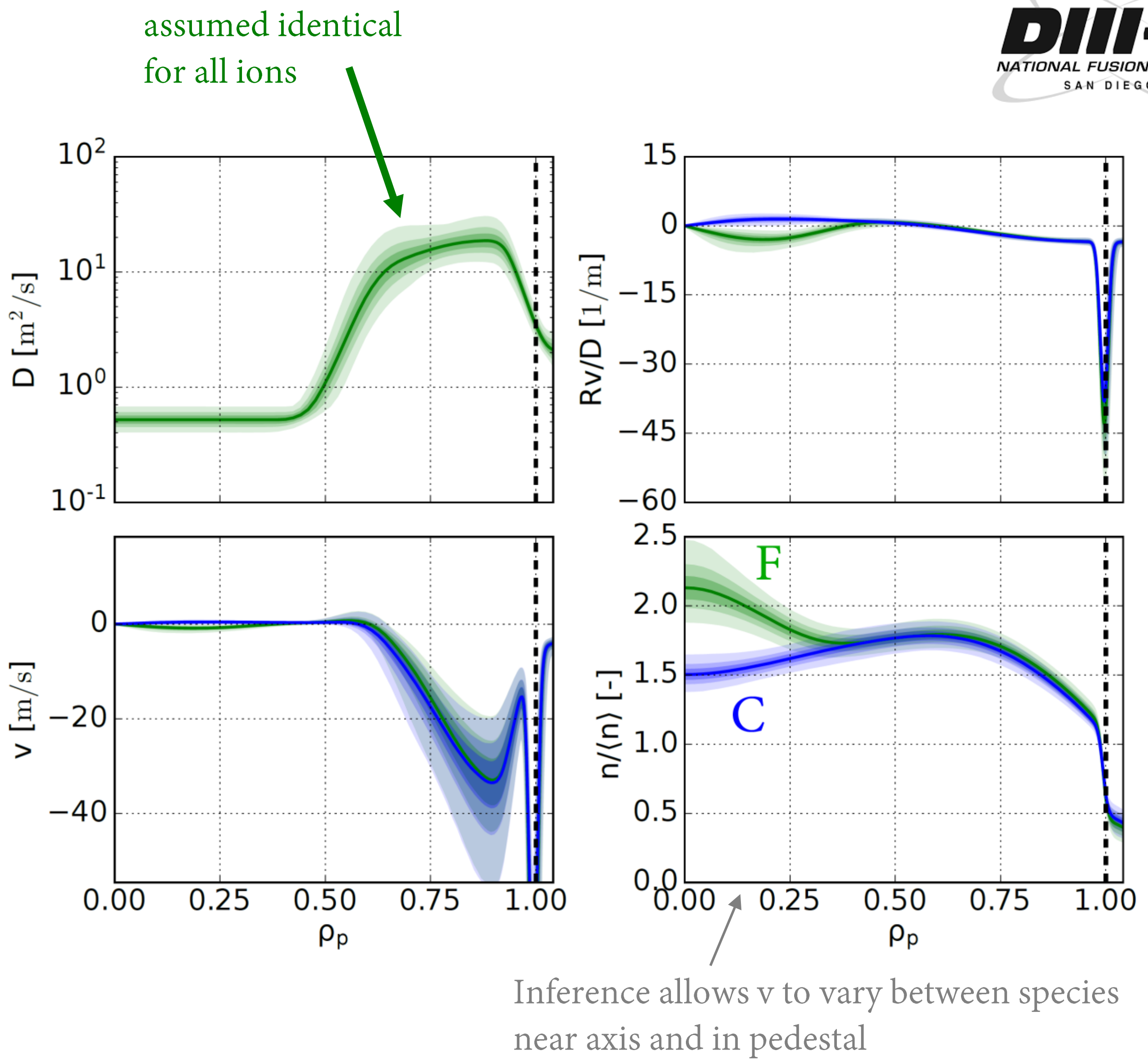




Further constraints on impurity transport from SXR and core-SPRED

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

**Multi-species impurity transport inference**

- F (LBO) and C (intrinsic)



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

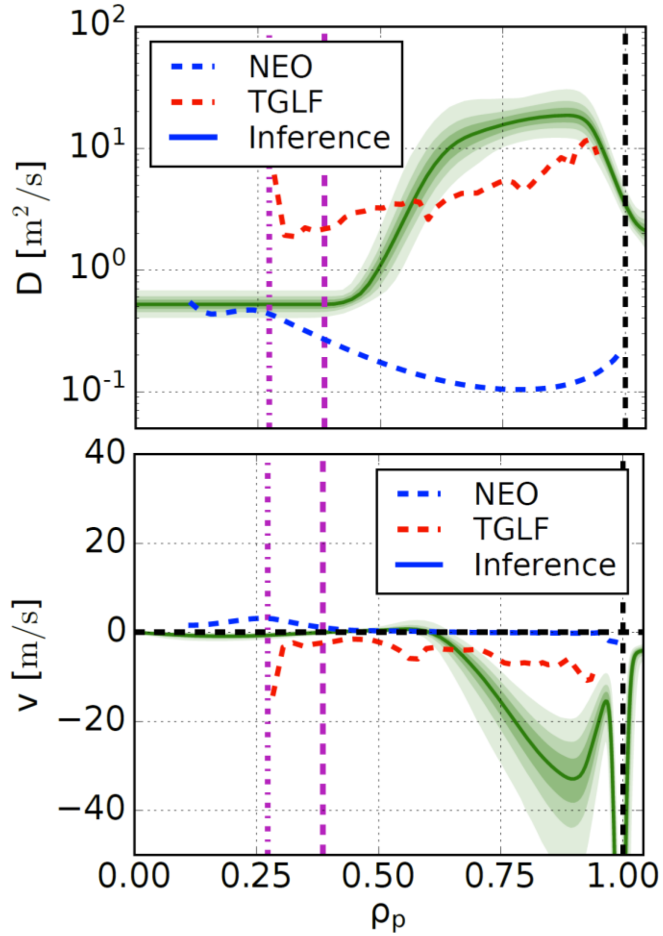
**Multi-species impurity transport inference**

- F (LBO) and C (intrinsic)

Comparison to theoretical models across multiple discharges suggests peaking mismatch

- **Experimental flat/hollow profiles often not captured by theory**

Fluorine

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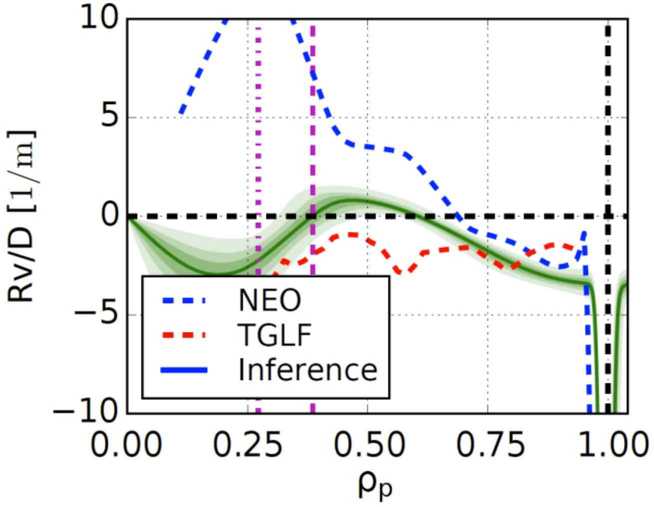

# Summary

Bayesian inference of particle transport coefficients on C-Mod and DIII-D

- Parameter Estimation, Uncertainty Quantification, Model Selection
- Focus on high physics-fidelity, including CX, multiple diagnostics, multiple species, etc.
- Techniques to improve Bayesian inferences *beyond particle/impurity transport*

| | Alcator C-Mod | DIII-D |
|---|---|---|
| Regimes | L-, I-, and EDA H-mode | Diverted $\delta < 0$<br>RMP ELM-suppressed H-mode |
| Experimental analysis | Modeling of Ca $\mathbf{K_\alpha}$ spectrum + EUV line ratios | Multi-species inferences with quasi-steady C + LBO-injected ions |

- Aurora + ImpRad make similar analysis **accessible** and **reproducible** by multiple researchers

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