

# Benchmarking of 3D Halo Neutral Calculation in TRANSP Code and Application to NSTX-U

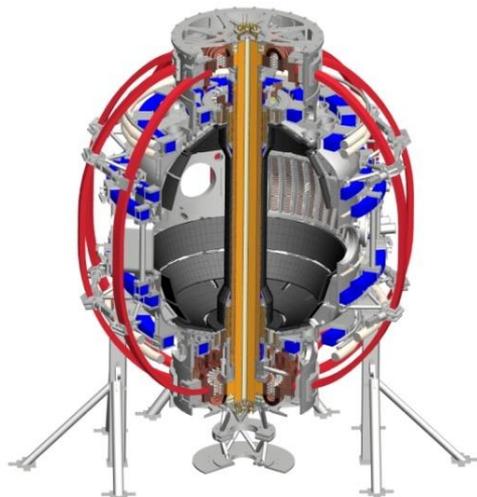
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**NSTX-U Monday Physics Meeting  
June 15, 2015**

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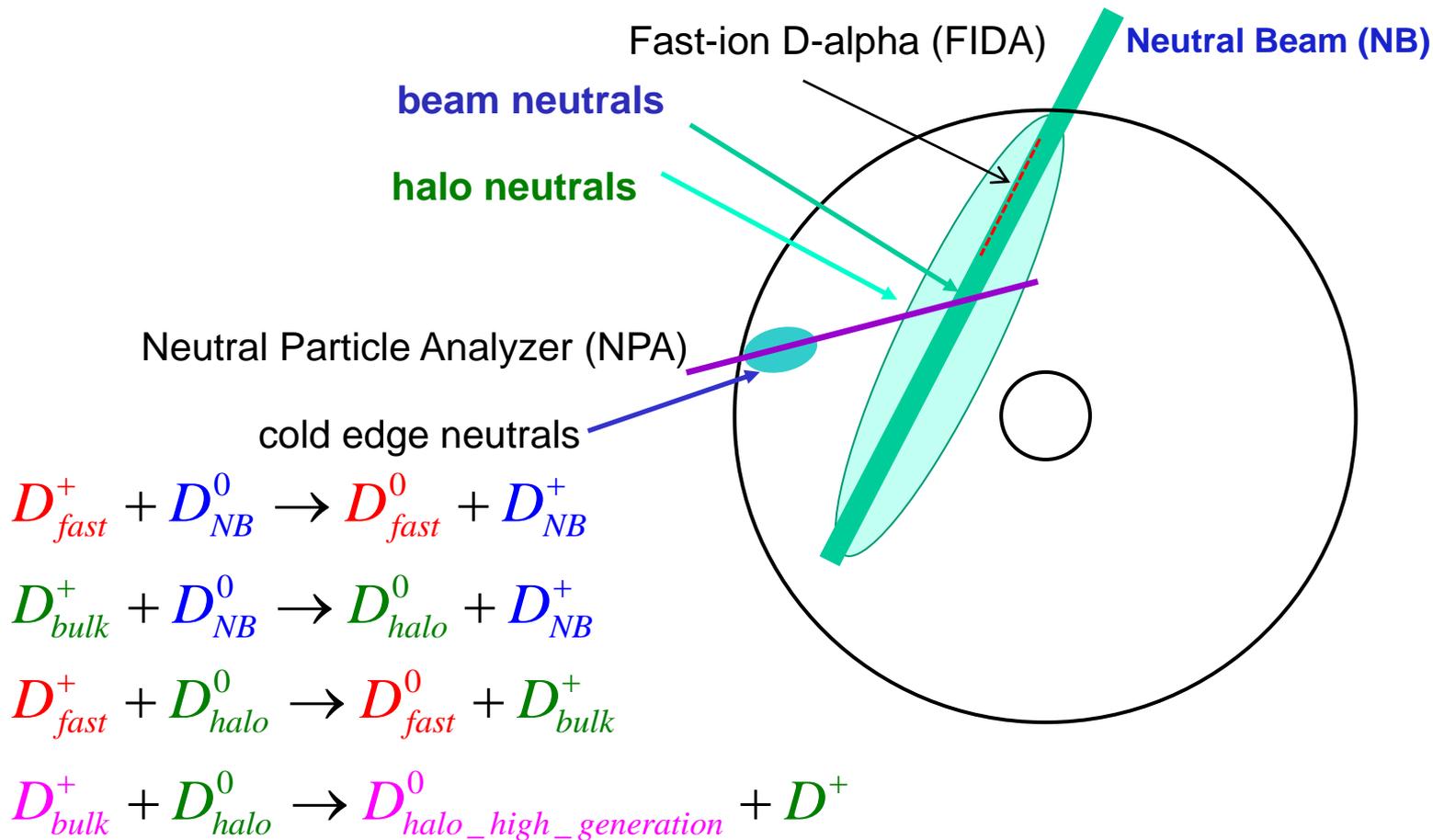


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# Outline

- Introduction: halo neutral and 3D halo neutral model in TRANSP
- Benchmarking of beam and halo neutral calculation in TRANSP with FIDA<sub>sim</sub>
- Effects of halo neutrals on NPA and FIDA synthetic diagnostics
- Effects of atomic cross sections on halo neutral calculation
- Summary

# Halo Neutrals are Created in the Vicinity of Neutral Beam Footprint through Charge-Exchange Reactions

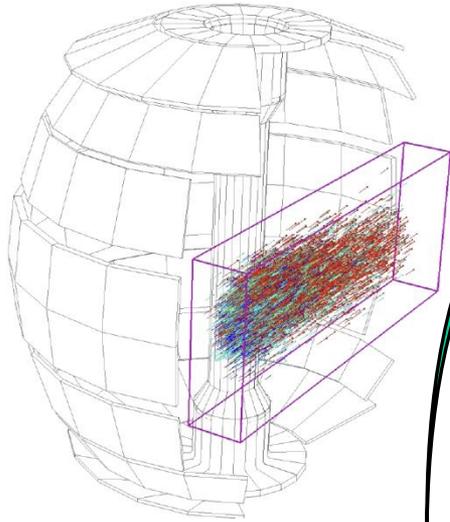


Both NPA and FIDA diagnostics rely on charge-exchange (CX) reactions between fast ions and beam/halo neutrals.  $Signal \propto n_{fi} n_{neutral} \langle \sigma v \rangle$

# Accurate Modeling of Halo Neutrals is Important for Proper Interpretation of Fast Ion Diagnostic Signals

- Halo neutral density is comparable with beam neutral density.
  - increase NPA and FIDA signal, critical for synthetic diagnostics
  - affect fast ion CX loss, thus impact basic TRANSP calculations, e.g. NB driven current, neutron yield, power balance
- Halo neutrals have a broader profile than beam neutrals
  - could affect spatial localization of NPA and FIDA diagnostics
  - could affect relative contribution to diagnostics from beam and halo neutrals
- A new 3D Halo model was recently developed in TRANSP/NUBEAM to replace the incorrect “volume averaged” halo neutral model.

# 3D Halo Model was Recently Developed in TRANSP/NUBEAM



➤ For each neutral beam source, a 3D box is aligned with and symmetrical around the NB centerline, and is divided into small cells.

1. Launch “weighted” beam neutrals (“markers”) at ion source location
  2. Track each marker, and record its entry and exit points and velocity vector when it crosses a cell
  3. Calculate the deposition probability and travel time in each cell  
→ beam neutral (or i-th gen. halo) density in the cell
  4. A deposition probability weighted random number generator determines whether and where a 1<sup>st</sup> (or i+1-th) gen. halo marker will be born.
    - “Nsplit\_geo” controls # of 1<sup>st</sup> (or i+1-th) gen. halos that will be generated from their parent neutral marker.
    - Assign new weight to 1<sup>st</sup> (or i+1-th gen.) halo neutral marker based on  $\sigma_{cx} v_{rel} / (\langle \sigma v \rangle_{cx} + \langle \sigma v \rangle_{ionization})$
    - Sample new velocity vector from Maxwellian (thermal halos) or non-Maxwellian (fast halos)
- Go back to step 2, until the weight is smaller than a minimum requirement.

\*Note: a neutral marker can be terminated by an ionization event, by reaching the minimum weight, or by exiting the 3D box

More details about 3D halo model in NUBEAM, see M. N. Gorelenkova’s 2014 APS poster and S. S. Medley’s paper (in preparation)

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# Halo Neutral Models in TRANSP and FIDAsim Differ in Atomic Physics

	3D Halo model in TRANSP	Halo model in FIDAsim
<b>Similarities</b>	3D Cartesian coordinates; Monte-Carlo approach; Include the effects of toroidal rotation;	
<b>Differences</b>	Ignore quantum energy levels (PREACT, ADAS, ADAS310), but cross section tables may include the effects of excited states (ADAS 310)	Solve collisional-radiative equations to get neutral density in each quantum energy level (n=1,2,..6) ADAS and Janev 2004 report
	Time dependent	Time independent (halos formed in ion-ion collision time scale << TRANSP/NUBEAM time step)
	Include thermal (and fast) halo neutrals from B-B interactions	Include thermal halos only

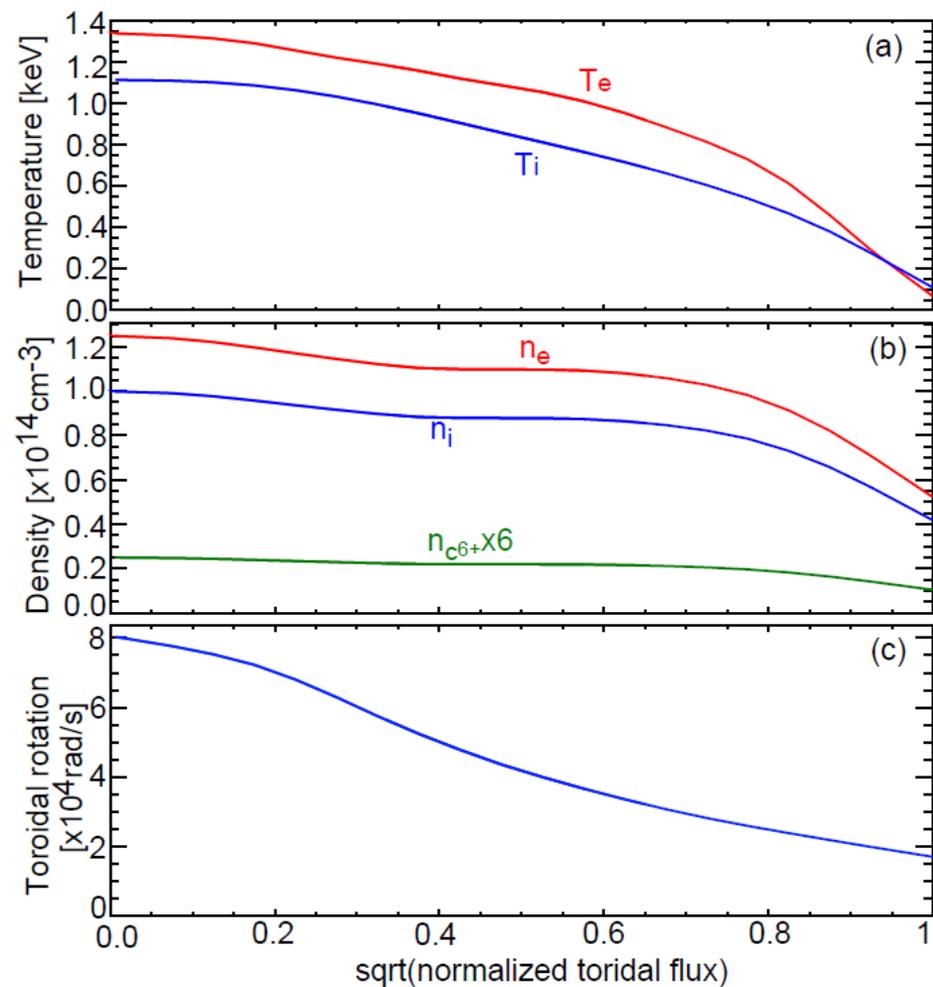
For the benchmarking purpose

- Use **ADAS ground state** cross sections in both codes, ignore quantum energy levels in FIDAsim.
- **Turn off fast halo neutrals** in TRANSP

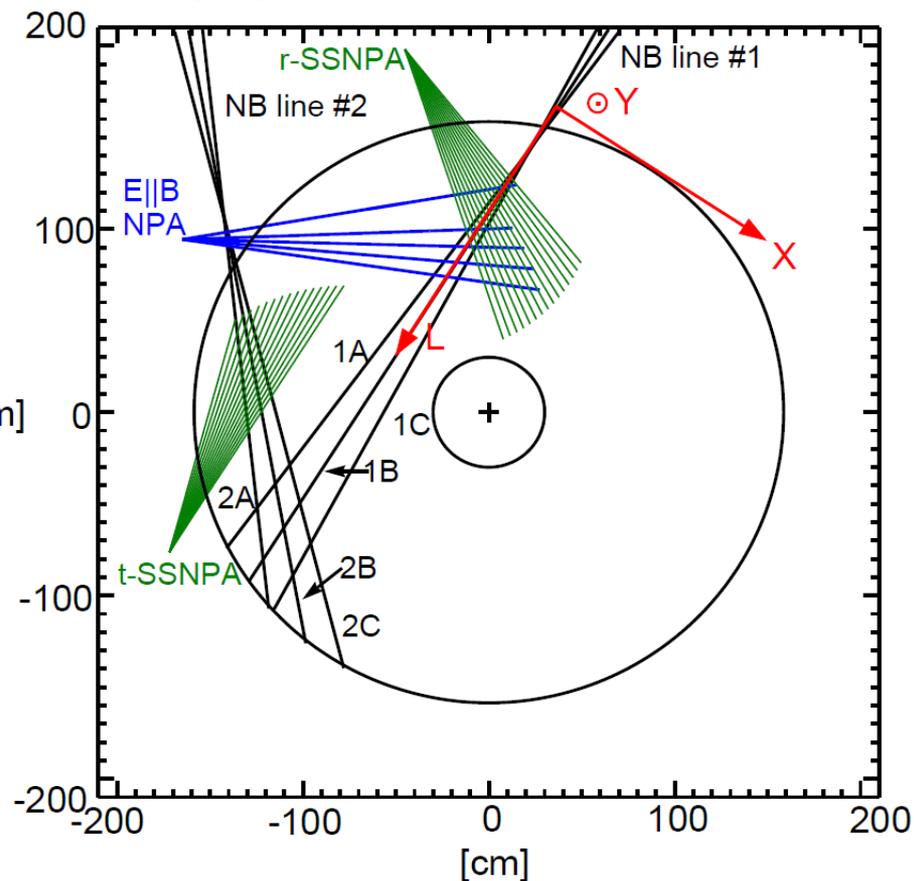
# Beam and Halo Neutral Density Modeling in TRANSP and FIDASim are Carefully Checked with a Series of Test Cases

- ✓ Case A: a perfectly collimated neutral beam (i.e. one source with one energy component, no divergence), flat plasma profiles, ADAS ground state cross section table, without rotation  
...
- ✓ **Case B:** case A, but w/ realistic neutral beam geometry (i.e. one source w/ three energy components, w/ focus & divergence), w/ realistic plasma profiles, w/ toroidal rotation
- ✓ Case C: case B, but with multiple neutral beam sources  
...
- **CASE D:** similar to Case B, but  
**TRANSP: ADAS310 atomic cross section tables**  
**FIDASim: cross section tables from ADAS & Janev 2004 report**

# Input Plasma Profiles and Coordinate System

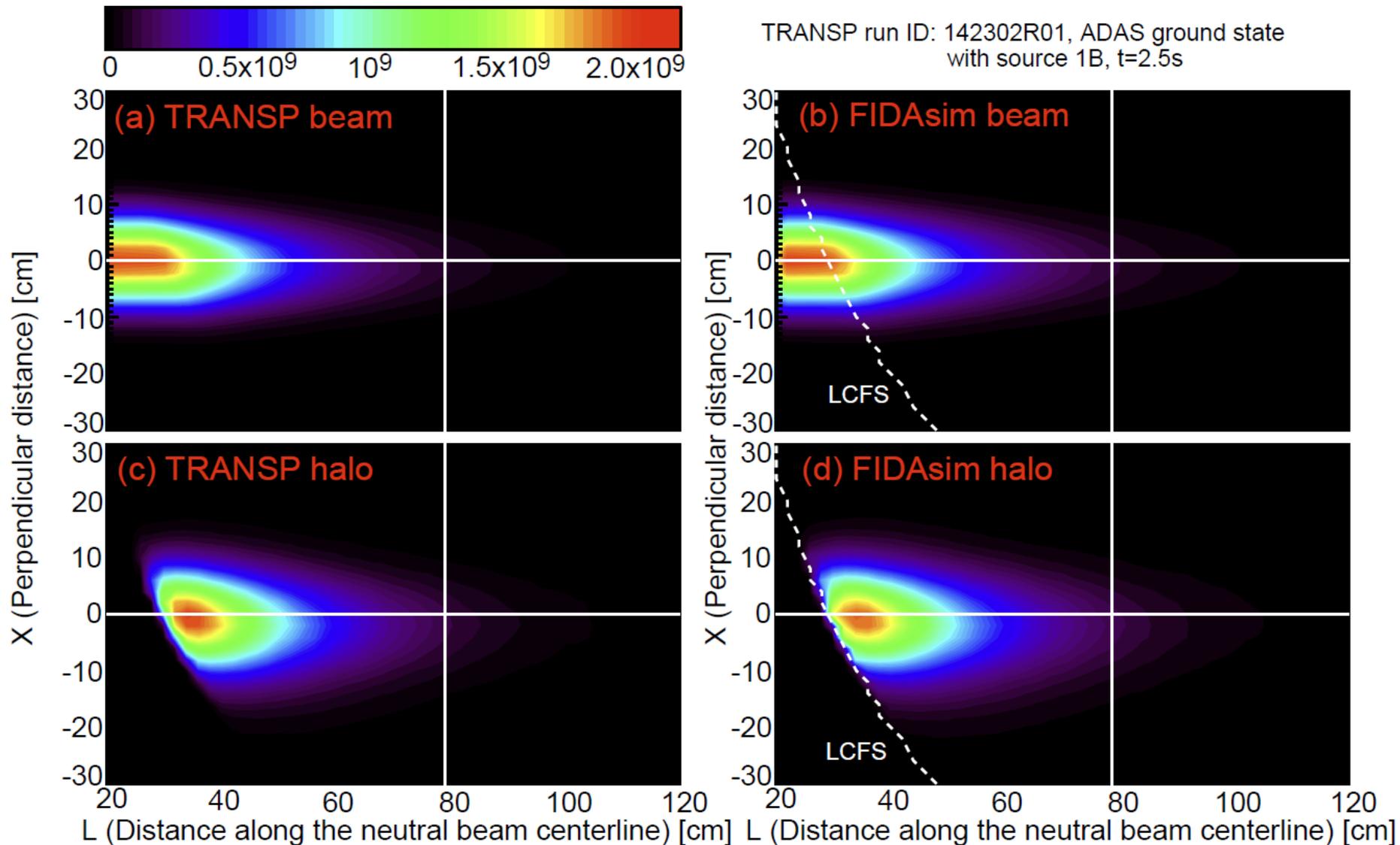


One beam (1B) is used in the benchmark case.

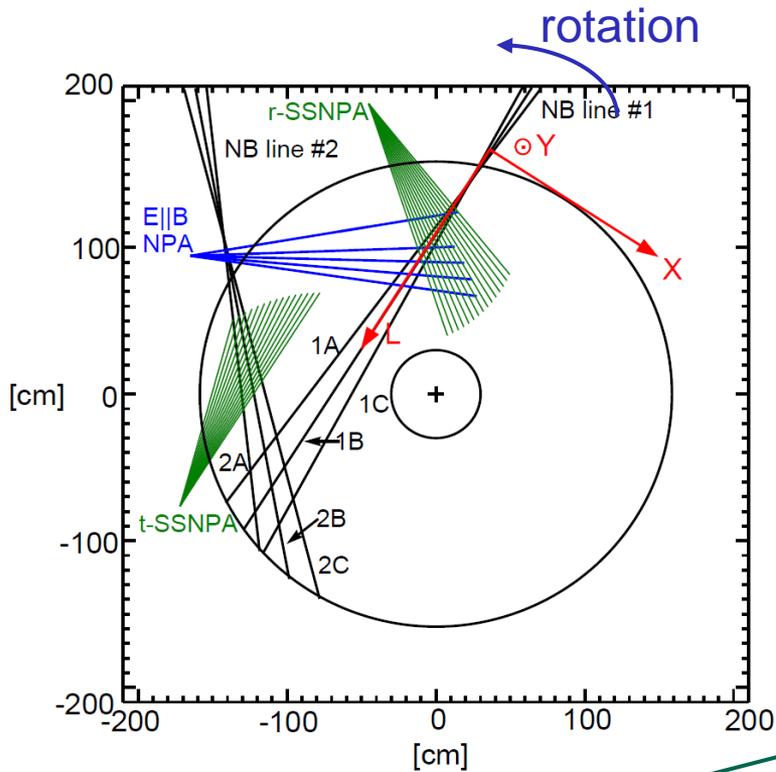


Note: Profiles are from a projected NSTX-U discharge in S. Gerhardt NF2012

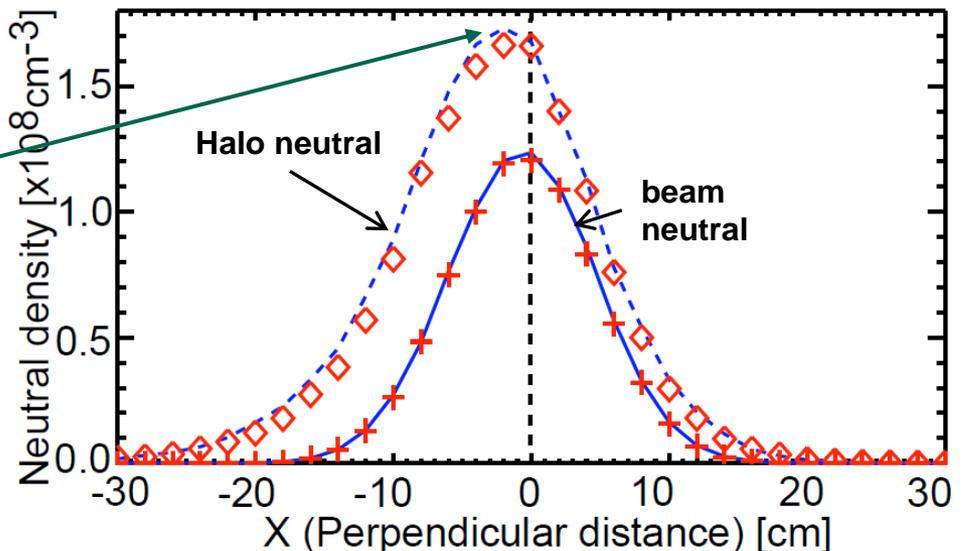
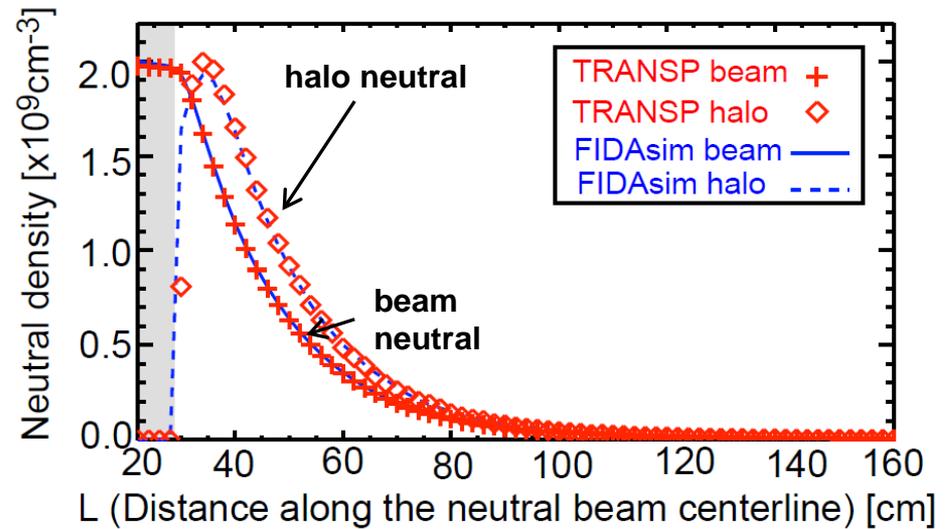
# Excellent Agreement between TRANSP and FIDAsim when Using the Same ADAS Ground State Cross Section Tables (1)



# Excellent Agreement between TRANSP and FIDASim when Using the Same ADAS Ground State Cross Section Tables (2)

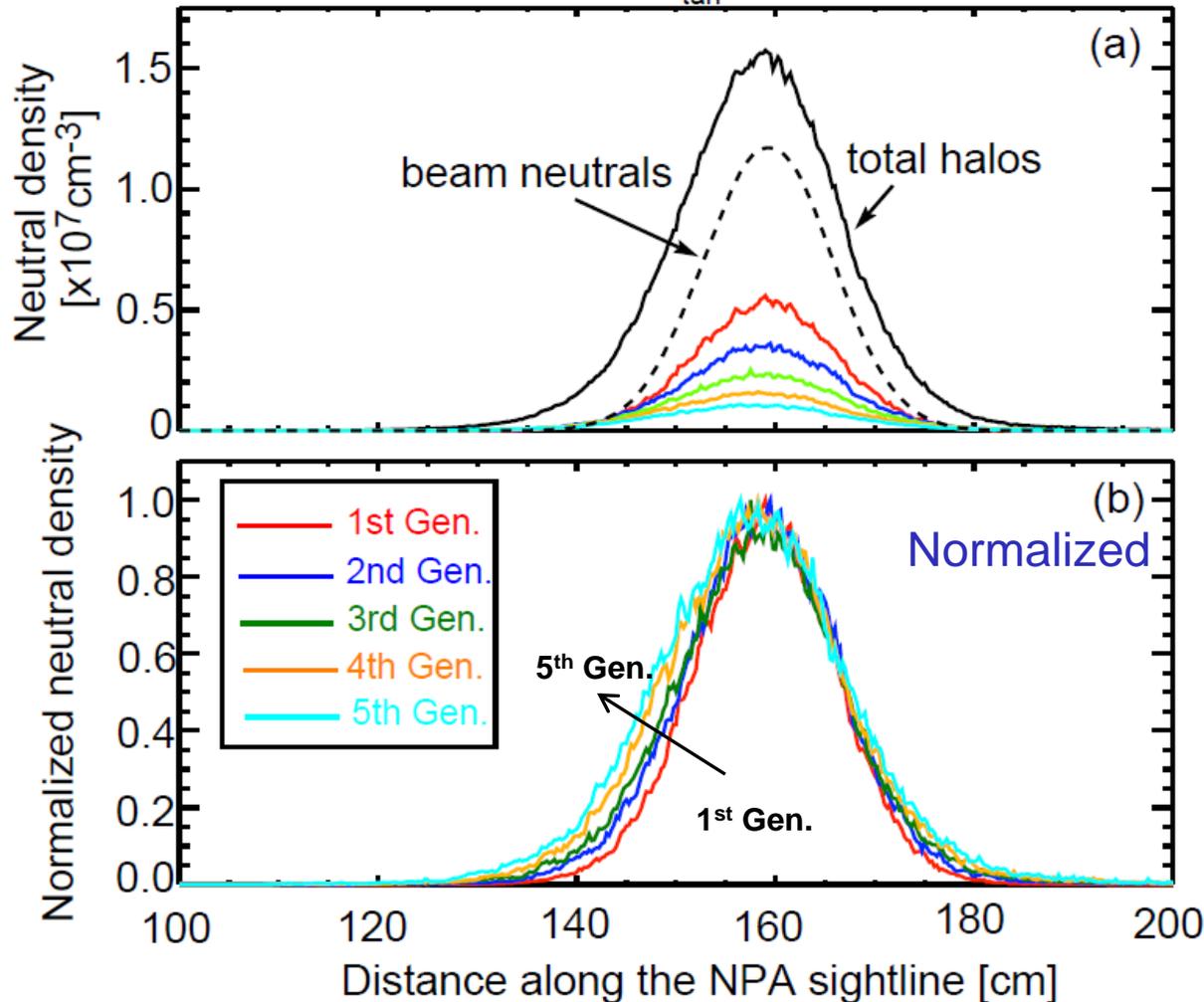


The peak of halo neutrals shifts in the same direction as toroidal rotation, as expected



# Halo Neutrals are Composed of Halos from Multiple Generations

TRANSP 142302R01 at  $t=2.5\text{s}$ , NPA  $R_{\text{tan}}=100\text{cm}$

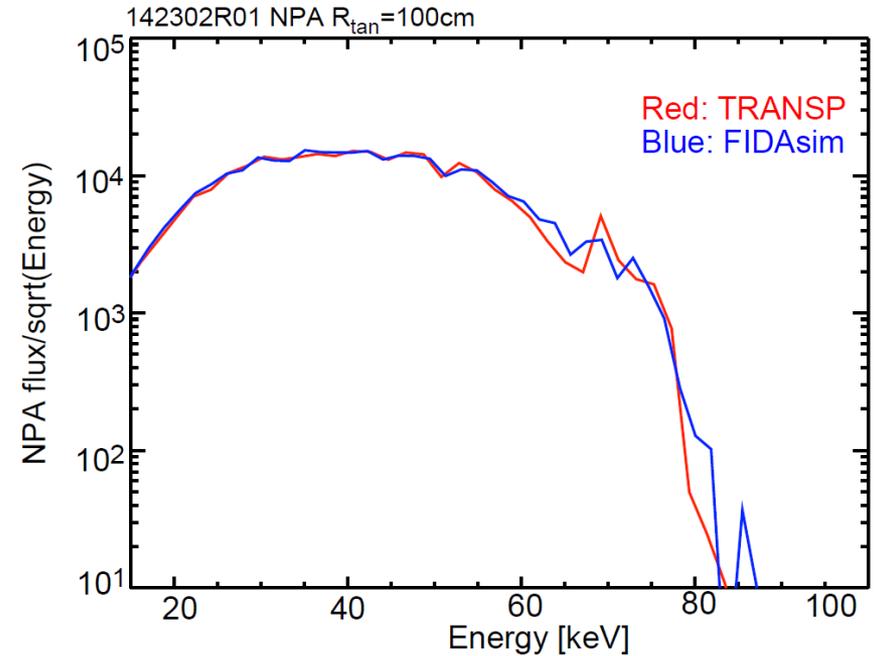
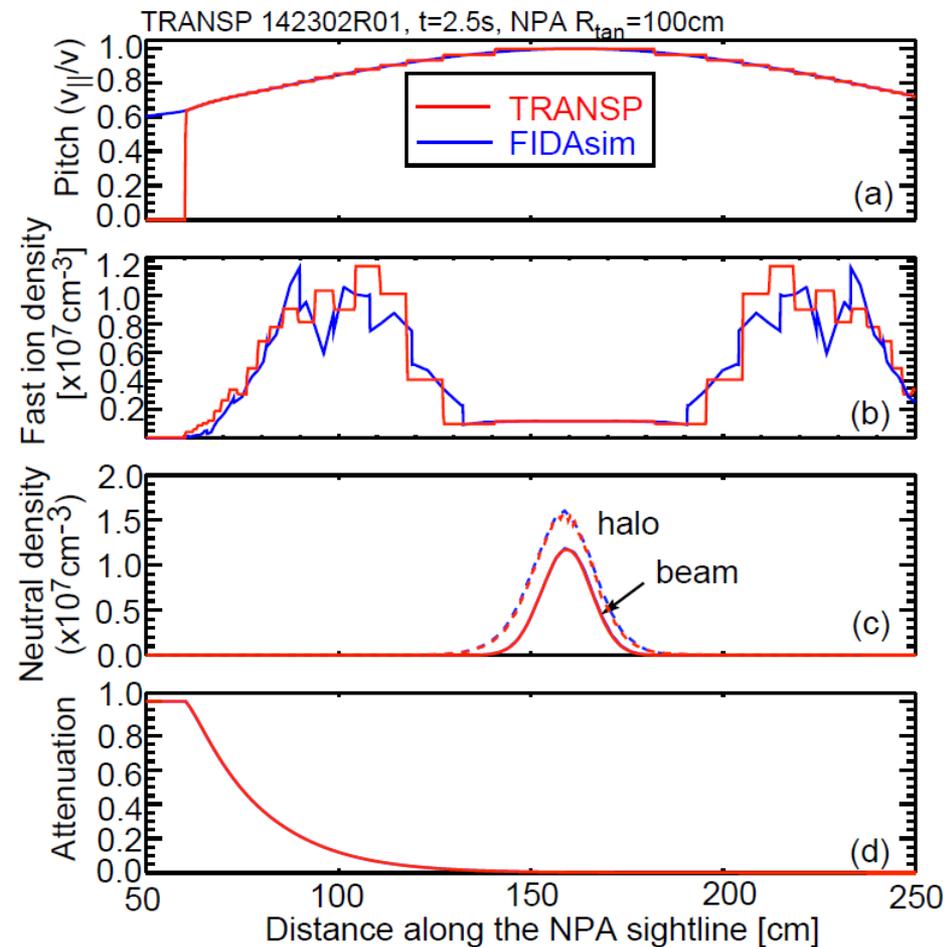


- Halo neutral density is comparable with beam neutral density.

- Halo neutrals spread wider than beam neutrals, and the spatial profile broadens with the increase in the halo generation.

# Verification of NPA Simulators in TRANSP and FIDASim

$$\Phi(E_i) = \int n_{fi}(r, E_i) n_n(r, E_i) \sigma_{cx}(E_{rel}^{i,n}) v_{rel}^{i,n} e^{-\lambda} dl$$



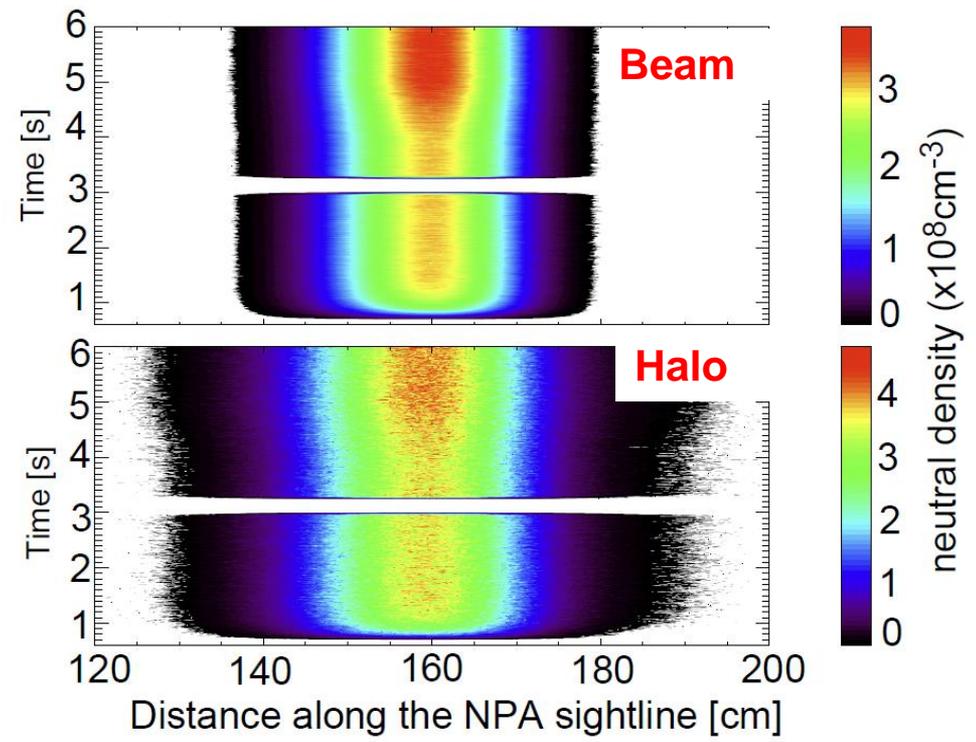
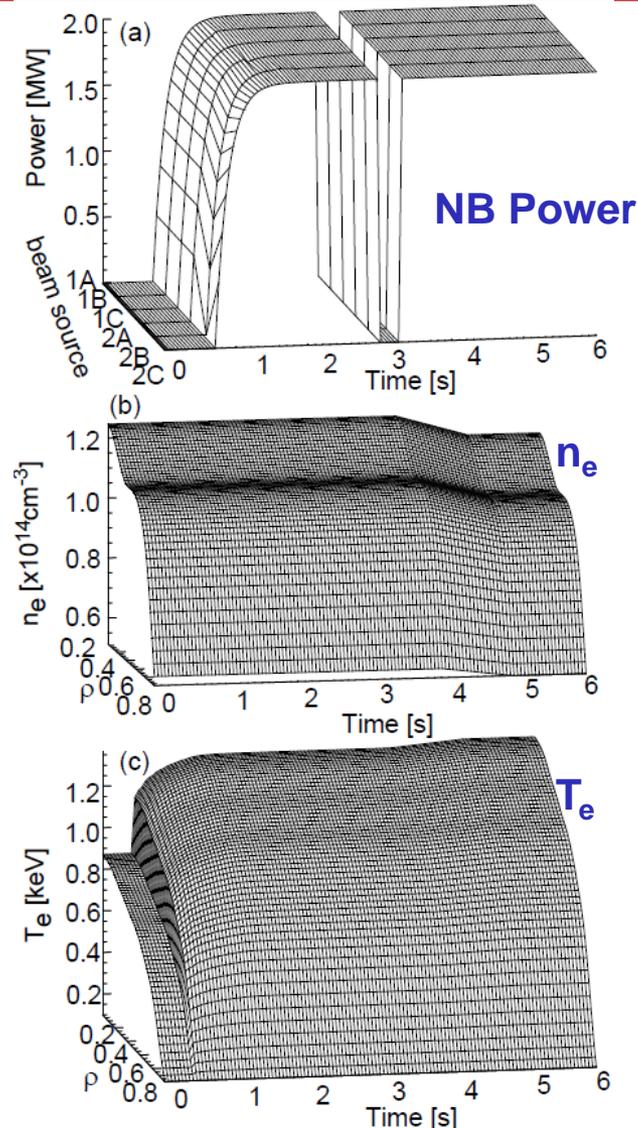
➤ NPA energy spectra from both NPA simulators agree with each other.

Note: only beam and halo neutrals are considered; edge neutrals from wall recycling and gas puffing are not included.

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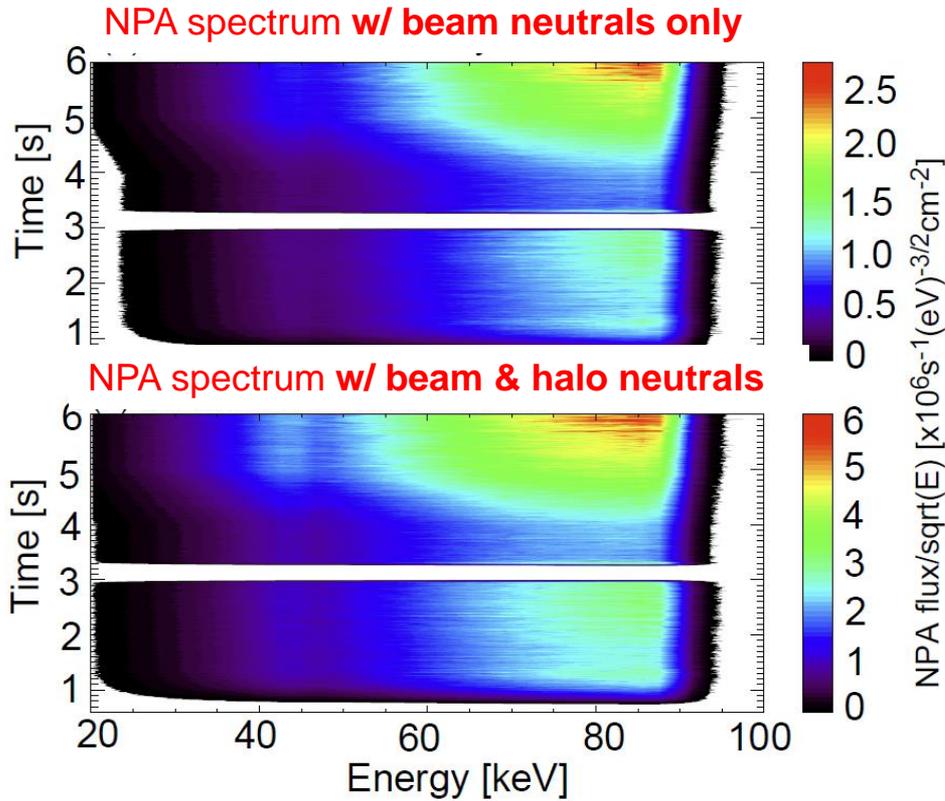
# Halo Neutral Density is Comparable with Beam Neutral Density and Halo Neutrals Spread Broader than Beam Neutrals



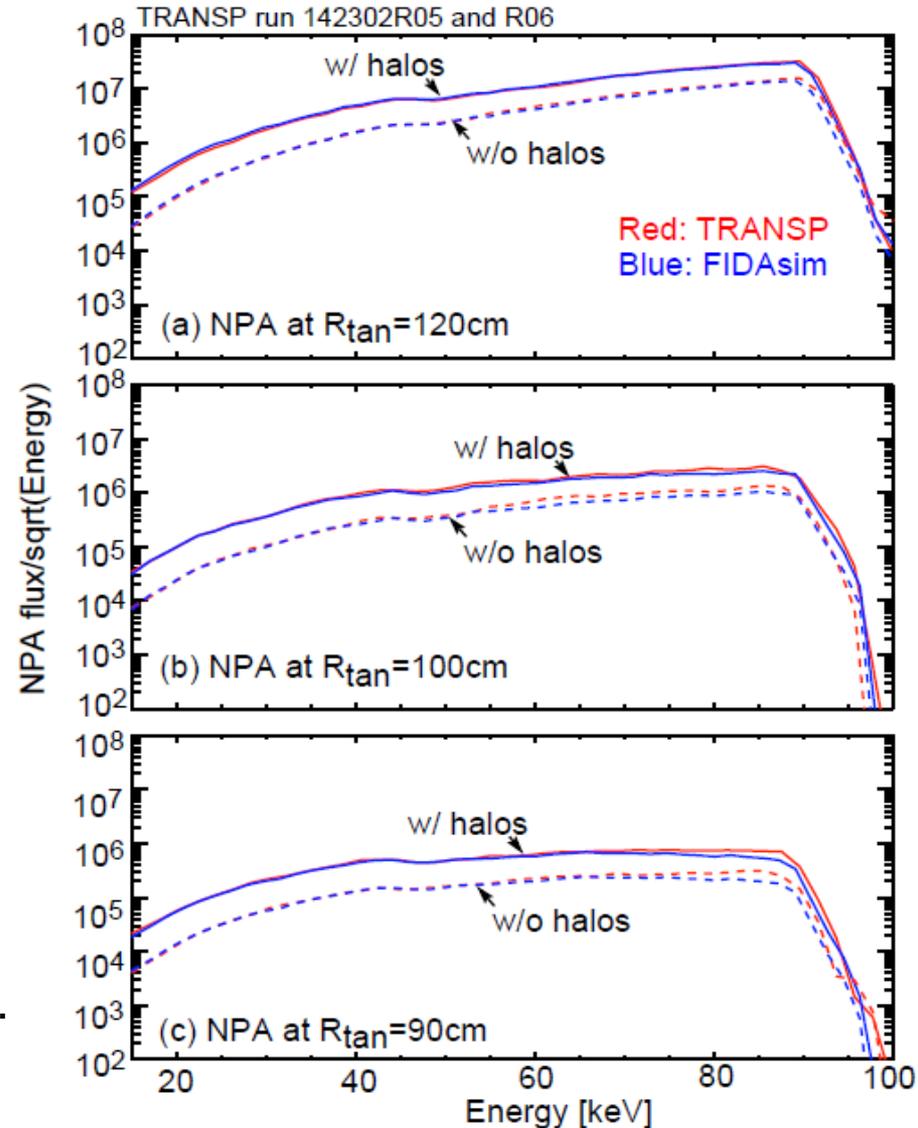
- Halos neutrals spread broader than beam neutrals
- Halo diffusion
  - Multi-generations

Note: Profiles are from a projected NSTX-U discharge in S. Gerhardt NF2012

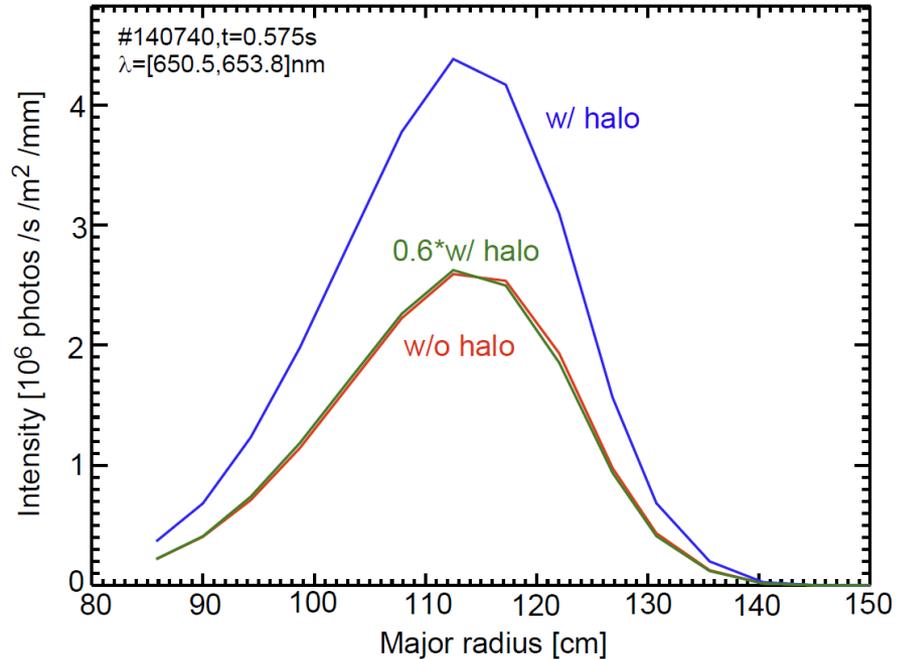
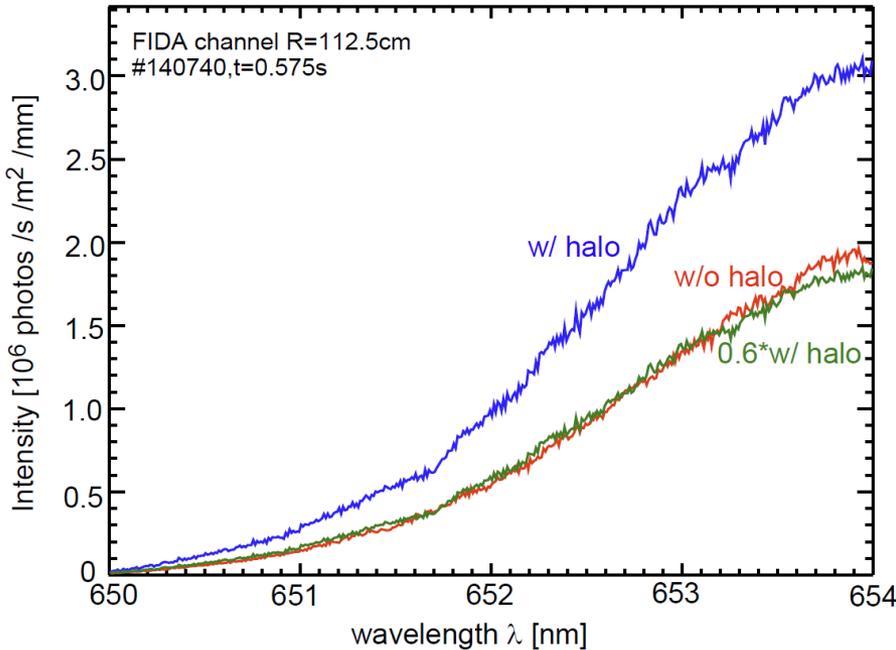
# Halo Neutrals Double NPA Flux



NPA flux in all channels double, but the shape of energy spectrum is weakly affected.



# Halo Neutrals Significantly Increase FIDA Signal, but Weakly Affect FIDA Spectrum and Spatial Profile



- FIDA signal is significantly increased due to large population of halo neutrals.
- The shape of FIDA spectrum and FIDA spatial profile is weakly modified.

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# Halo Neutral Density is Sensitive to The Choice of Atomic Cross Section Tables

## Options of atomic cross section tables in TRANSP

(1) ADAS ground (LEV\_NBIDEP=2 and NSIGEXC=0) :ground state only

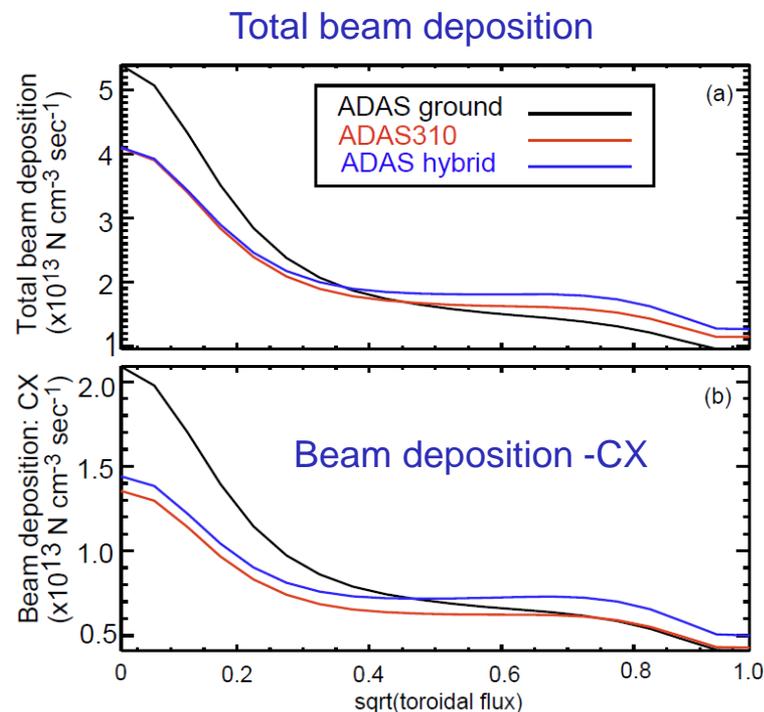
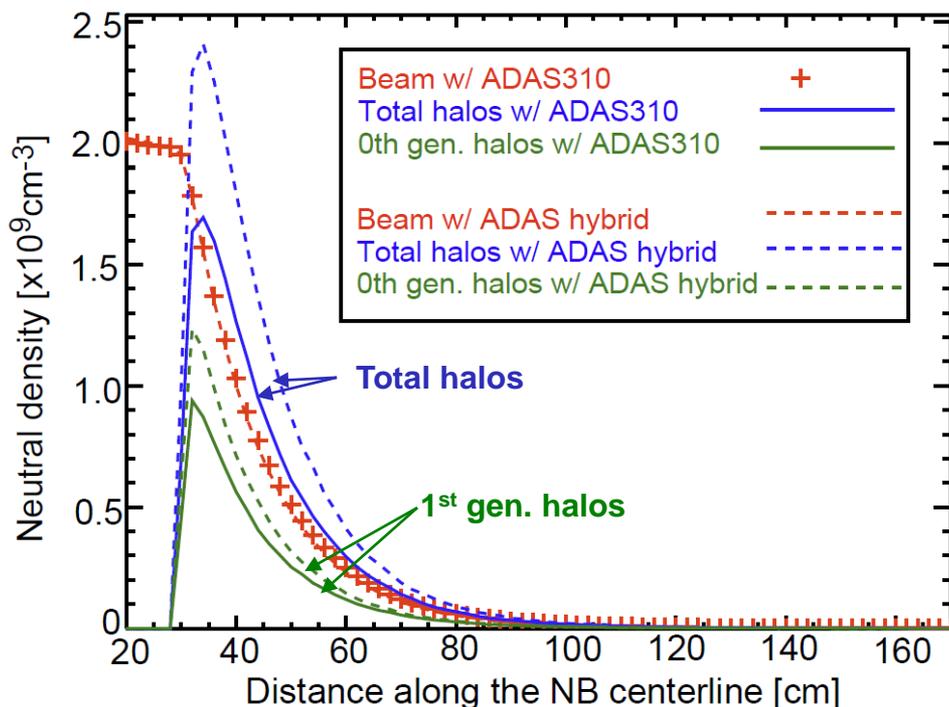
(2) ADAS hybrid (LEV\_NBIDEP=2 and NSIGEXC=1)

A simple excited states deposition model using enhancement factor

(3) ADAS310 (LEV\_NBIDEP=2 and NSIGEXC=3) (recommended for TRANSP runs)

A consistent excited state model

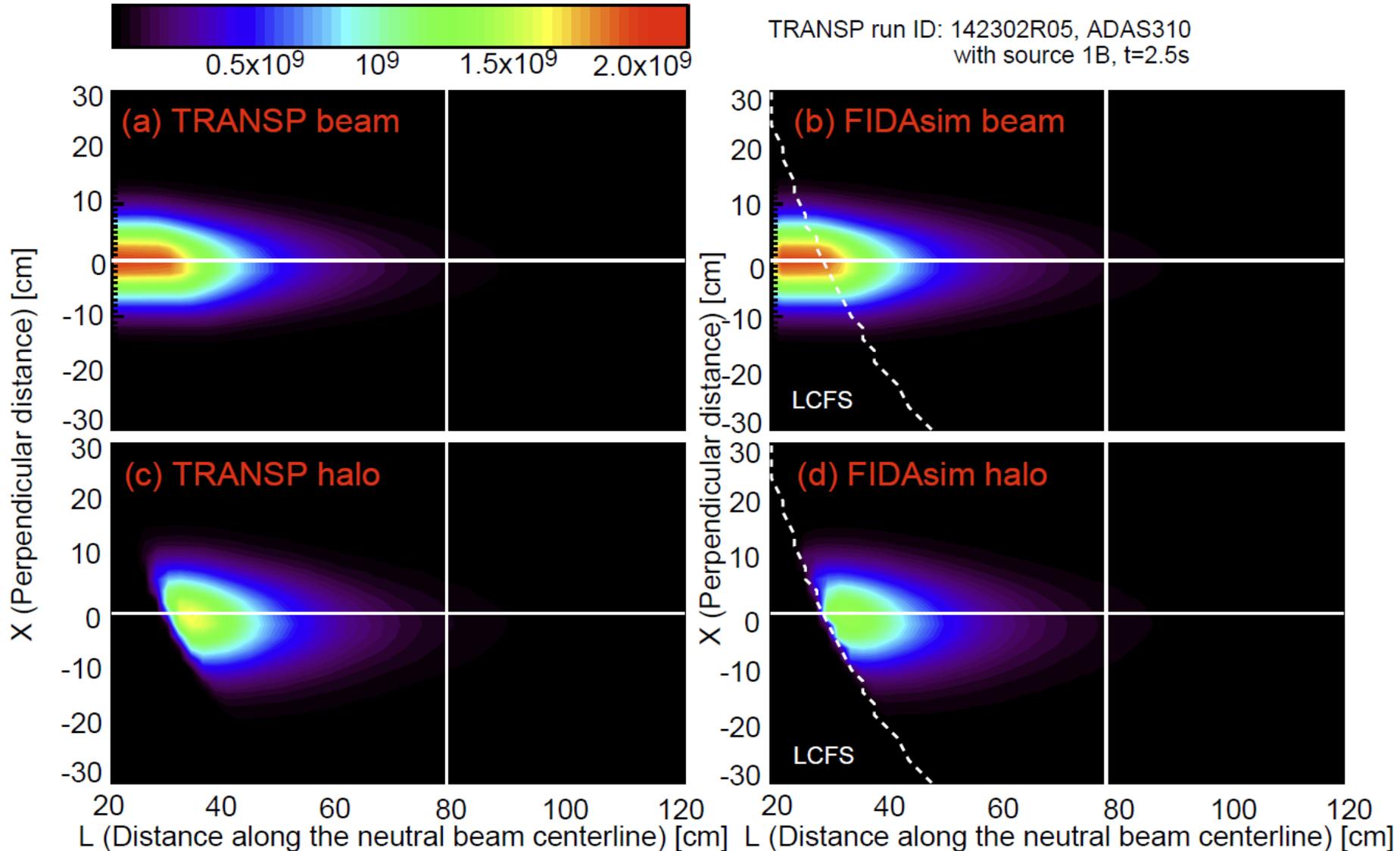
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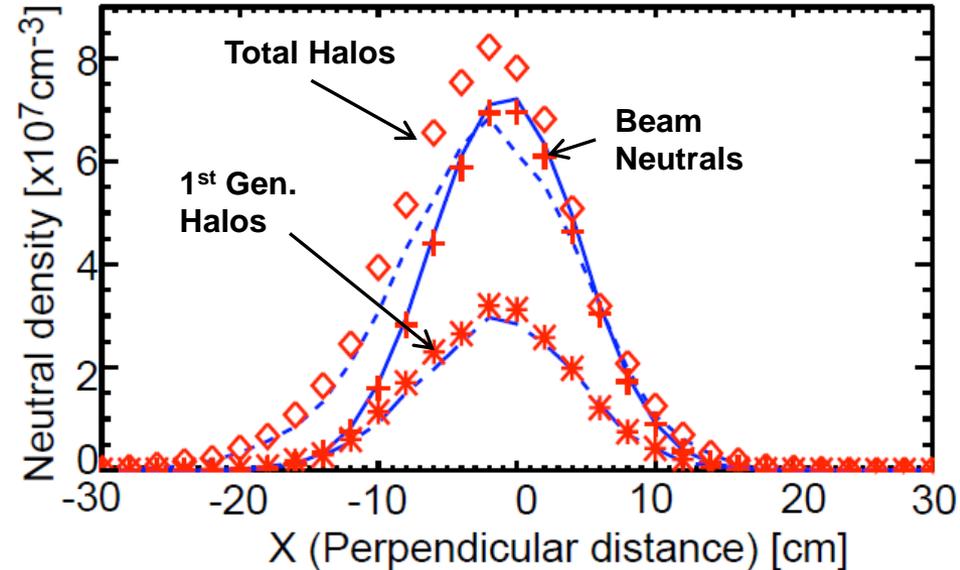
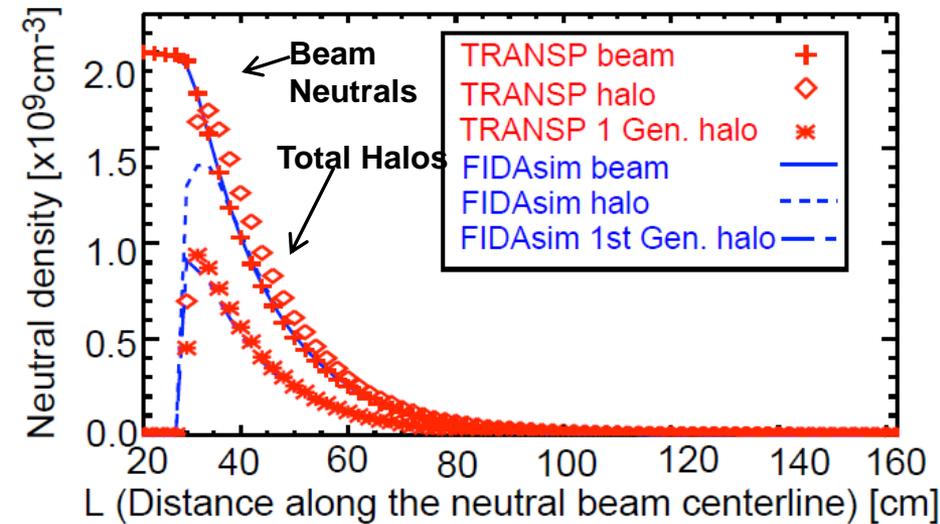
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- **CASE D:** similar to Case B, but  
**TRANSP: ADAS310 atomic cross section tables**  
**FIDAsim: cross section tables of different quantum energy level from ADAS & Janev 2004 report**

# Case D: TRANSP and FIDAsim Predictions of Halos are Similar in Shape, but Different in Magnitude (1)

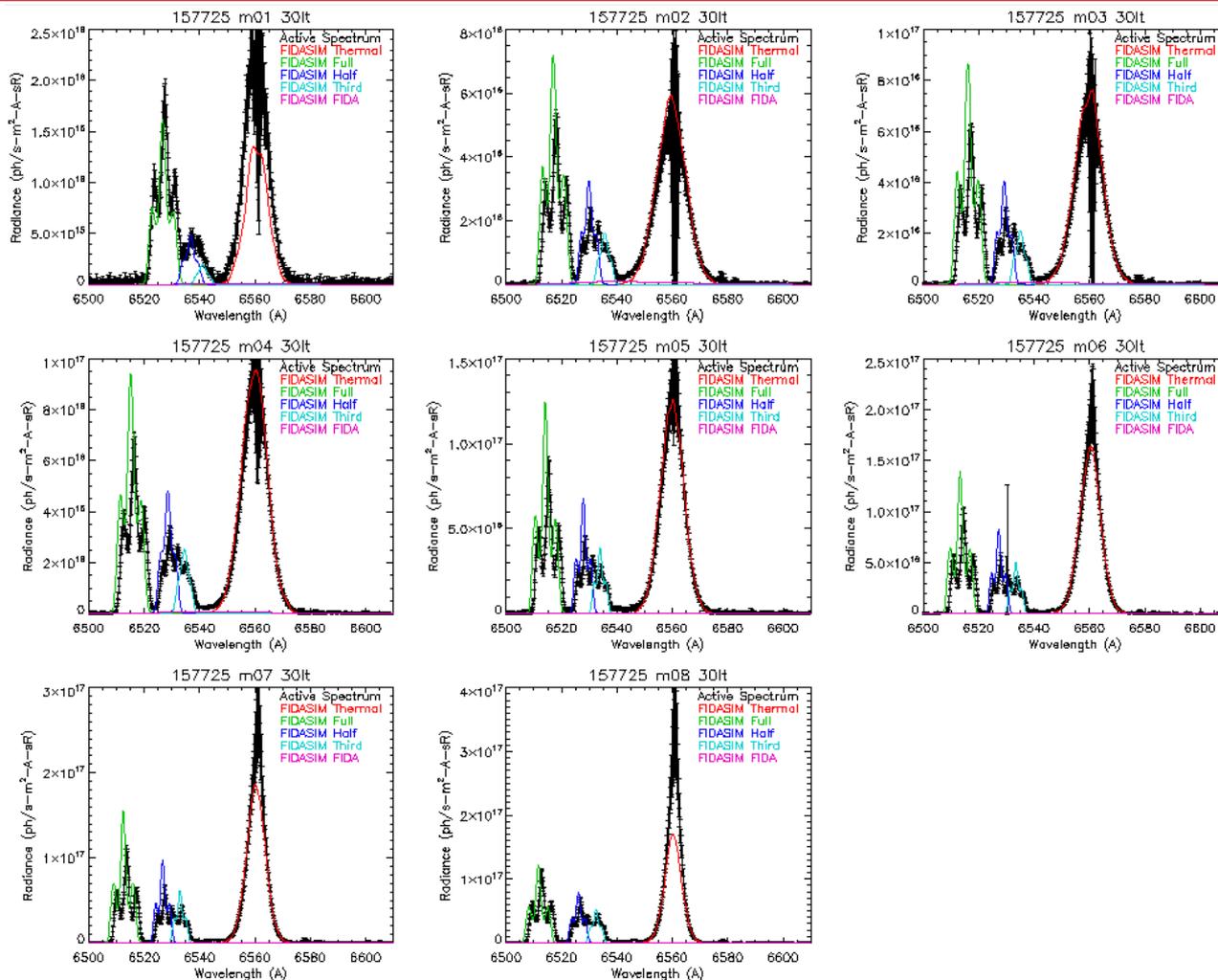


## Case D: TRANSP and FIDASim Predictions of Halos are Similar in Shape, but Different in Magnitude (2)



- TRANSP calculated halo neutral density is ~20% larger than FIDASim prediction because different atomic cross sections tables are used in TRANSP and FIDASim.

# Beam and thermal Emissions from FIDASim Simulations Agree with Experimental Measurements



Data from Main-Ion  
Charge Exchange  
Spectroscopy on DIII-D

B. Grierson

FIDASim calculated beam and thermal emission agrees well with experimental measurements  
→ Beam and halo neutral density and profile from FIDASim (and TRANSP) are reasonable.

# Summary

- When using the same cross section databases, TRANSP & FIDA<sub>sim</sub> predictions of beam & halo neutral densities get excellent agreement in both magnitude & spatial profile.  
→ verify the halo models in TRANSP and FIDA<sub>sim</sub>
- Halo neutral density is comparable with beam neutral density and halo neutrals spread broader than beam neutrals due to multi-generations and halo diffusion.
- Halo neutrals significantly increase the NPA flux and FIDA emission, but they have minor effects on NPA energy spectrum or FIDA spectrum/spatial profile.
- The calculation of halo neutral density (and also fast ion density, NBCD, neutron rate) is relatively sensitive to the choice of atomic cross section databases.

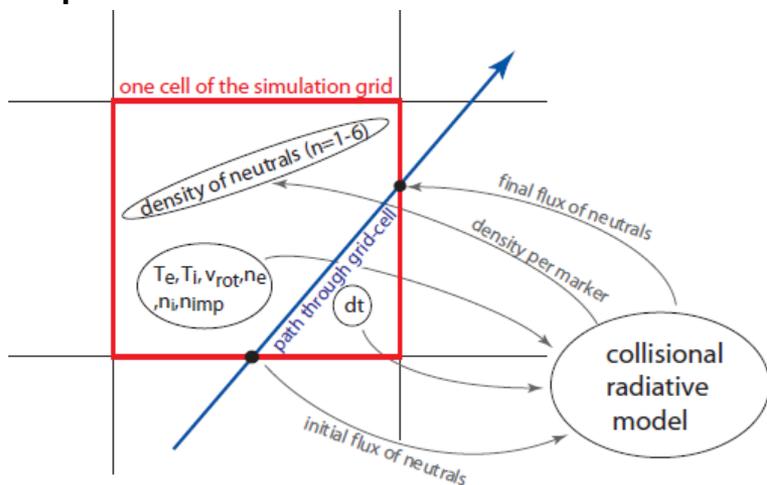
# Backup Slides

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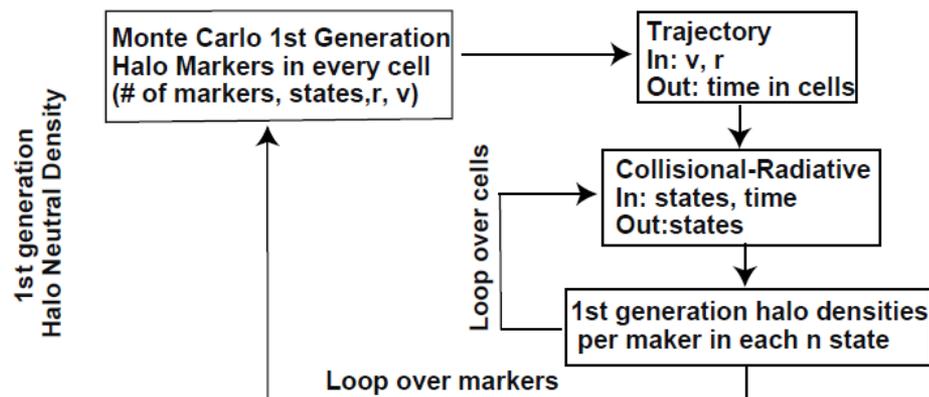
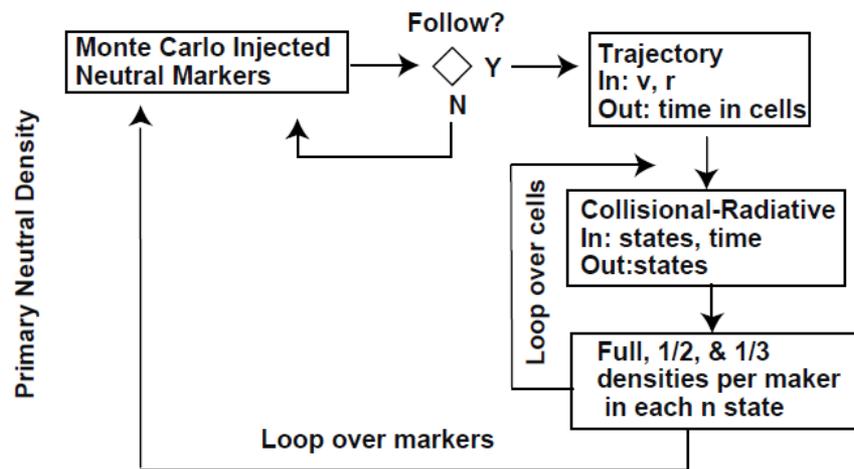
# Beam and Halo Neutrals are Calculated Self-consistently with Monte-Carlo Method in FIDASim

FIDASim: a synthetic diagnostic code that uses forward modeling to calculate Doppler shifted  $D_\alpha$  spectrum, and NPA particle flux at a particular time slice.

The core of the code is collisional-radiative equation with energy level  $n$  up to 6.



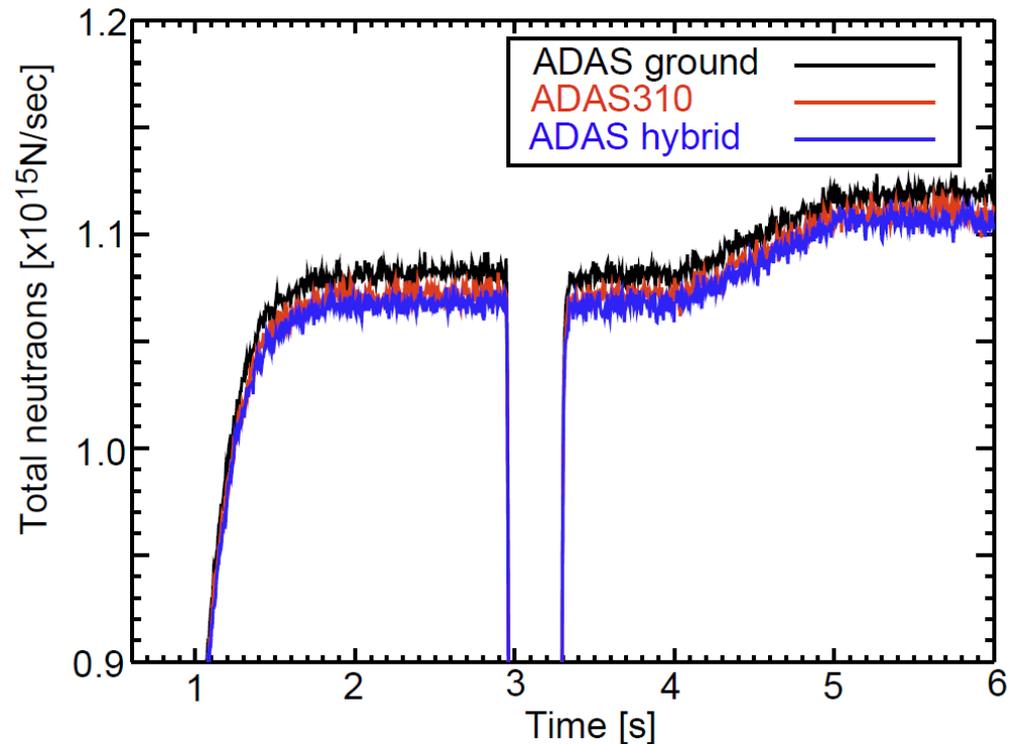
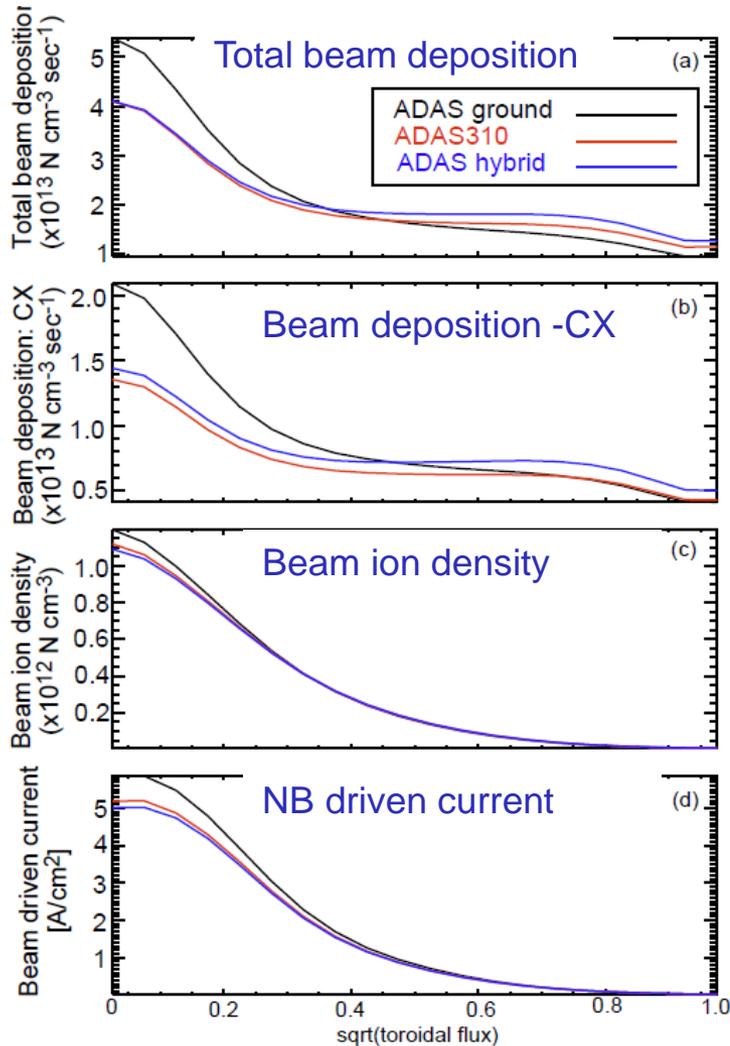
B. Geiger 2012 PhD Thesis



$i$ -th Generation Halos: similar to 1st generation except the number of marks is proportional to  $(i-1)$ th generation halos

\*More details about FIDASim code, visit, <https://github.com/D3DEnergetic/FIDASIM/>

# Effects of Choices of Atomic Cross Section Tables



# Benchmark Work Benefits both FIDAsim and TRANSP

- The benchmark work help resolve a few issues in both FIDAsim and TRANSP codes.
  - **FIDAsim code**
    - (1) Improve the NPA attenuation calculation
    - (2) Improve the mapping of fast ion density along the NPA sightline
  
  - **TRANSP/NUBEAM code**
    - (1) Fix a bug in the calculation of relatively velocity
    - (2) Fix a bug related with the sign of rotation
    - (3) Resolve left-handed or right-handed coordinate system confusion
    - (4) Resolve the inconsistency between 3D box output data and NPA sightline diagnostic output
    - (5) Improve the control of statistics of halo neutral calculation