

**PSI** Center for Neutron and  
Muon Sciences

# Neutronic study of Hydrogen Deuteride as a Cold Neutron Moderator

ICANS XXV

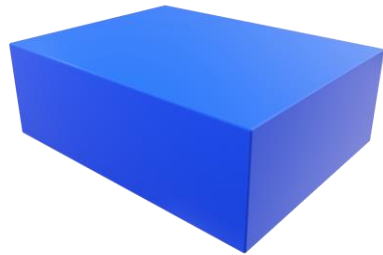
Nicola Rizzi

Malmö, 13.04.2026

# Brightness vs Intensity

**Brightness:** Phase-space density. Invariant under ideal transport thanks to Liouville's theorem

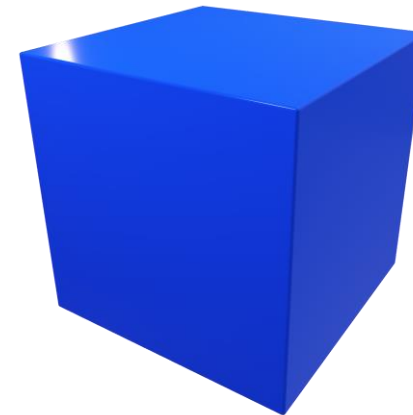
Liquid  $H_2$  and pure para- $H_2$  offer high proton density and scattering  $\sigma$  leading to small volumes or even 1D design



Short MFP at thermal energies limits emission surface. Risk of under-illuminated guides. Larger surfaces lead to strong spatial inhomogeneity.

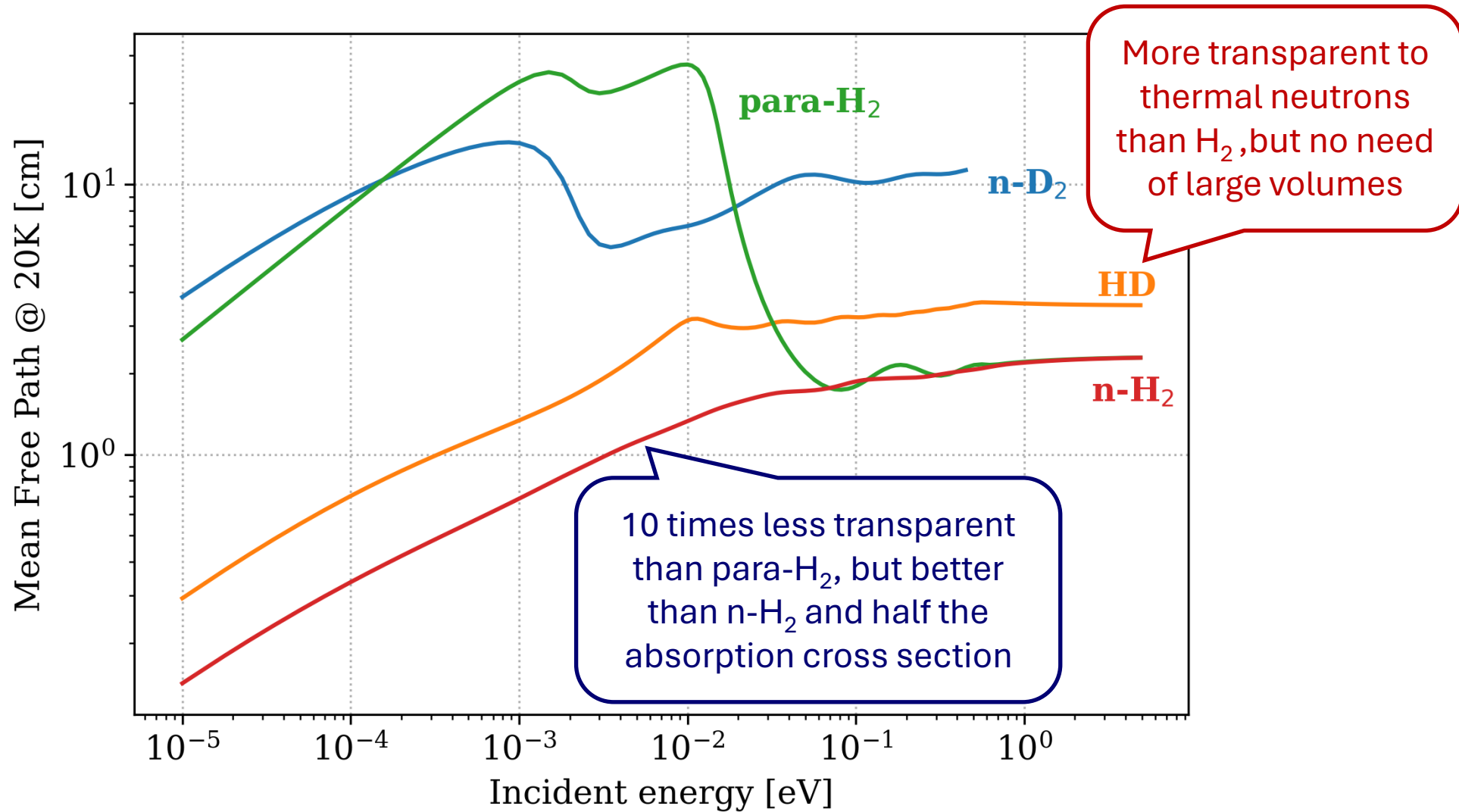
**Intensity:** Neutrons available when we integrate over the emission surface.

Liquid  $D_2$  permits large emission surfaces thanks to its exceptionally small thermal  $\sigma$



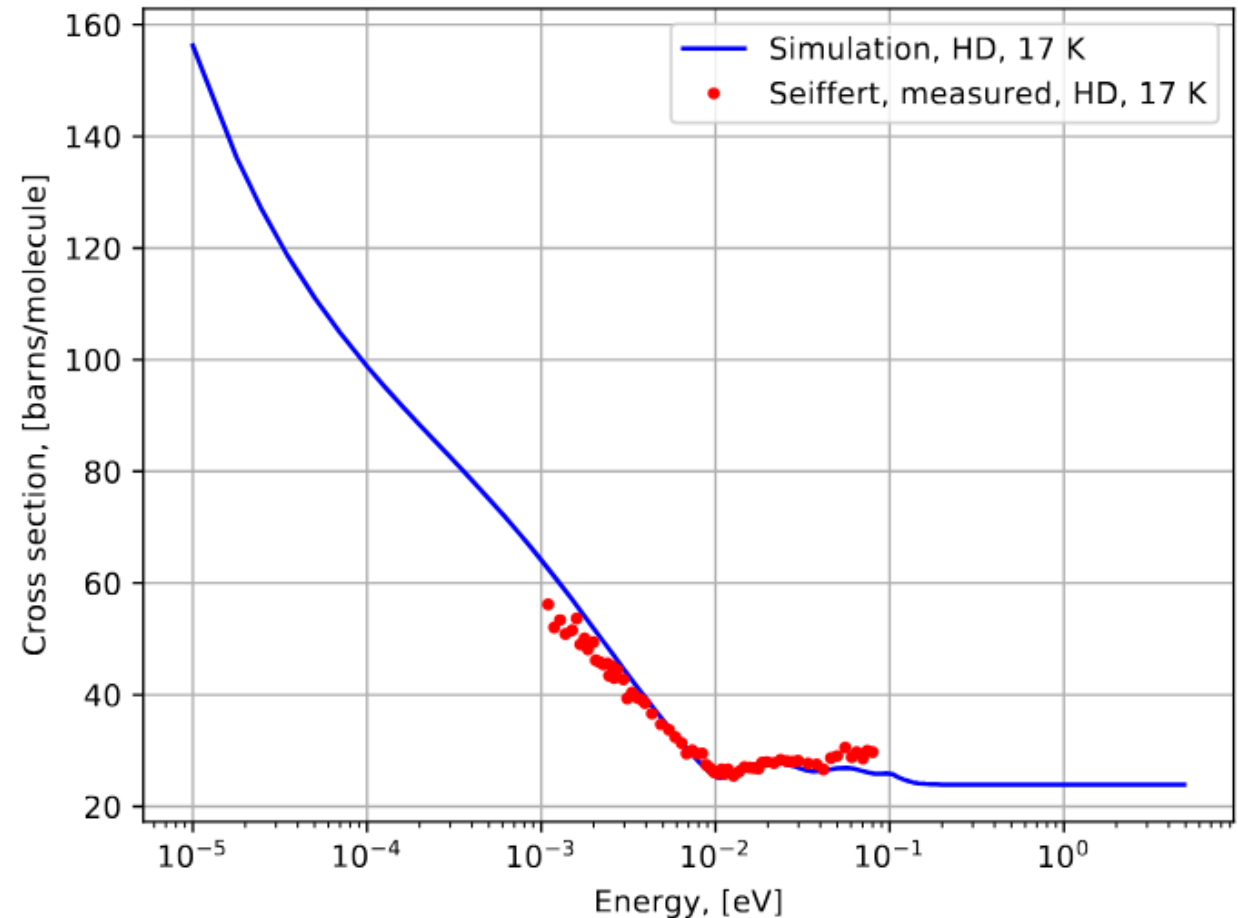
Large volumes to ensure enough collisions for thermal equilibrium. Isotropic emission compromises brightness.

# HD: Intermediate neutronic



# TSL from RPMD

- New Thermal Scattering library based on the work of Alexander Huusko<sup>1</sup> with improved epithermal coupling.
- Only 1 cross section dataset available for validation at 17K<sup>2</sup>



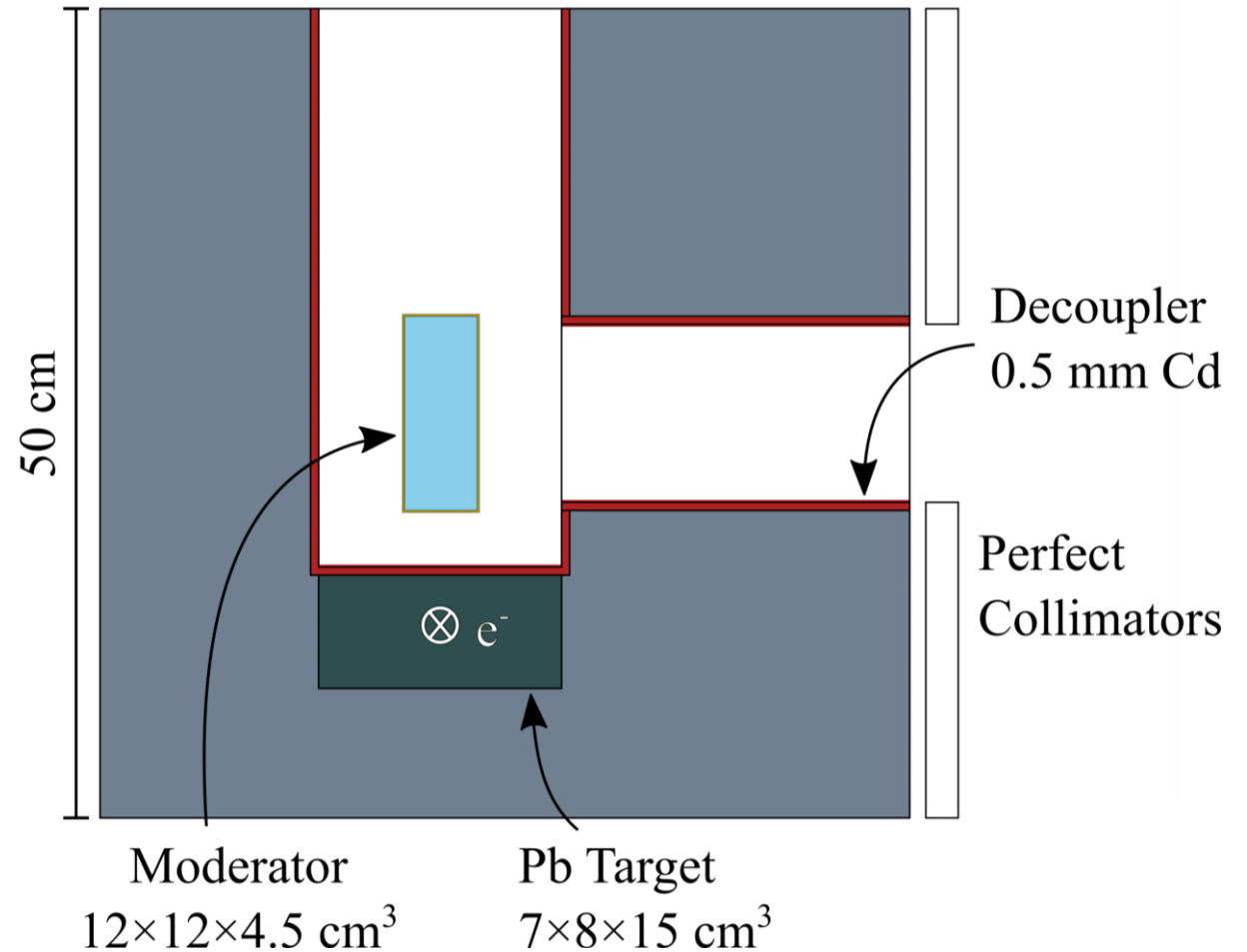
<sup>1</sup>Huusko, Alexander, 2022. Calculation of neutron scattering libraries for liquid ortho-deuterium and hydrogen deuteride. Student Paper

<sup>2</sup>Seiffert, W.D., Weckermann, B., Misenta, R., 1970. Messung der Streuquerschnitte von flüssigem und festem Wasserstoff, Deuterium und Deuteriumhydrid für thermische Neutronen. Zeitschrift für Naturforschung A 25, 967–972.

# TSL Validation: Hokkaido Linac

## MCNP6.3 Simulation Flow

- 1 Electron-to-Gamma (el03):** 34 MeV electron beam impinges on the lead block. Emission of bremsstrahlung gammas.
- 2 Gamma-to-Neutron (ENDF7u):** Photonuclear production of neutrons within the target.
- 3 Decoupled Source:** neutrons generated as a uniform and isotropic volumetric source in the lead block. Energy-dependent probability distribution from previous step.
- 4 Moderation:** 97% purity D in liquid HD and natural para-ortho 1:3 ratio in liquid H<sub>2</sub> modeled using JEFF 3.3 at 18K.



# Energy Spectrum

## Intrinsic Efficiency Parametrization

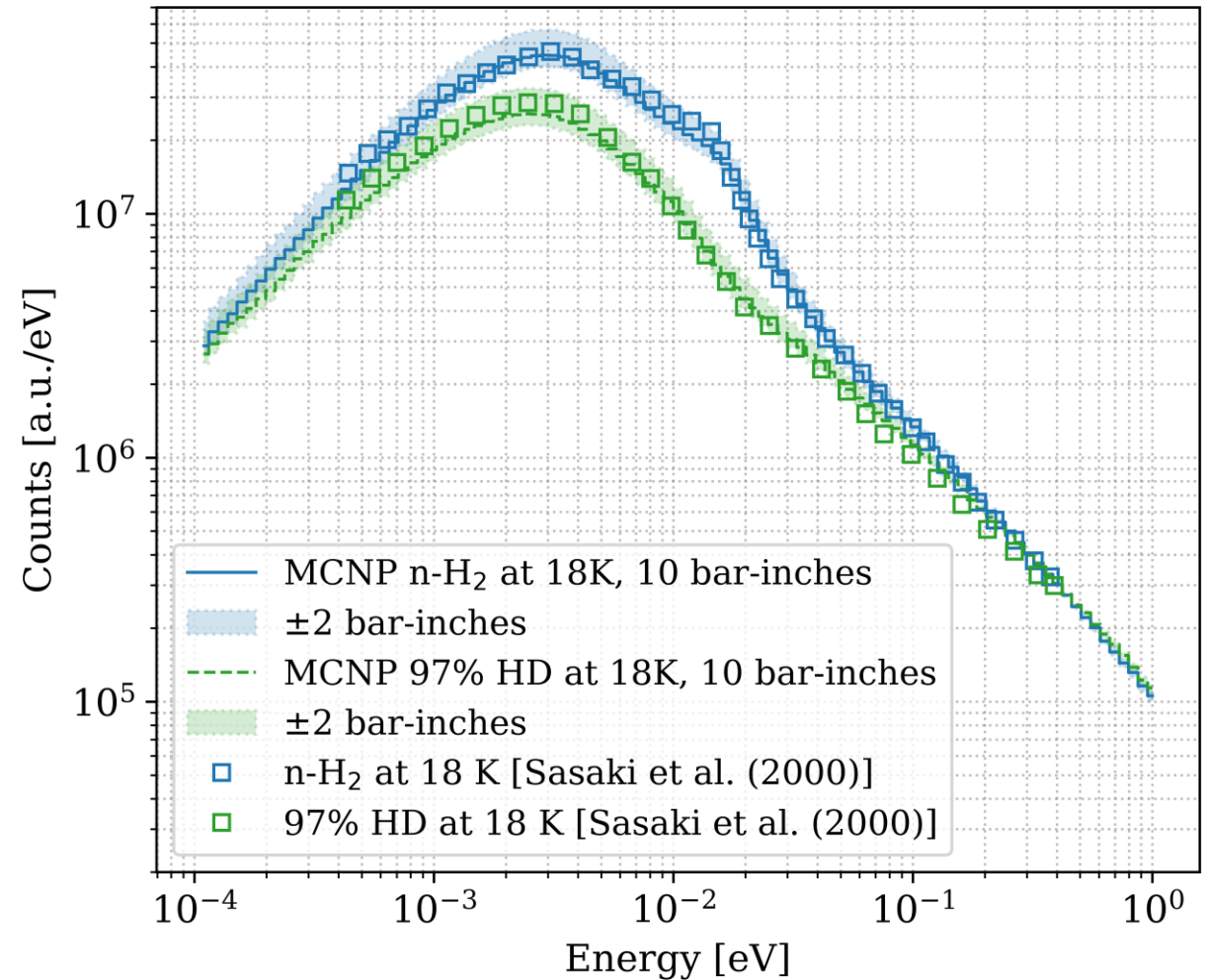
$$\varepsilon(E) = 1 - \exp\left(-\frac{P \cdot D}{RT} N_A \sigma(E)\right)$$

$P \cdot D$  = gas pressure x detector diameter  
(uncertainty treated as systematic error)

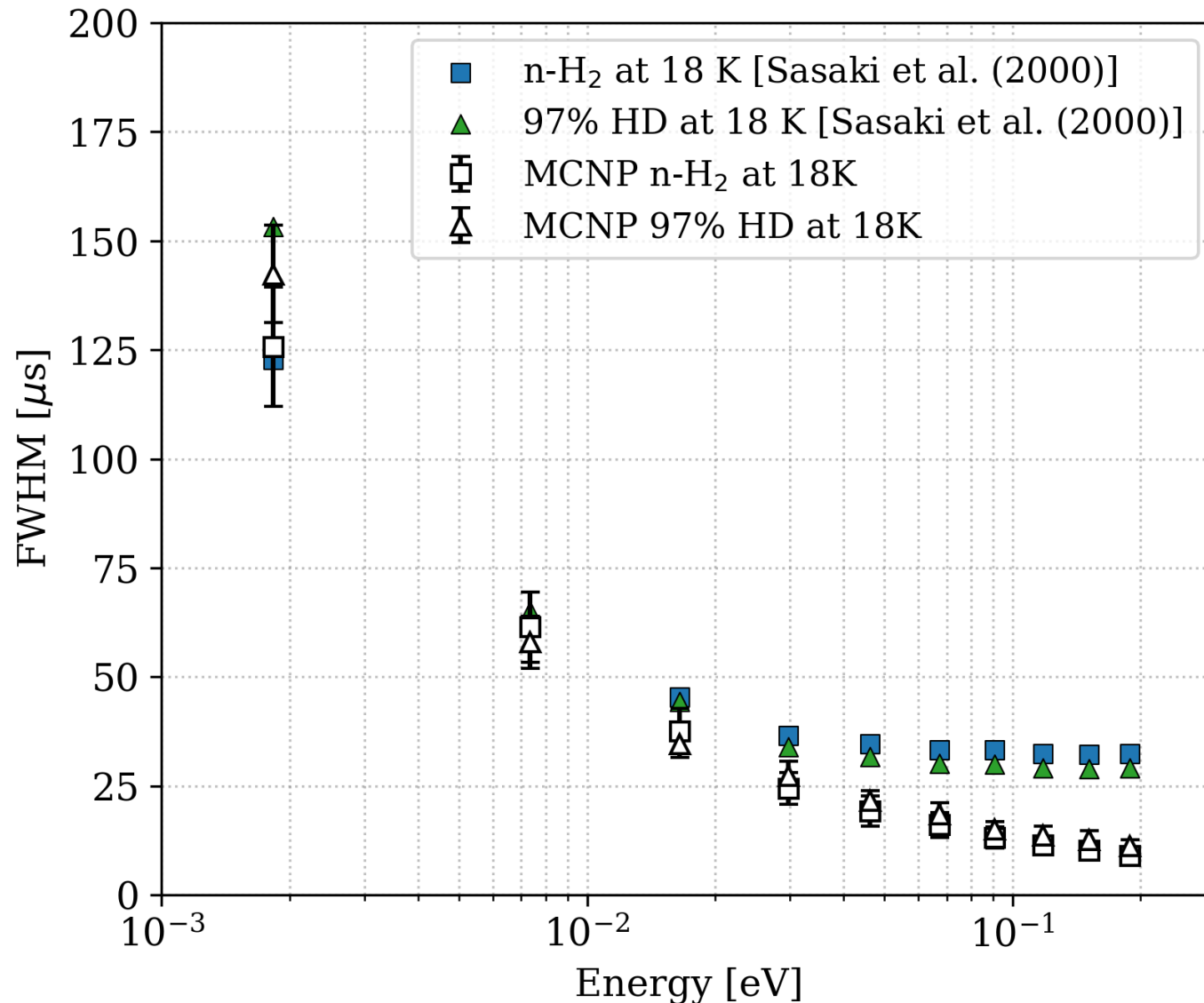
$\sigma$  =  $^3\text{He}$  microscopic absorption cross-section  
(1/v law from 5330 b at 25 meV)

### Conclusion

The simulation data, renormalized at 0.37 eV where scattering does not depend on molecular dynamics, accurately reproduces the physical peak energy at 2.4 meV and cold-to-thermal neutron ratio for HD.



# Pulse Shape Validation



## Systematic Error

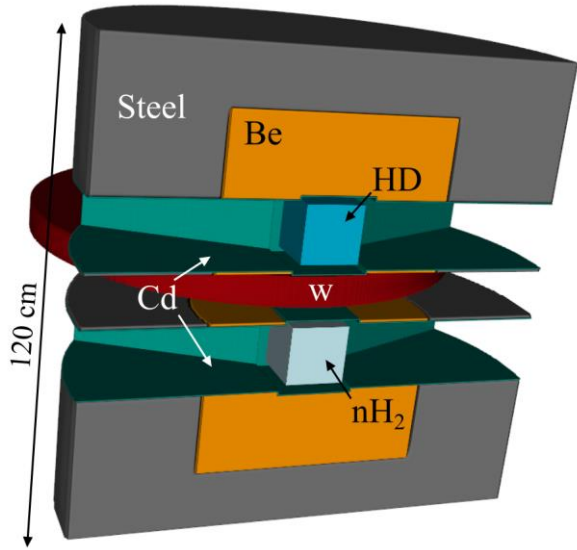
Error bars in the FWHM derived from combining pulse width uncertainty (0.01 to 3  $\mu\text{s}$ ) with wavelength resolution (5-10% from pyrolytic graphite Bragg diffraction)

## Conclusion

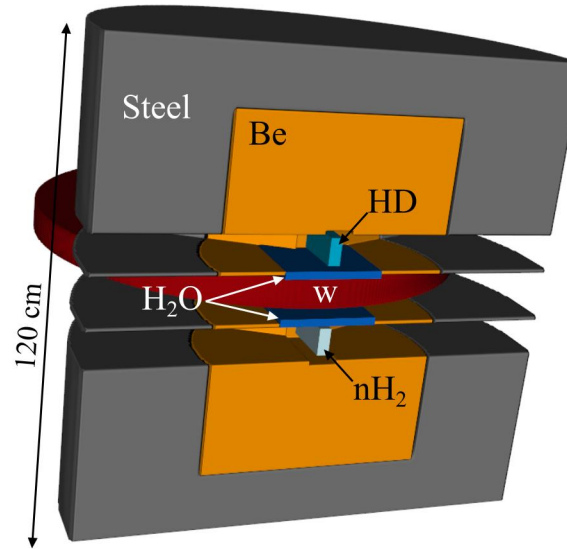
Strong agreement (within 10%) for slower neutrons. Discrepancies at higher energies fall outside standard range of interest for cold neutron applications and may stem from instrument limitations.



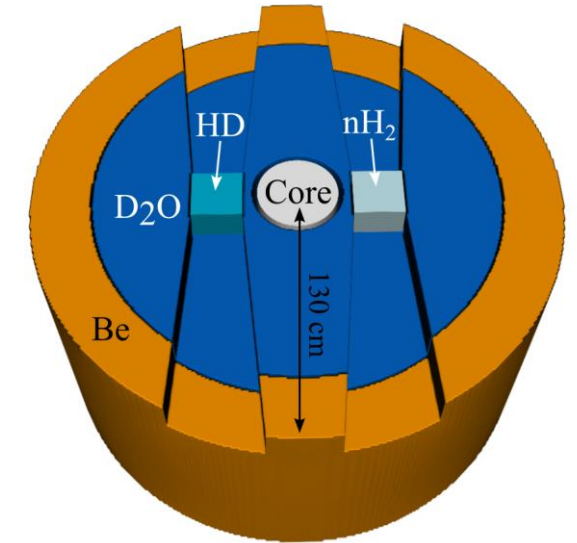
# The simulation study



**Decoupled Source**



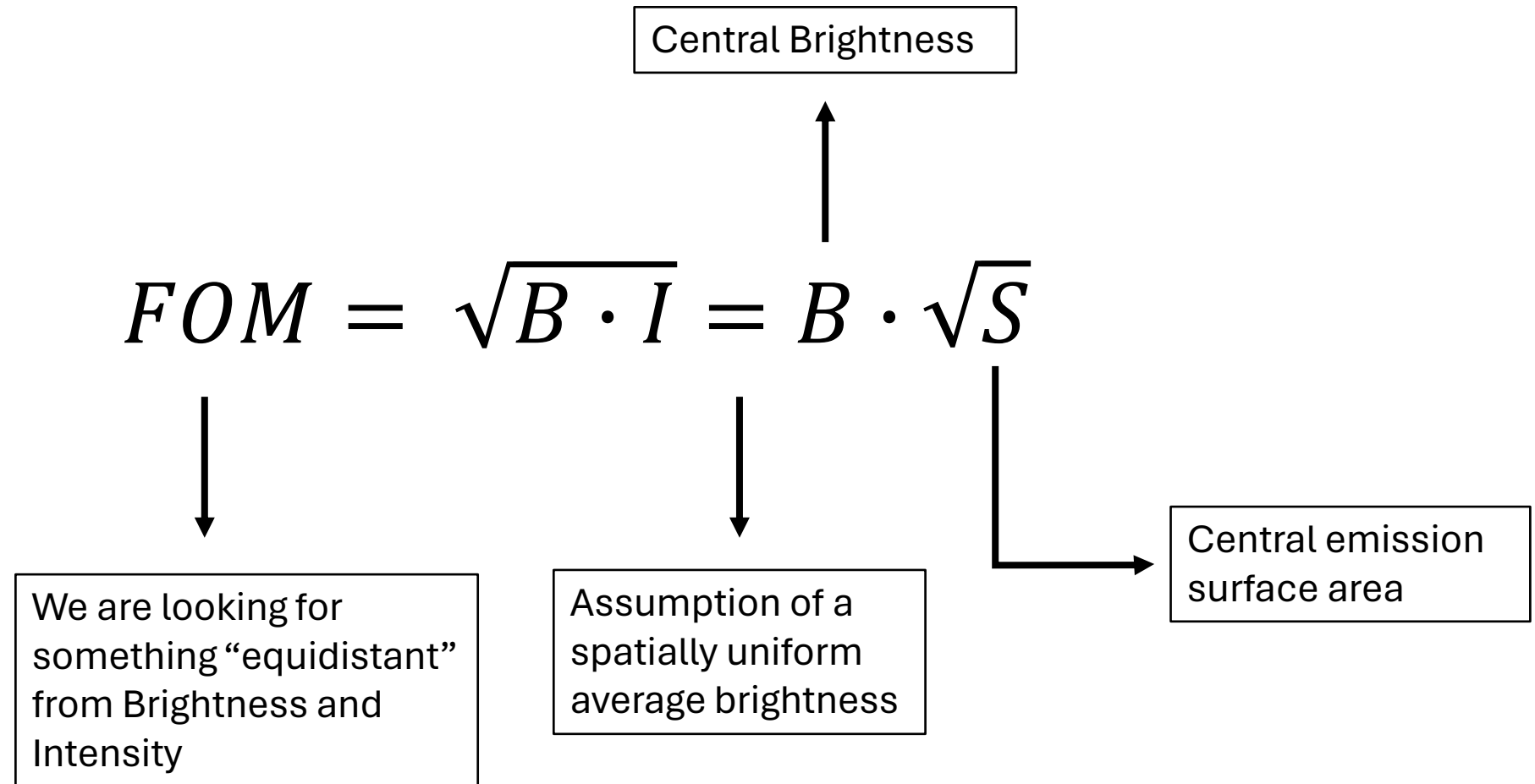
**Coupled Source**



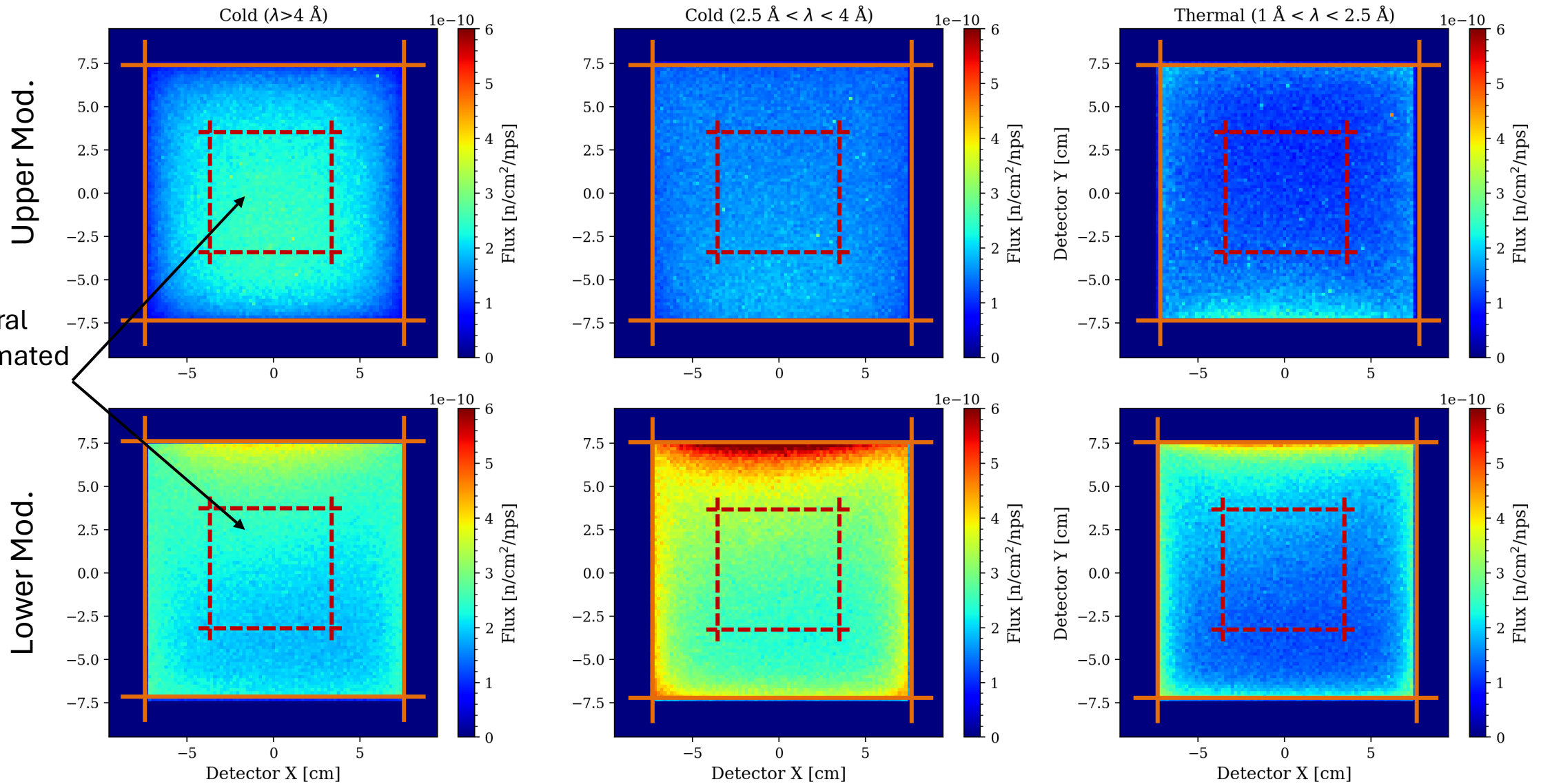
**Reactor-like Source**

<b>Setup</b>	Pulsed accelerator-driven spallation source. Cd decouplers.	Pulsed accelerator-driven spallation source. Room temperature water pre-moderator	Continuous steady source. Heavy water and beryllium reflectors.
<b>Incoming Flux</b>	High fast-neutron component	High thermalized component	Dominant thermal component (heavily coupled)
<b>Goal</b>	Sharp neutron pulses for energy resolution	Maximize time-integrated brightness. Relaxed constraint on time resolution	Voluminous sources for high intensity feeding many guides.

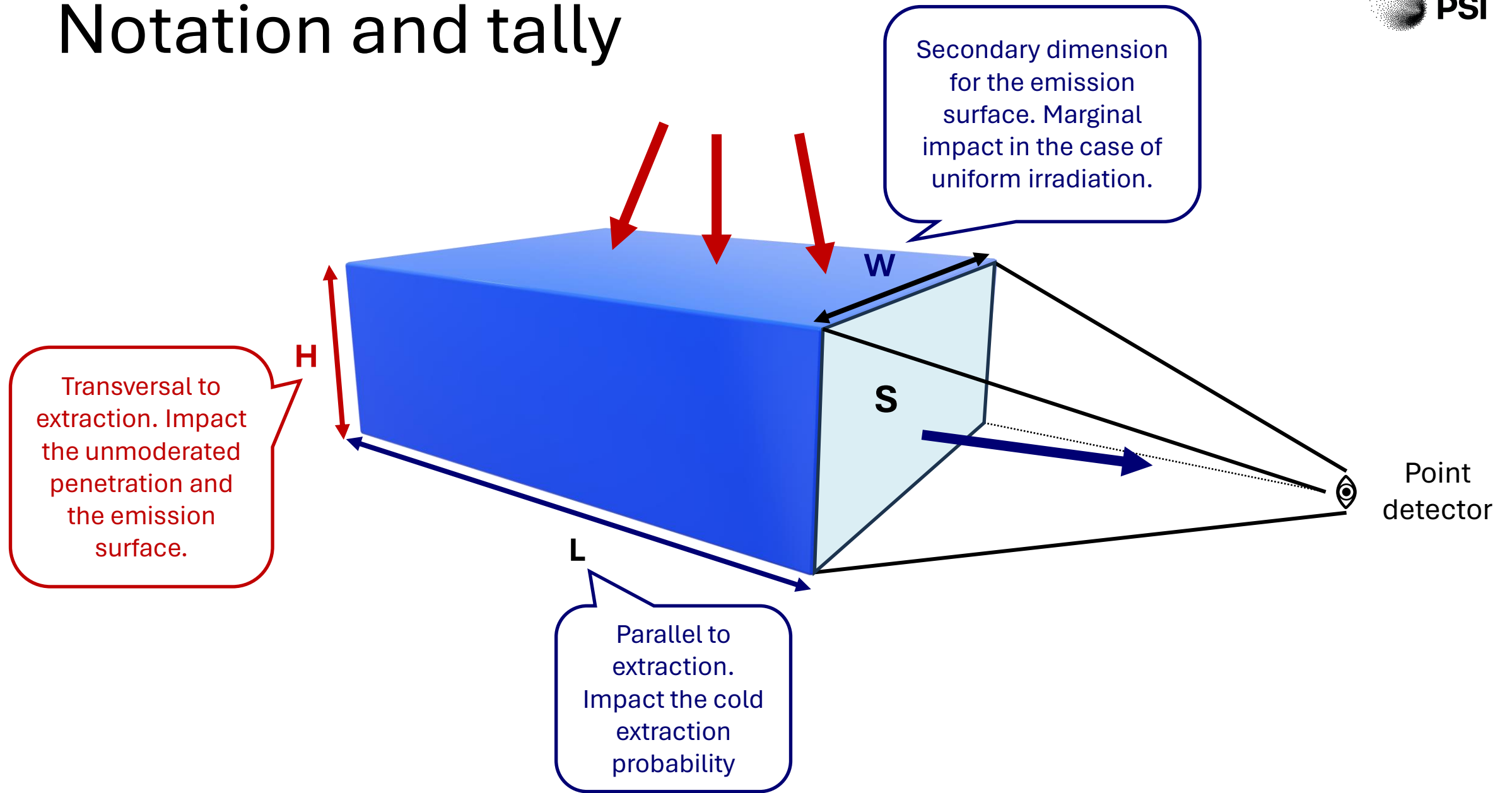
# FOM



# Exclude border effect



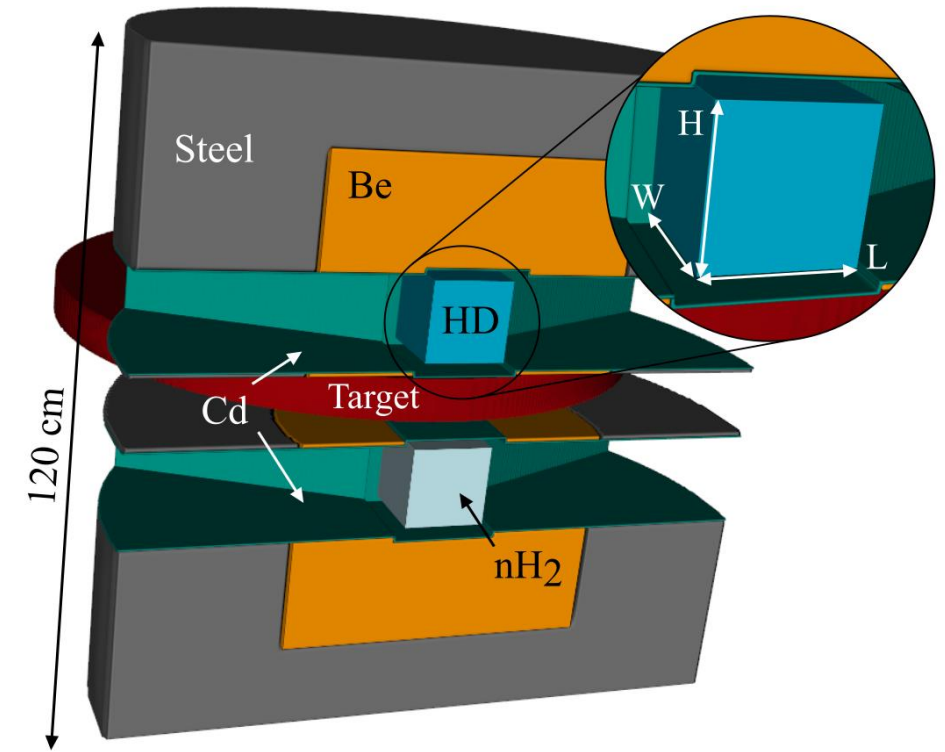
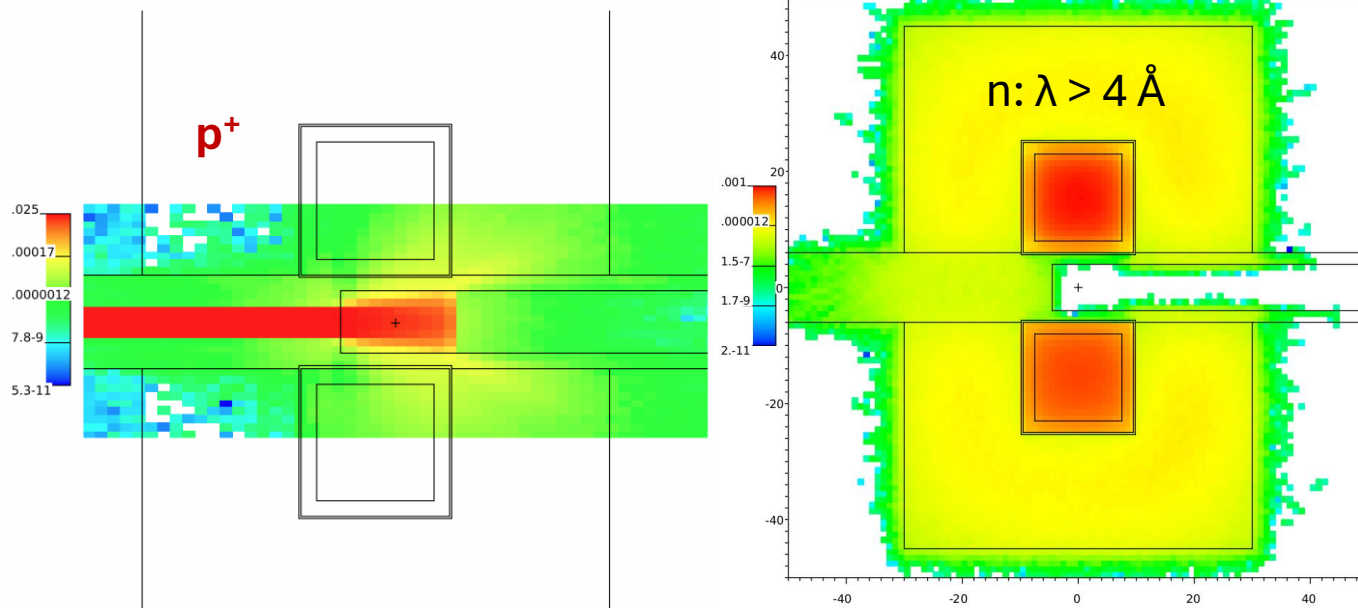
# Notation and tally



# Decoupled Source

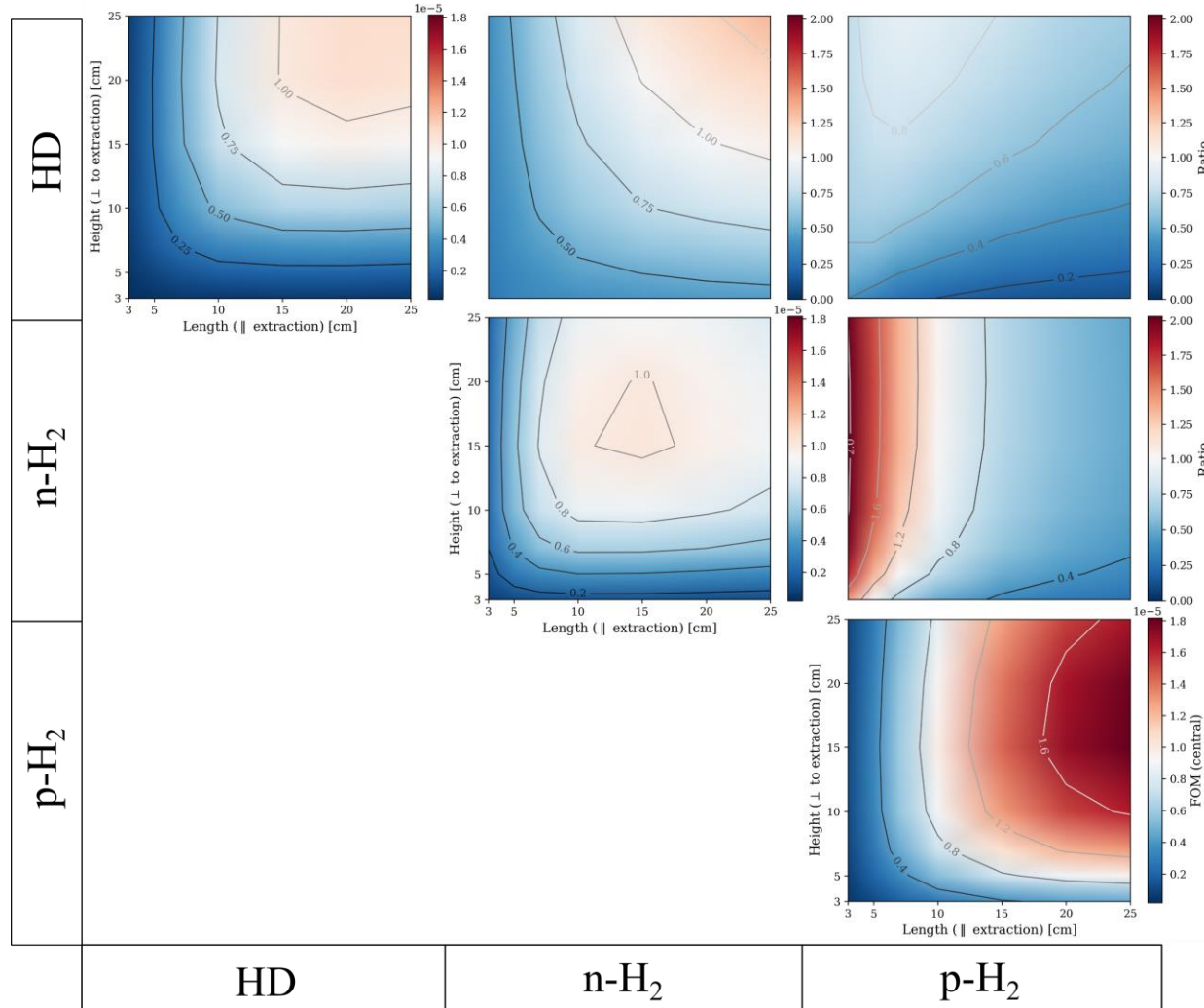
## System Parameters

- **Proton Beam:** 500-MeV, 1  $\mu$ s pulse width
- **Target:** Tungsten wheel ( $\rho = 15.3 \text{ g/cm}^3$ ). Spallation model CEM3.03.
- **Decoupling Layer:** 0.3 cm Cadmium
- **Reflector:** Beryllium ( $\rho = 1.85 \text{ g/cm}^3$ )



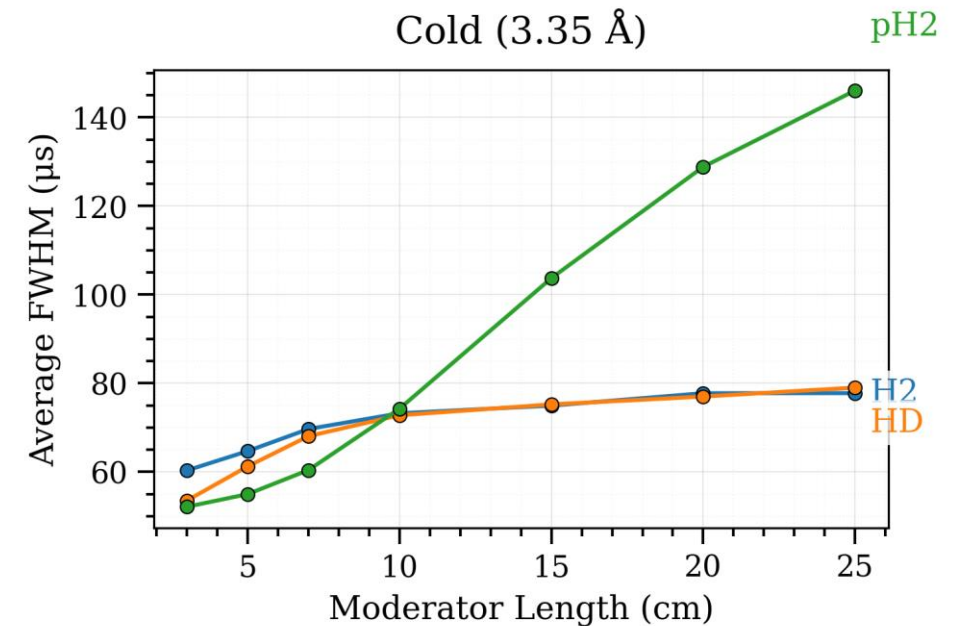
# Results

$\lambda = 4 - 10 \text{ \AA}$ .  $W = 15 \text{ cm}$



## Performance Outcome

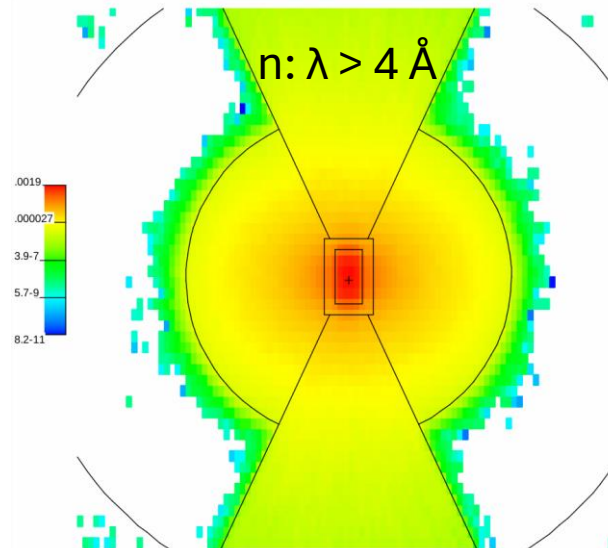
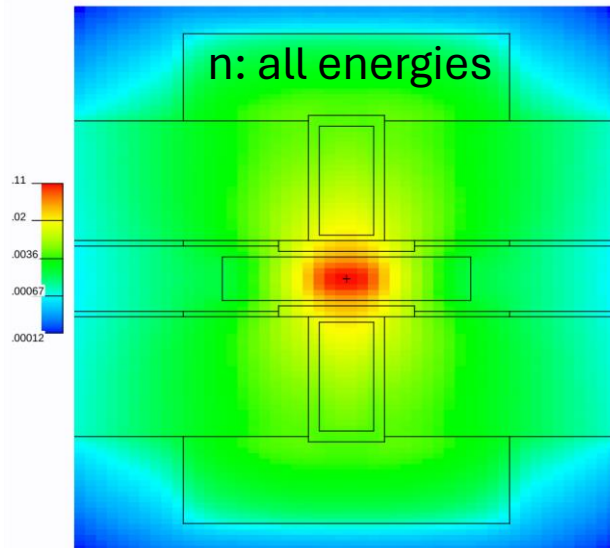
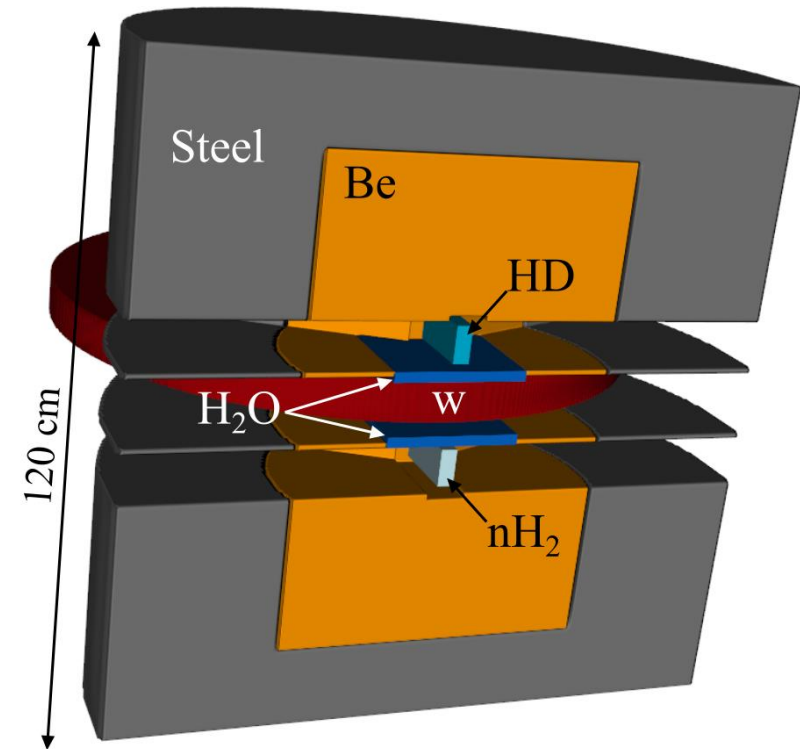
- HD yields fewer cold neutrons than both n-H<sub>2</sub> and pure para-H<sub>2</sub> across the majority of geometries.
- The transparency of para-H<sub>2</sub> entirely outclasses HD in voluminous decoupled setups.
- The choice is between n-H<sub>2</sub> for a thin, fast response moderator, or para-H<sub>2</sub> for maximum brightness.



# Coupled Source

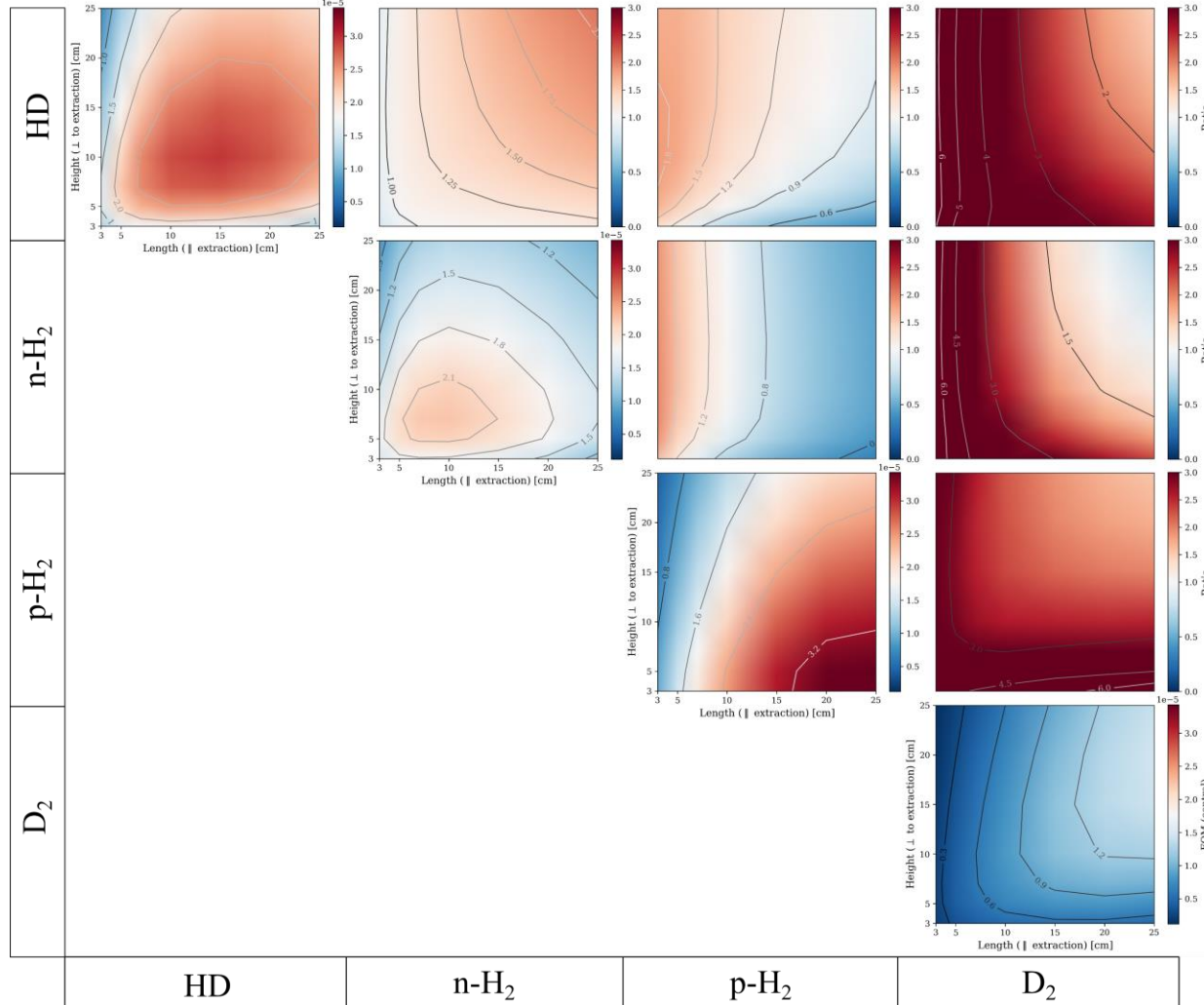
## System Parameters

- **Proton Beam:** 500-MeV, 1  $\mu$ s pulse width
- **Target:** Tungsten wheel ( $\rho = 15.3 \text{ g/cm}^3$ ). Spallation model CEM3.03.
- ~~Decoupling Layer: 0.3 cm Cadmium~~
- **Pre-Moderator:** 25 x 25 x 2  $\text{cm}^3$  room temp.  $\text{H}_2\text{O}$
- **Reflector:** Beryllium ( $\rho = 1.85 \text{ g/cm}^3$ )



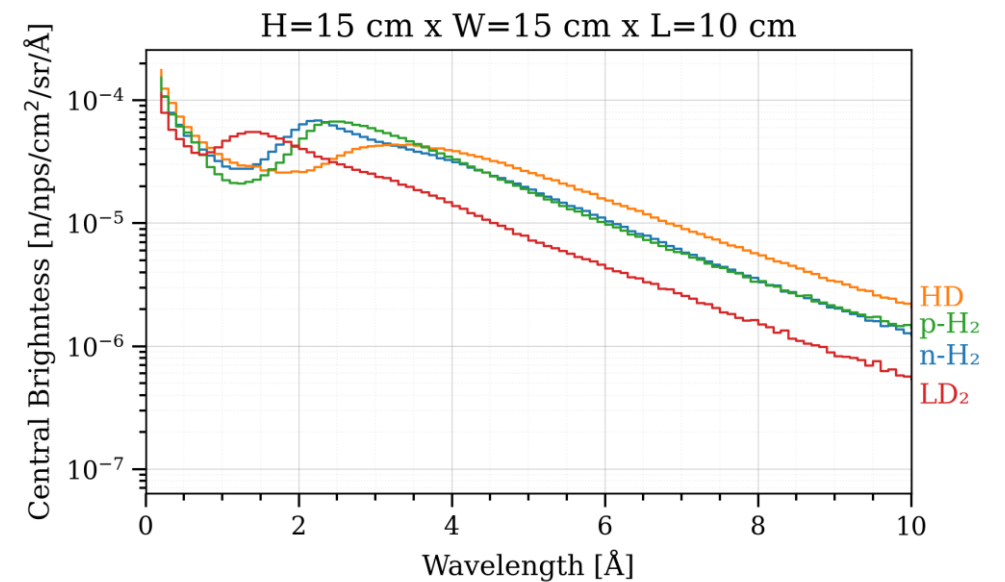
# Results

$\lambda = 4 - 10 \text{ \AA}$ .  $W = 15 \text{ cm}$



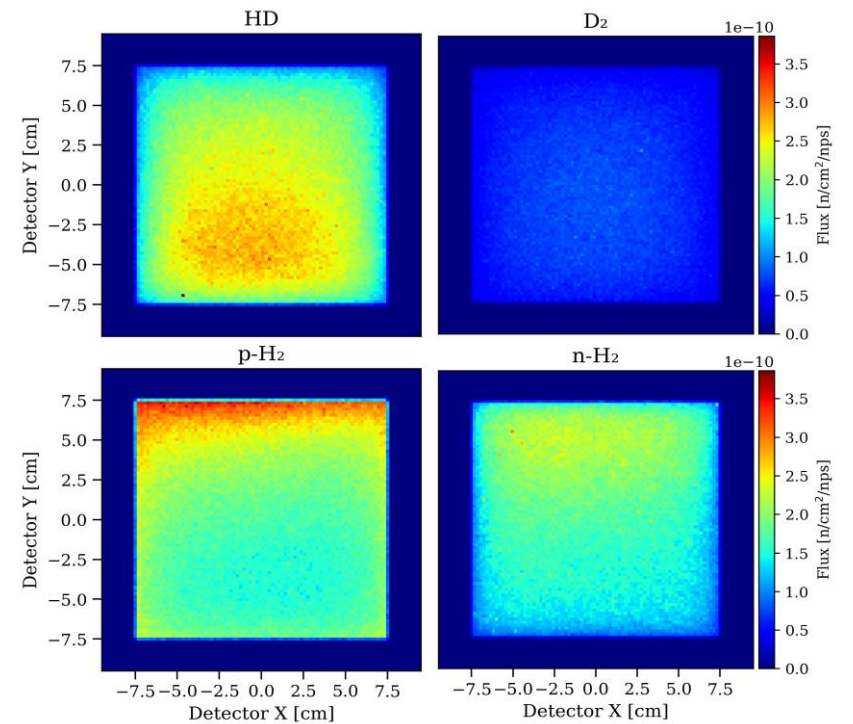
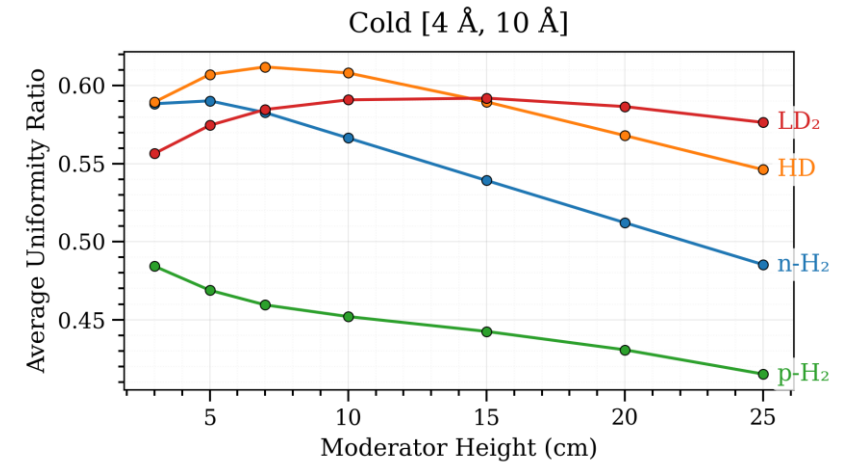
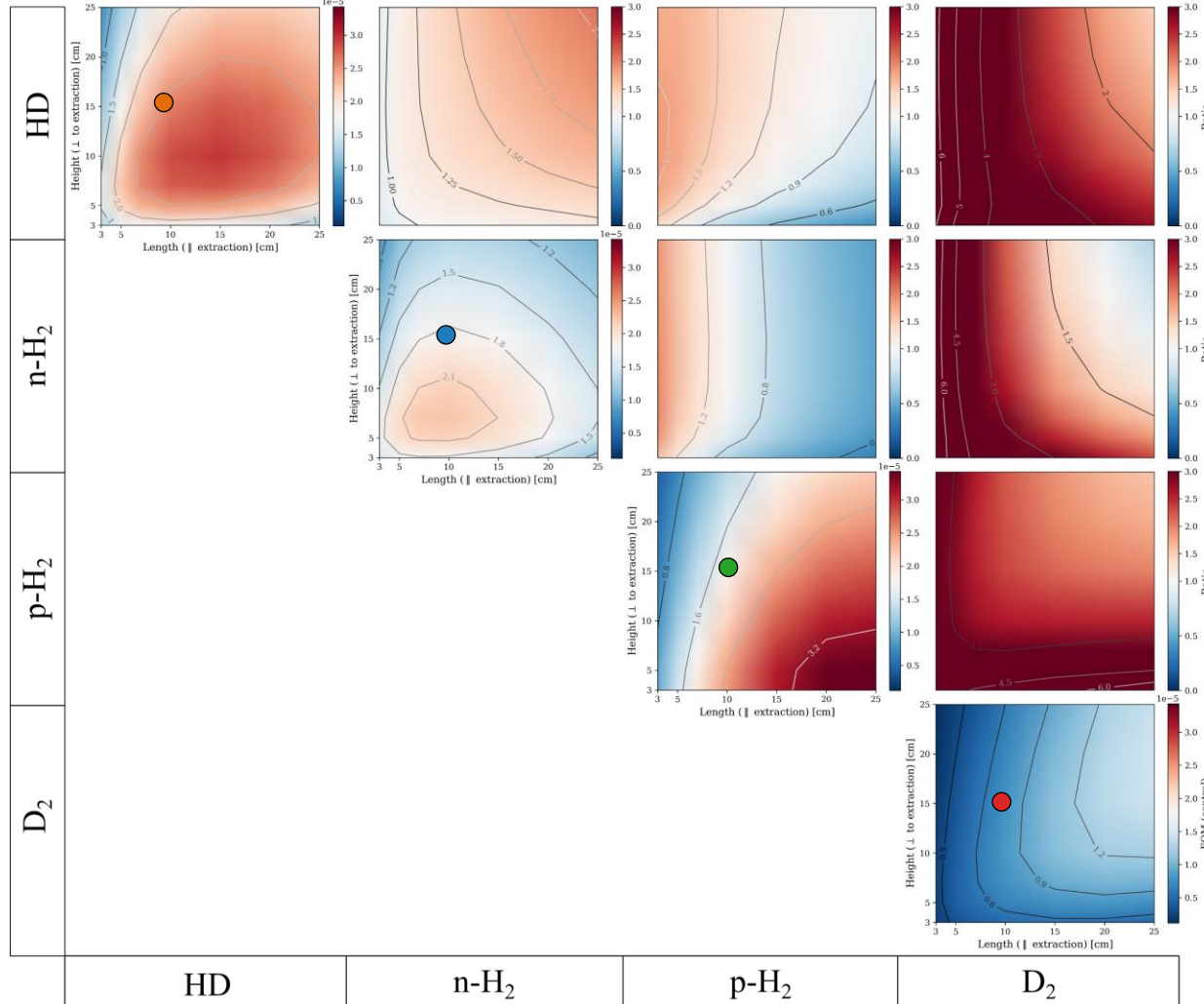
## Performance Outcome

- HD demonstrates a clear FOM advantage in compact regimes ( $L < 15 \text{ cm}$ ). Similar to n-H<sub>2</sub> for  $L < 5 \text{ cm}$
- HD yields a 60% higher FOM than n-H<sub>2</sub> for neutron wavelengths  $> 10 \text{ \AA}$ , regardless of the moderator height.



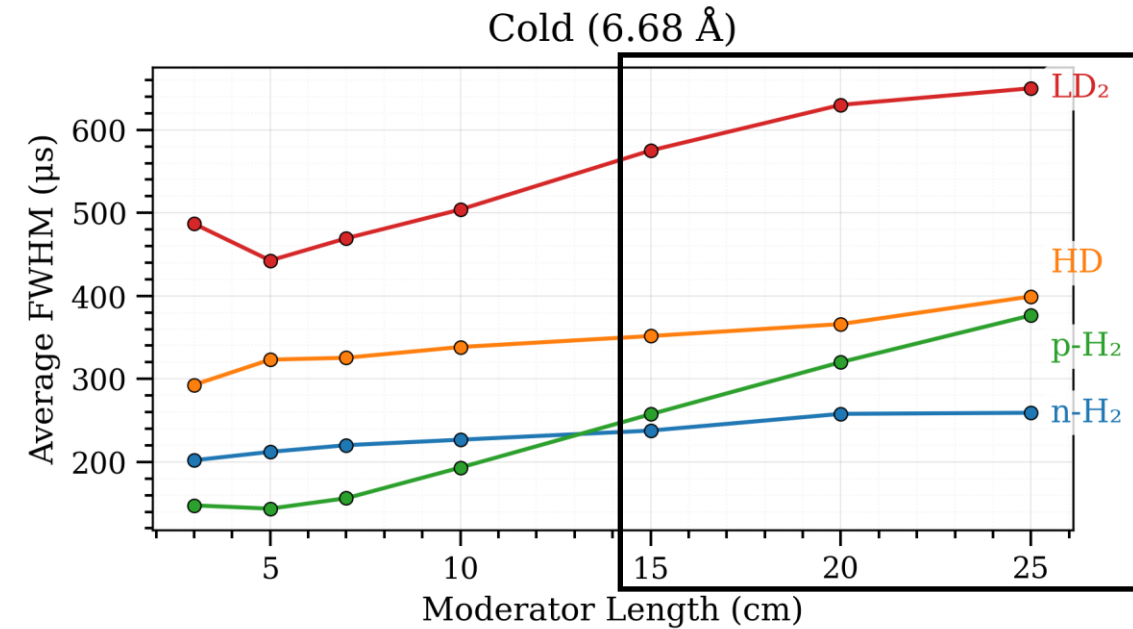
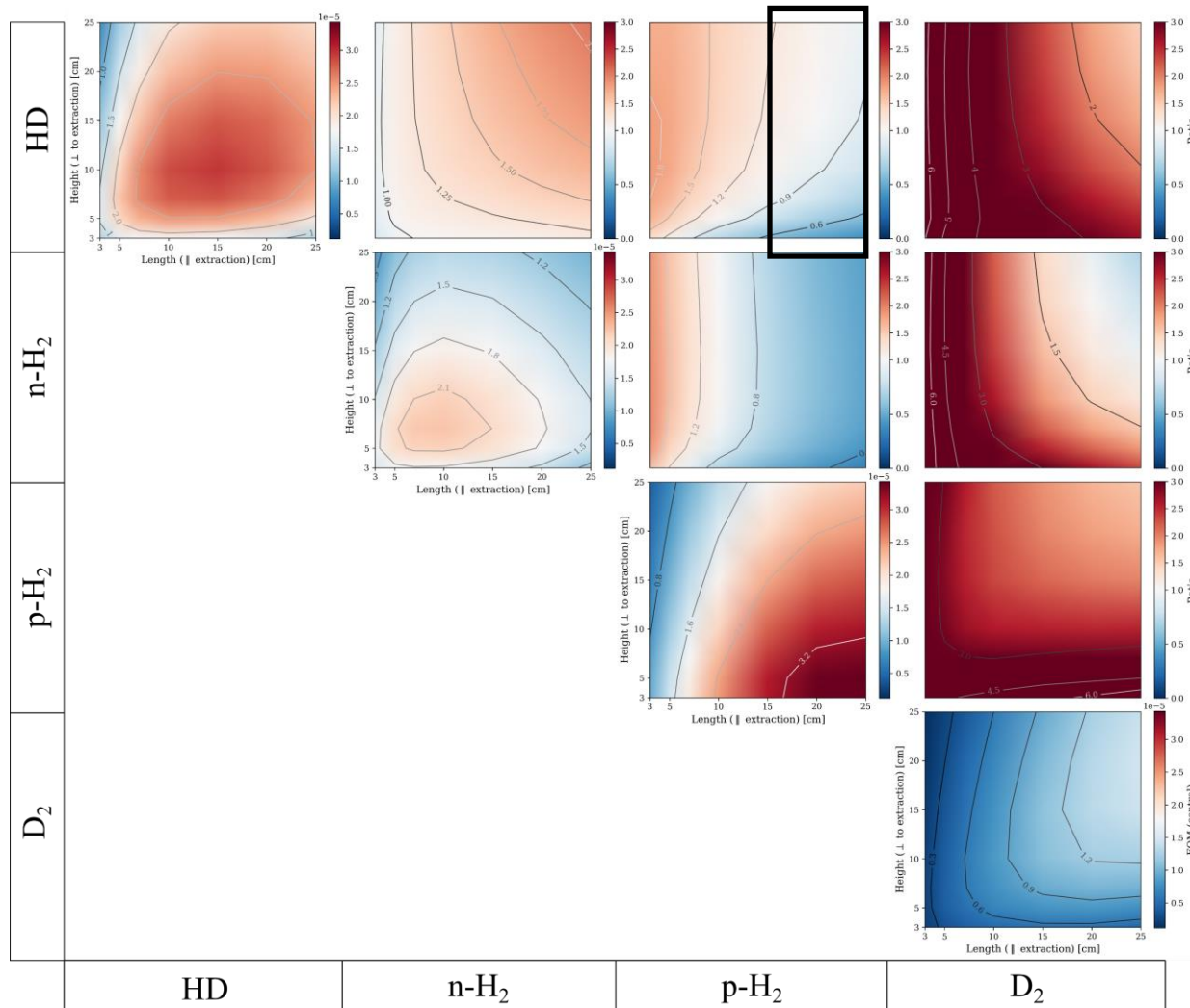
# Uniformity

$\lambda = 4 - 10 \text{ \AA}$ .  $W = 15 \text{ cm}$



# FWHM pulse shape

$\lambda = 4 - 10 \text{ \AA}$ .  $W = 15 \text{ cm}$

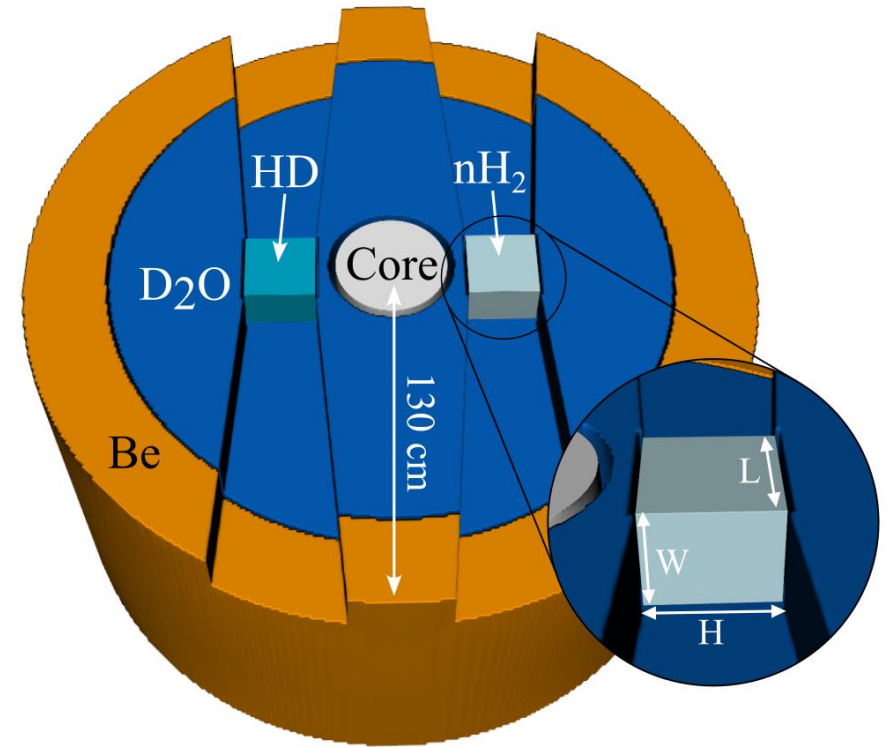
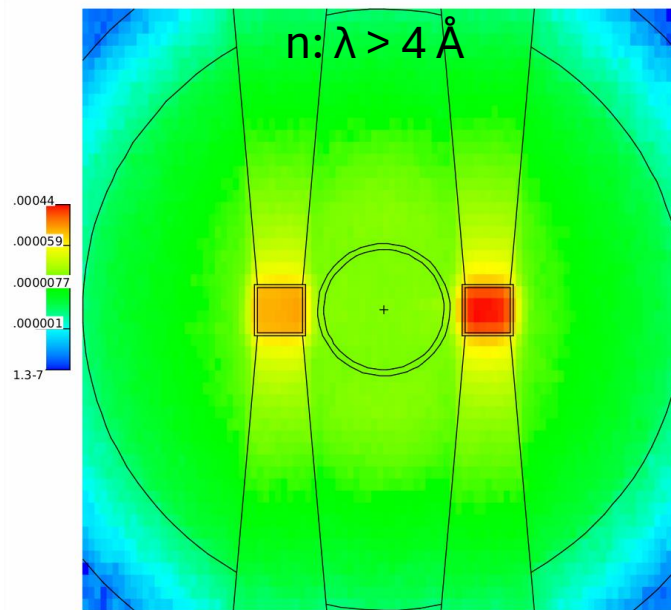
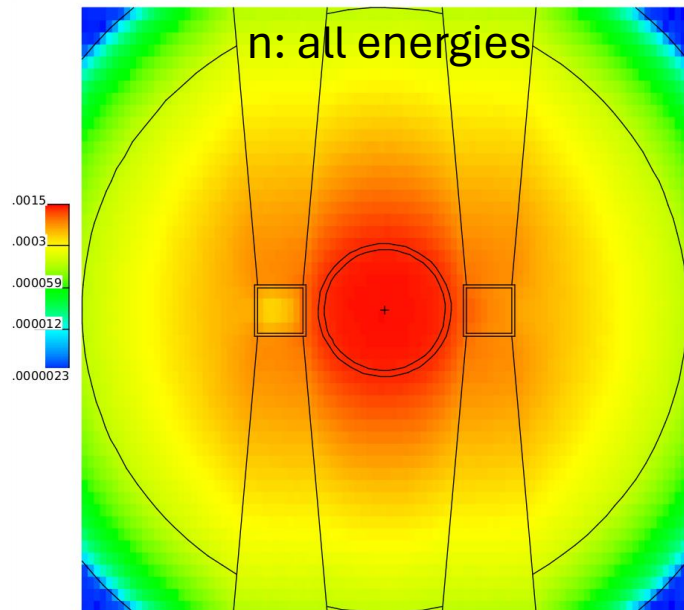


- HD yields in general a broader cold pulse than hydrogen.
- But for long moderator, where para-H<sub>2</sub> excels, this gap soon disappears.

# Reactor-like Source

## System Parameters

- **Source:** dummy core region emitting neutron according to a validated peripheral code spectrum<sup>1</sup>
- **Reflector:** Inner D<sub>2</sub>O (r=100 cm) and Outer Be (r=130 cm)

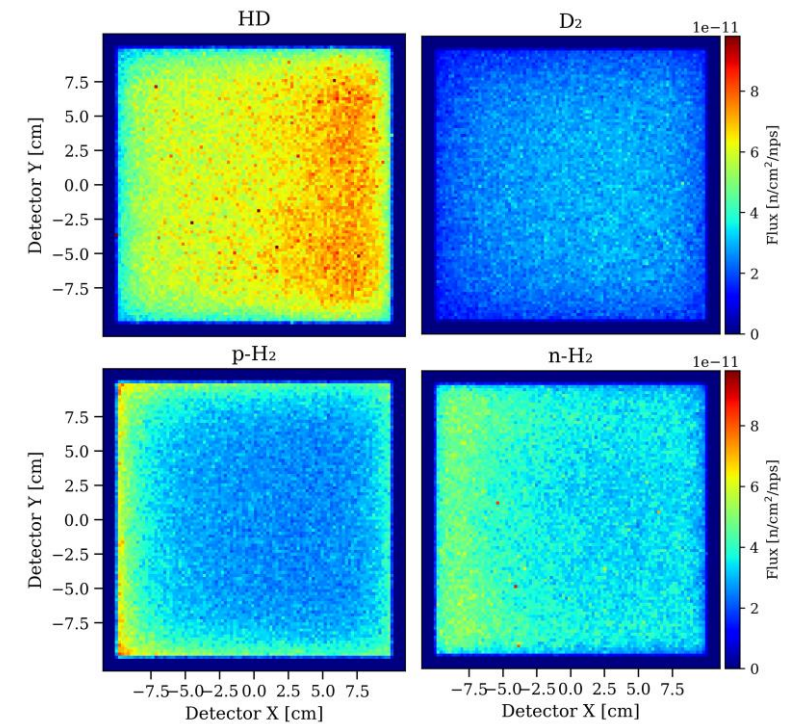
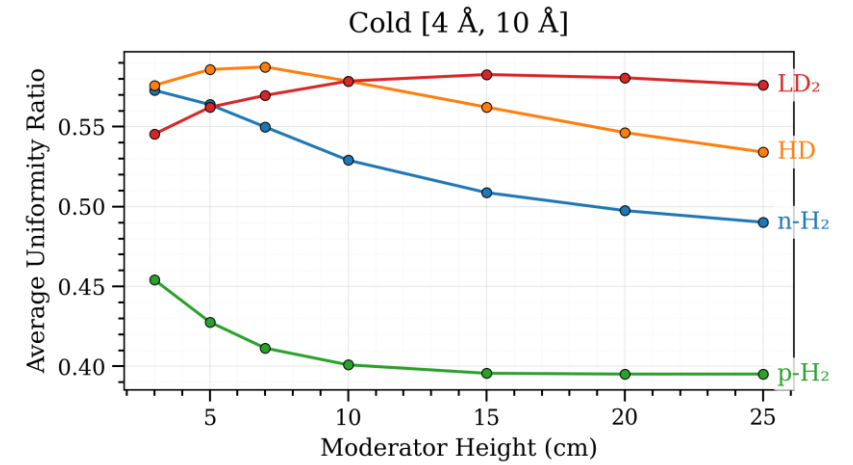
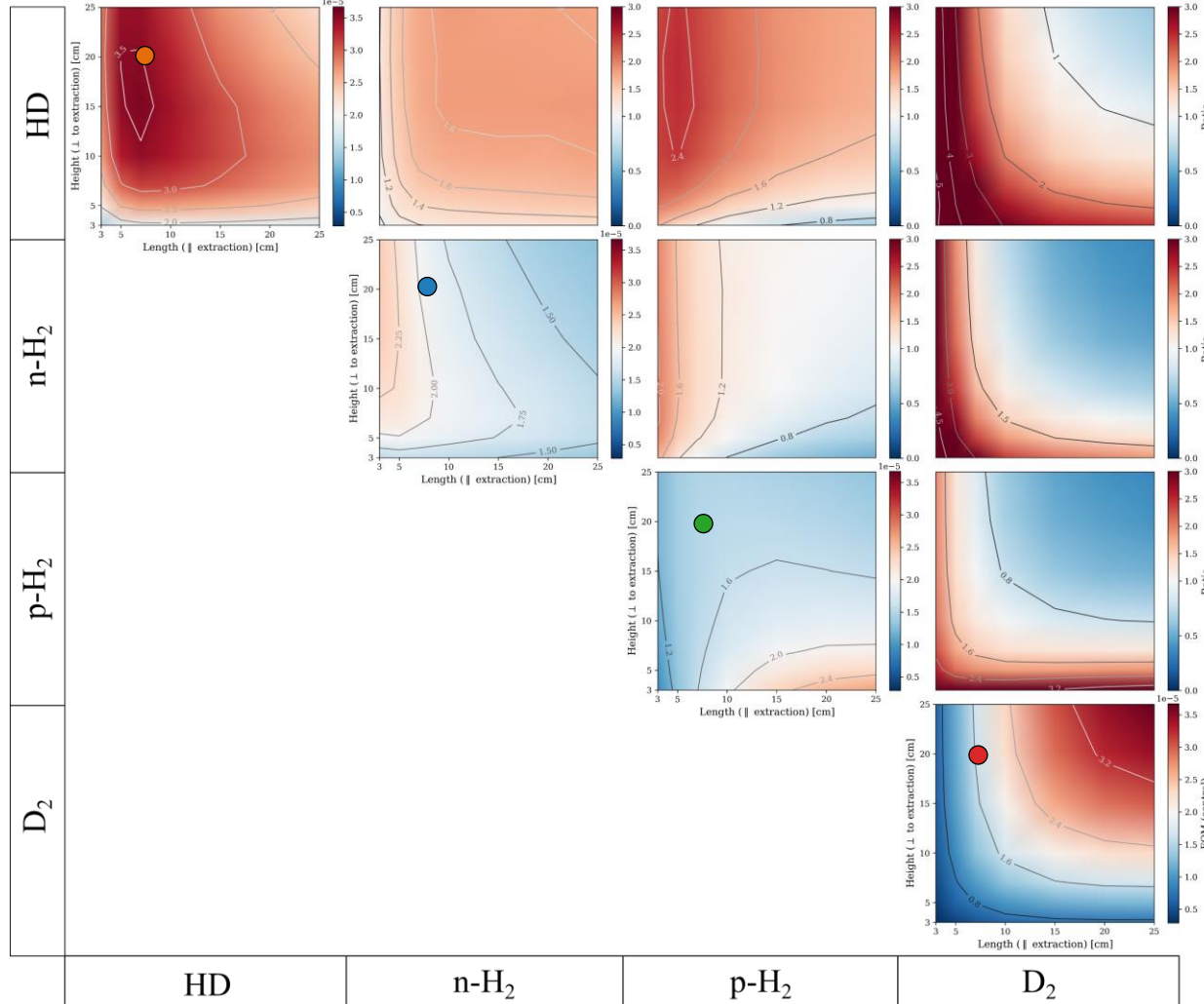


<sup>1</sup>Jiang, Y., Laureau, A., Lamirand, V., Frajtag, P., Pautz, A., 2020. In-core dosimetry for the validation of neutron spectra in the CROCUS reactor.



# Uniformity

$\lambda = 4 - 10 \text{ \AA}$ .  $W = 20 \text{ cm}$

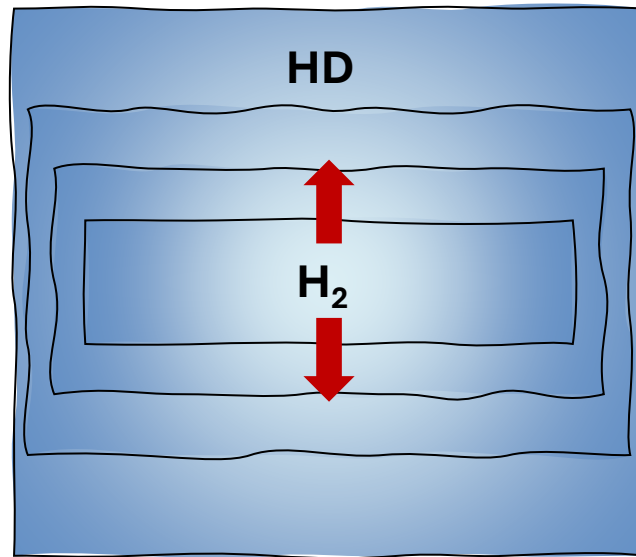


# HD vs H<sub>2</sub> vs D<sub>2</sub>

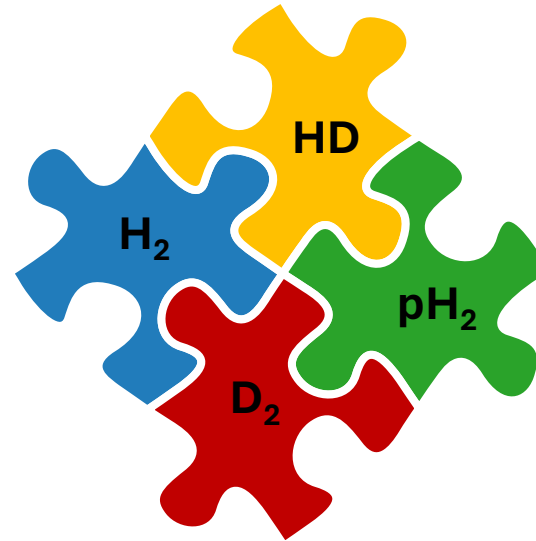
	Para-H <sub>2</sub>	n-H <sub>2</sub>	HD	D <sub>2</sub>
Decoupled (Fast)	 Best overall	 Optimal for thin moderators		
Coupled (Mixed)	 Best L > 15 cm	 Good	 Best L < 15 cm	
Reactor-like (Thermal)		 Good	 Best overall	 Best for large volumes

# Conclusions

## Larger Surfaces

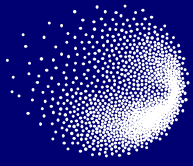


## Geometric Niche



## Future Developments



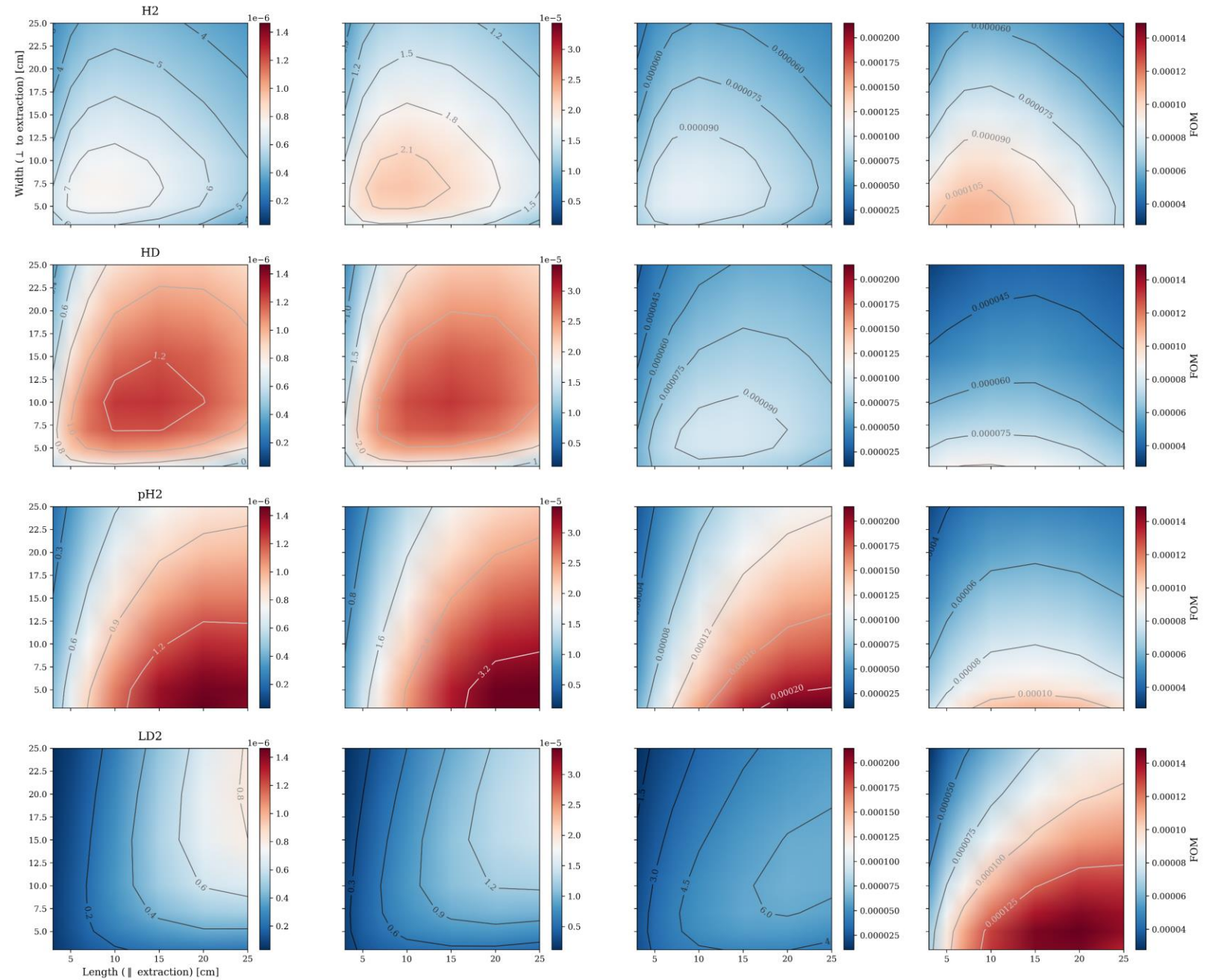


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Thank You  
for your attention



# Coupled All





# Reactor All

