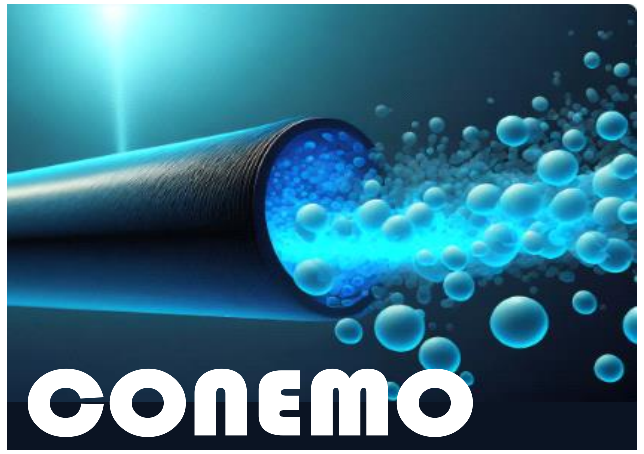
OpenMC simulations of a low dimensional cold neutron moderator for the ICONE project

Richard Wagner, LLB 17.4.2024

LENS/ELENA Workshop
Paris, France



ICONE
Neutrons for
Materials Sciences

Outline

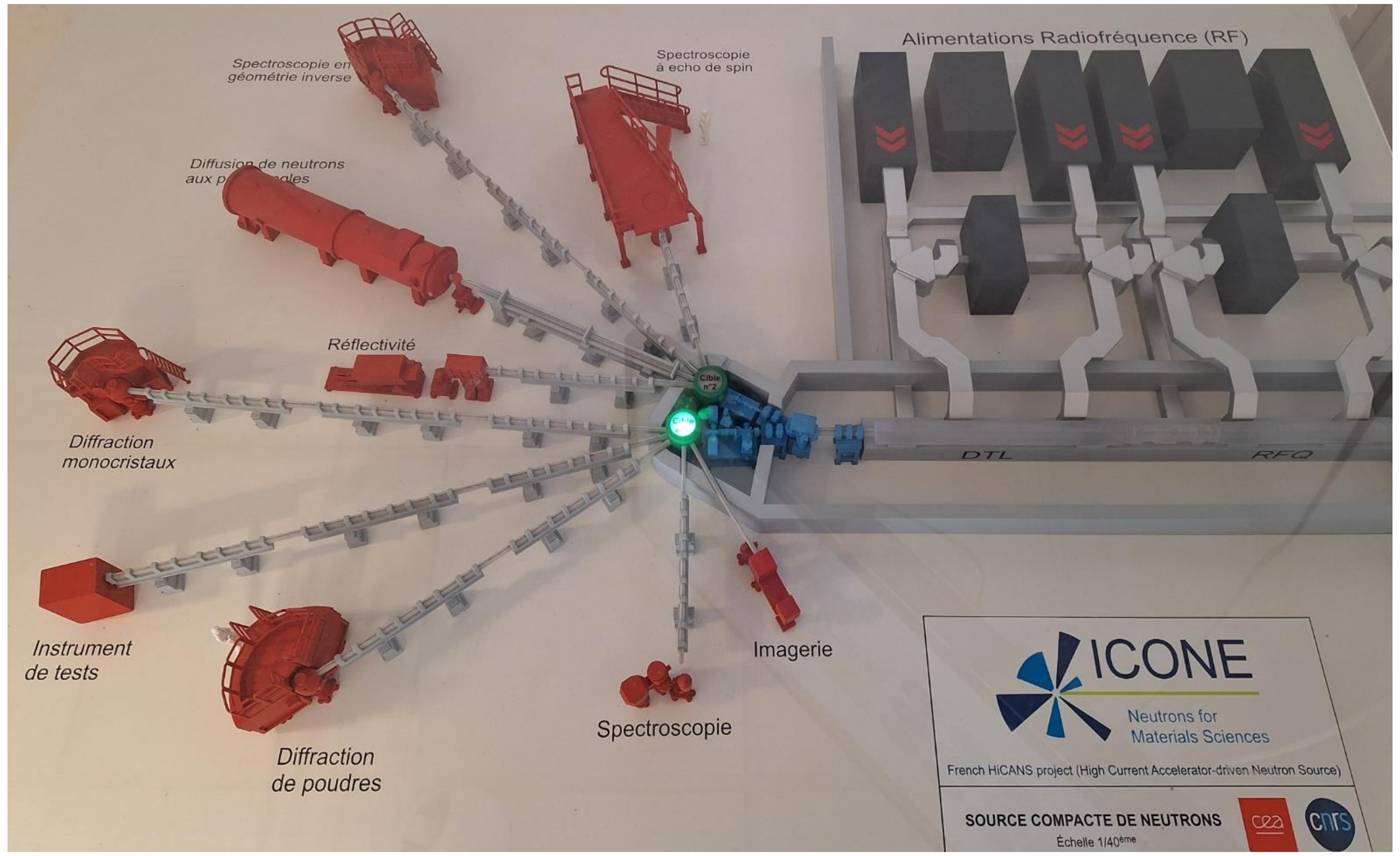
- ICONE project
- OpenMC and simulation strategy
- CONEMO project
- Cross-sections of Para- and Ortho- Hydrogen
- Simulations
  - Spectrum
  - Flux
  - Brilliance
- Source
- Outlook

The ICONE Project

(formerly known as Sonate NEUTRONS FOR MATERIALS SCIENCE)

The Installation COmpact de Neutrons (**ICONE**) project

- a french based and operated High Current Accelerator-driven Neutron Source (HiCANS) for the neutron scattering community



Key Figures

Proton Accelerator: ~20-30 MeV, ~60-100 mA

High Resolution Configuration: ~200µs@100Hz

High Flux Configuration : ~2ms@20Hz

2-3 **Targets**

8-12 **Instruments**

- **APD** (avant projet détaillé) Phase Launched (~Detailed Technical Design Study)

ICONE White Book published 2023

Details in the talk of Frédéric tomorrow

OpenMC I

- Community-developed Monte Carlo neutron and photon transport simulation code
- Originated 2011 at the MIT by members of the *Computational Reactor Physics Group* .
- User and development base broadened over time; various universities, laboratories and organizations contribute now to the development of OpenMC.

OpenMC - https://openmc.org/

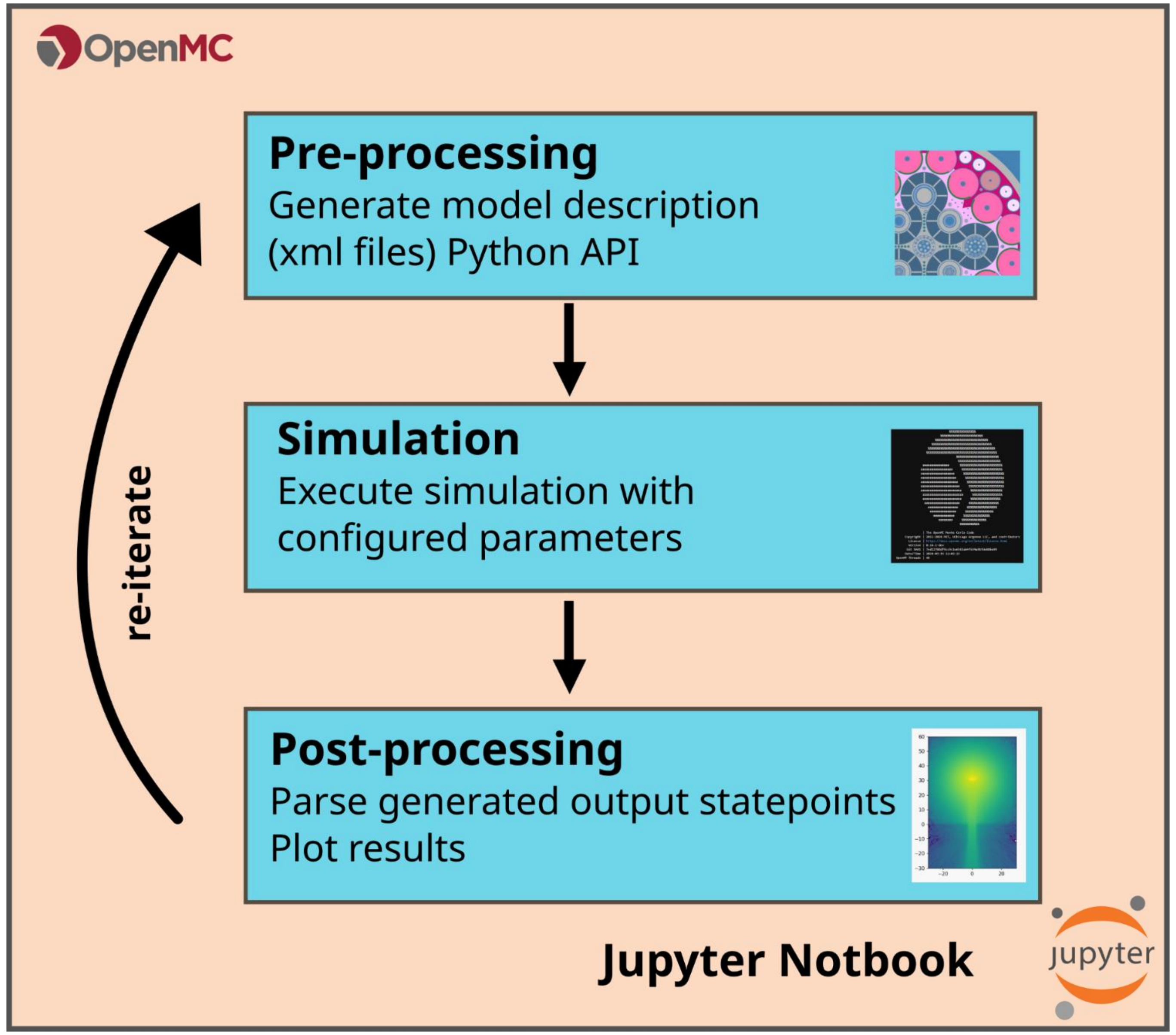
- Capable of simulating neutrons either in fixed source or k-eigenvalue problems
- On models built from assemblies of solid geometric objects or from CAD representation.
- Supports both continuous-energy and multigroup transport.
- Parallelism is enabled via a hybrid MPI and OpenMP

OpenMC II

- **Advantages**
  - Open Source -> Easy and on short term available and accessible (especially important for students)
  - Python API – easy to learn
  - Source Code accessible – possibility to extend/fix code
  - Interfaces to NCrystal (provides interface to include physics of new/complex scattering processes)
  - Supports MCPL – Format
- **Disadvantages**
  - OpenMC cannot model accelerated charged particles (i.e. protons)
  - Point Detectors (Tally F5 MCNP)
  - Surface flux like the F2 tally MCNP
    - Especially no direction weighting (cos(α))
  - Mesh Surface filtering still buggy

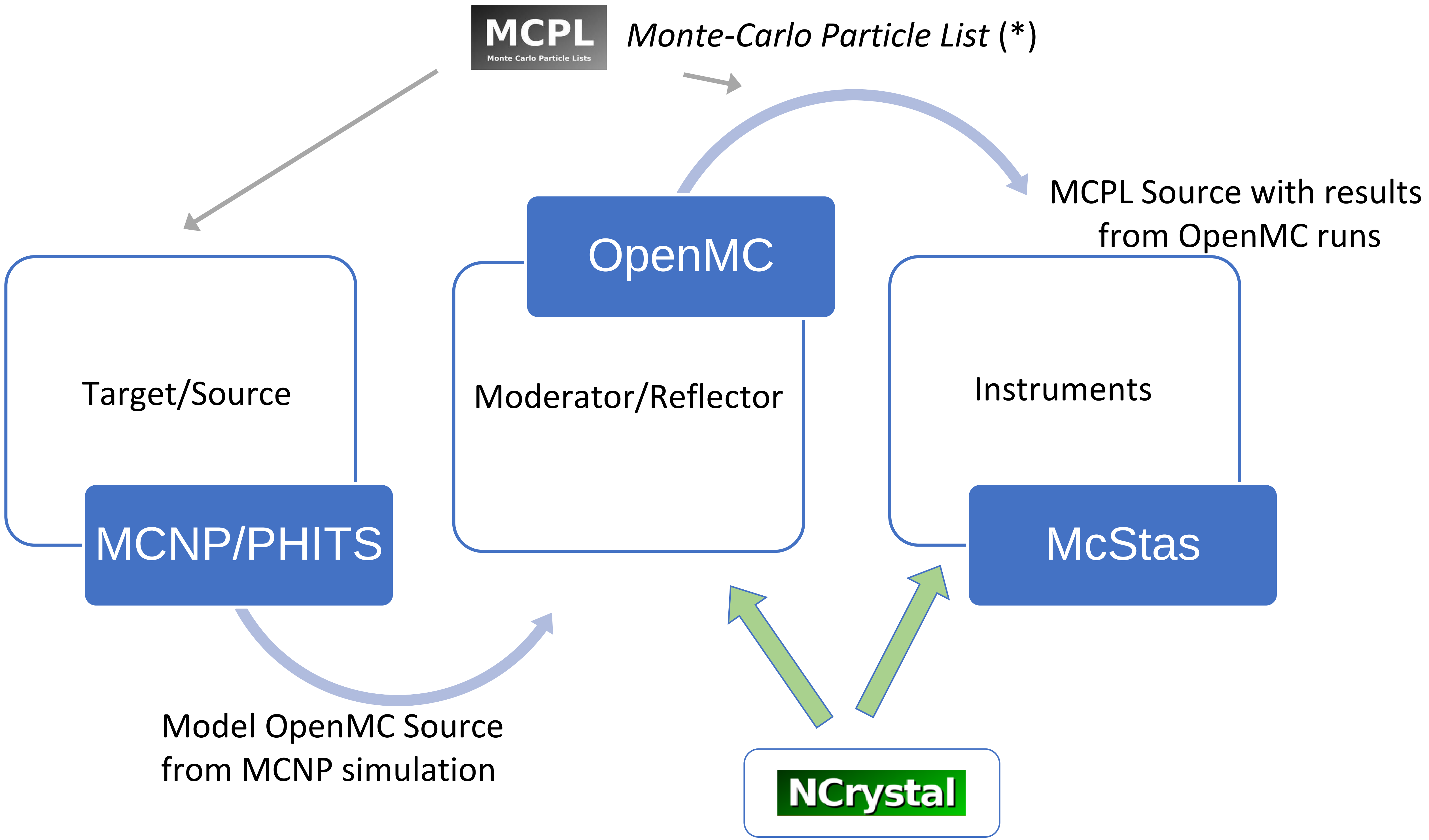
[OpenMC - https://openmc.org/](https://openmc.org/)

OpenMC III



[OpenMC - https://openmc.org/](https://openmc.org/)

General Simulation Strategy

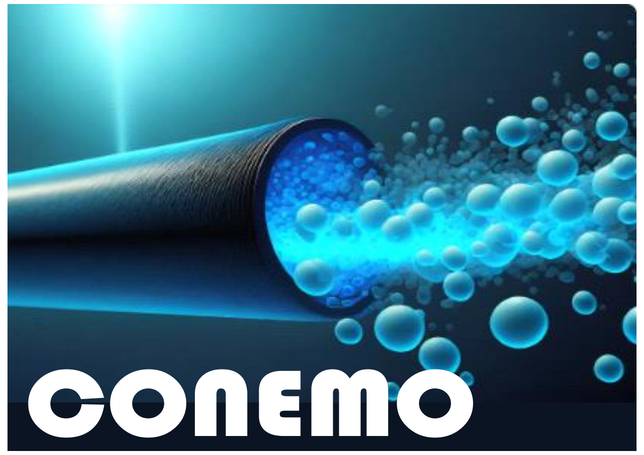


Library for thermal scattering transport (**)
Extend physics beyond limits of different
scattering library formats (e.g. reflector materials)

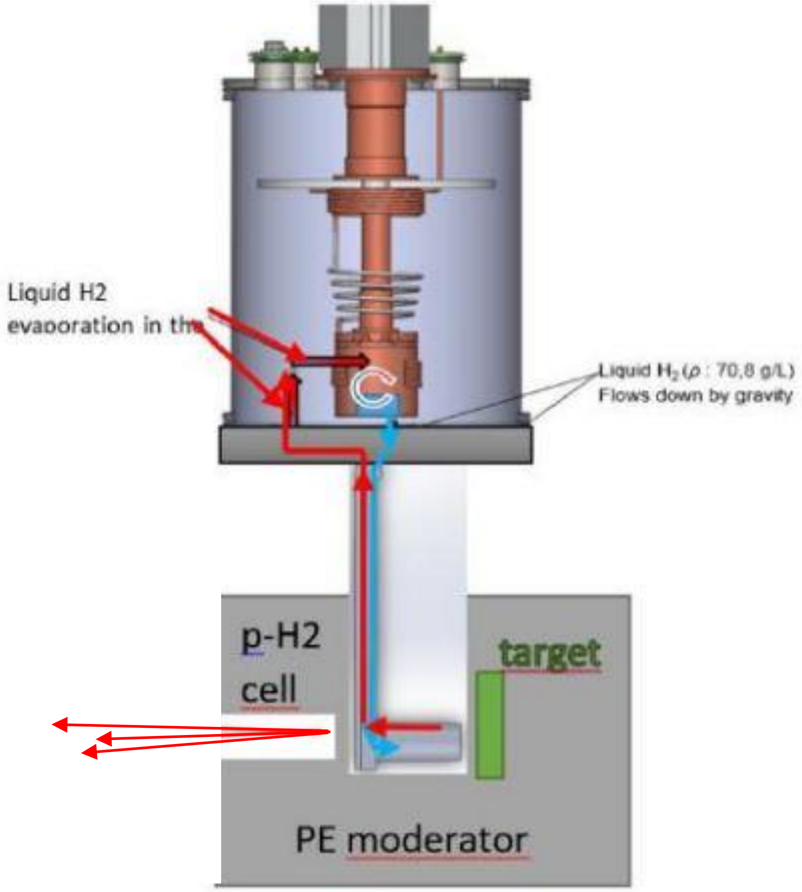
(*) https://mctools.github.io/mcpl/
(**) https://github.com/mctools/ncrystal/wiki

CONEMO

Cold neutron moderators using para hydrogen are predicted to significantly increase their performance when their dimensionality is reduced (e.gh disc shape(2D) or pencil shape (1D).
Mezei er al. (2014) https://doi.org/10.3233/JNR-140013

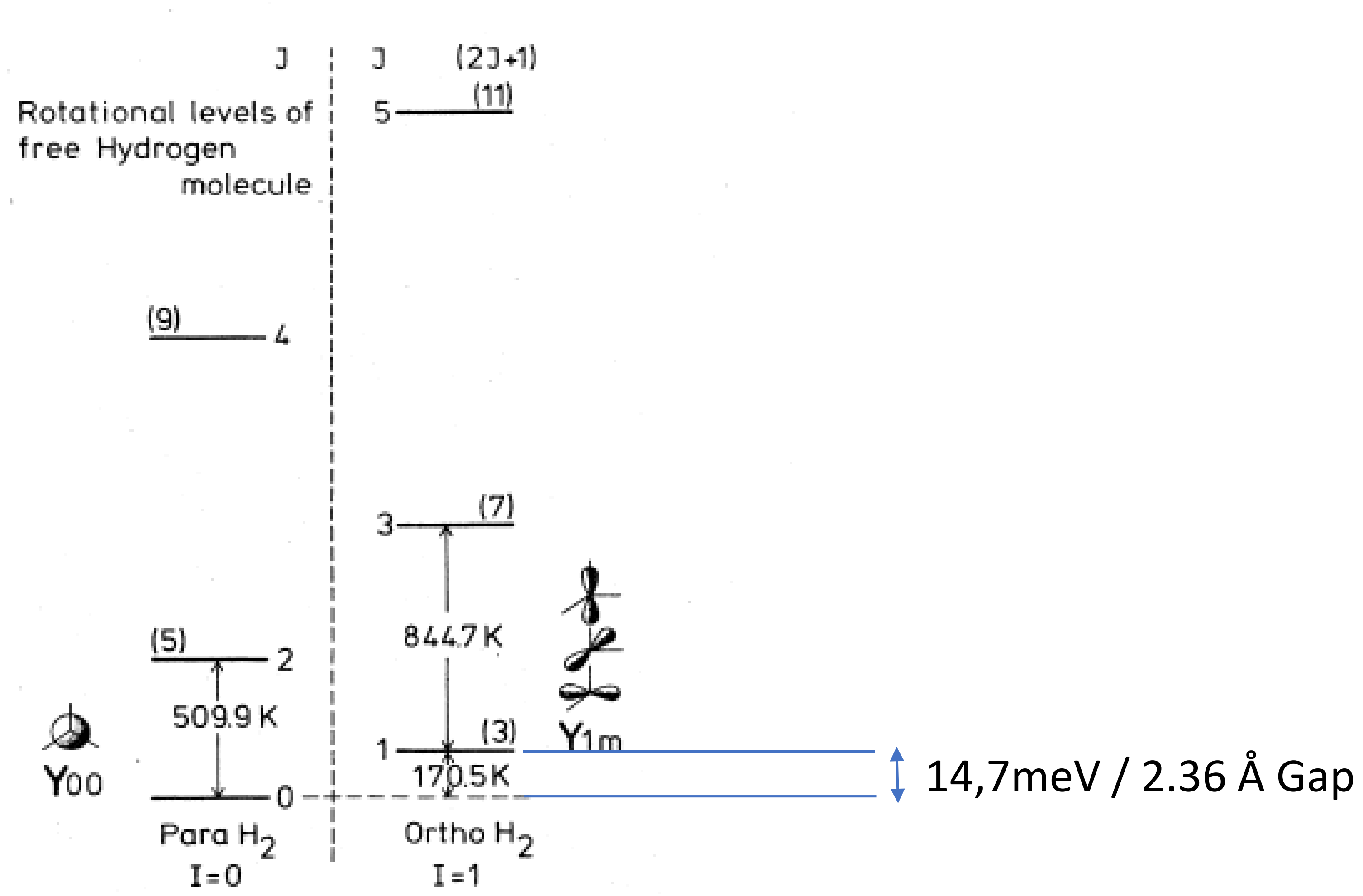


- The objective of the CONEMO (Cold Neutron Moderator) project is:
  - to develop the tools and methods for modeling the integrati of these low dimensional moderators around CANS sources
  - to build and integrate a prototype of a one-dimensional moderator and to validate its performance (neutron radiography, reflectometry, SANS)

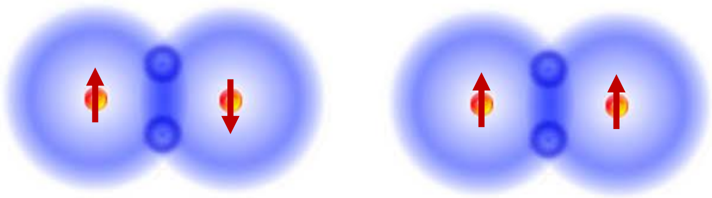


➢ This talk only simulation/optimization aspects

Para- Ortho Hydrogen



Singlet State

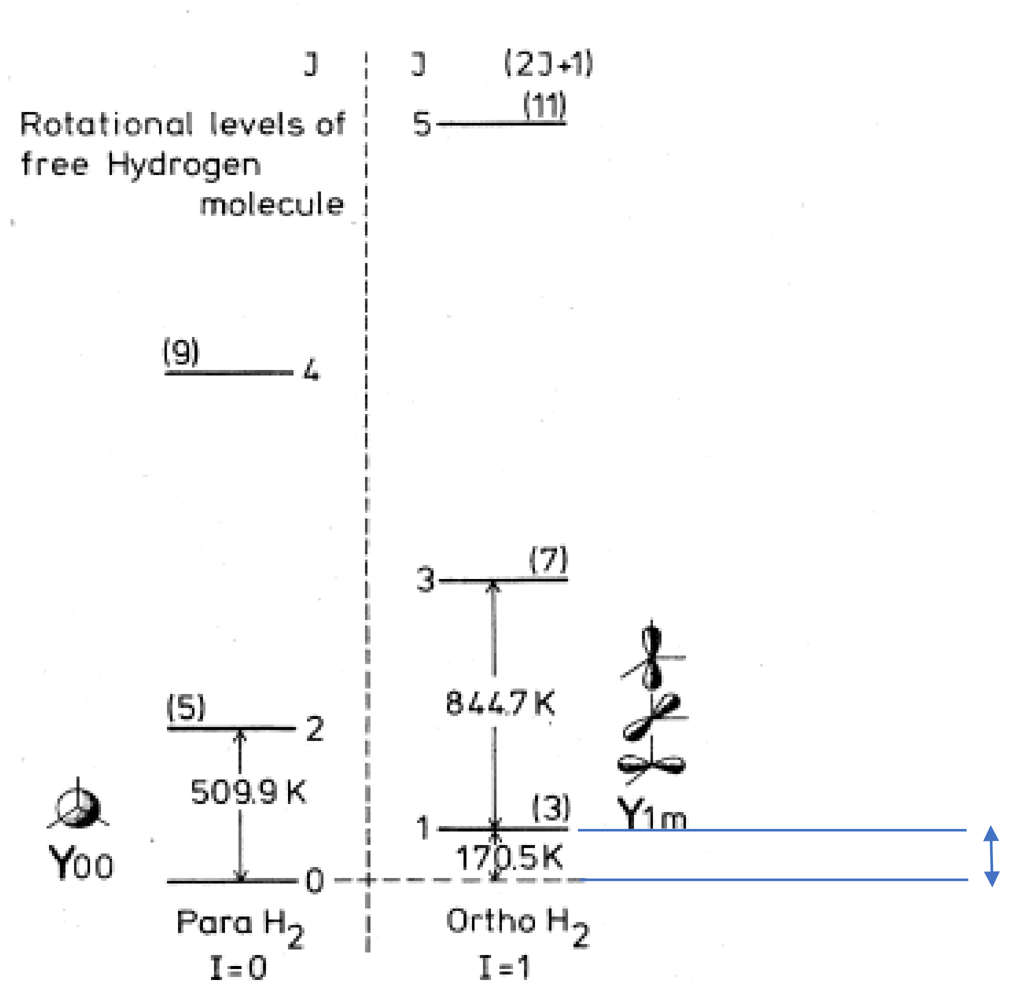


Triplet State

From:

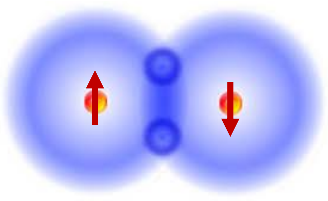
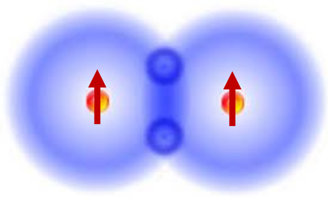
Silvera, Isaac F. "The Solid Molecular Hydrogens in the Condensed Phase: Fundamentals and Static Properties." *Reviews of Modern Physics* 52, no. 2 (April 1, 1980): 393–452. https://doi.org/10.1103/RevModPhys.52.393.

Para- Ortho Hydrogen



14,7meV / 2.36 Å Gap

- Neutrons with energy less than 14.7 meV -> only elastic scattering in para-H2
- In ortho-H2 down-scattering still possible

Singlet State   Triplet State

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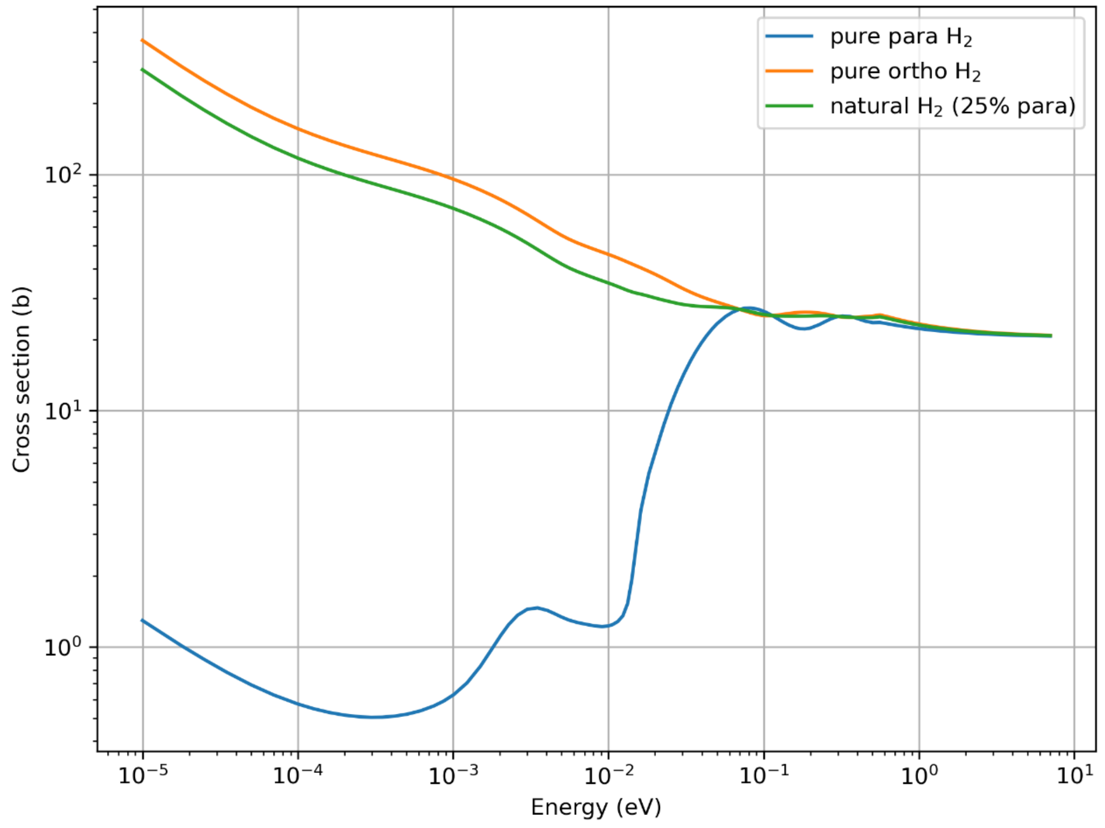
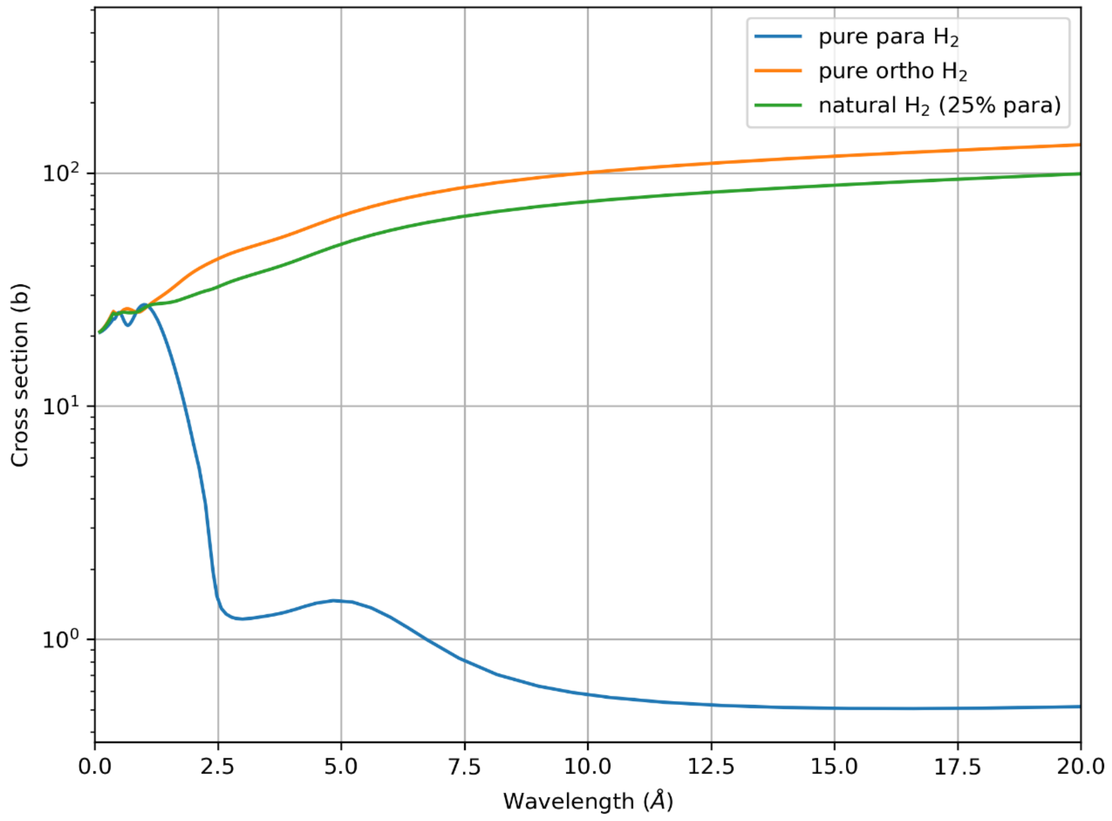
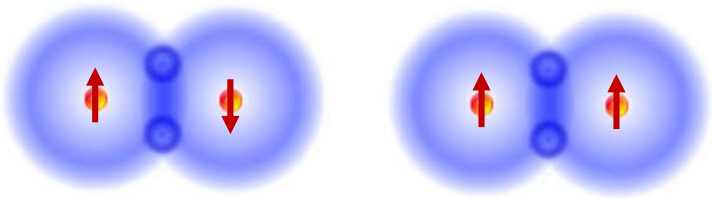
Para- Ortho Hydrogen

Cross Section



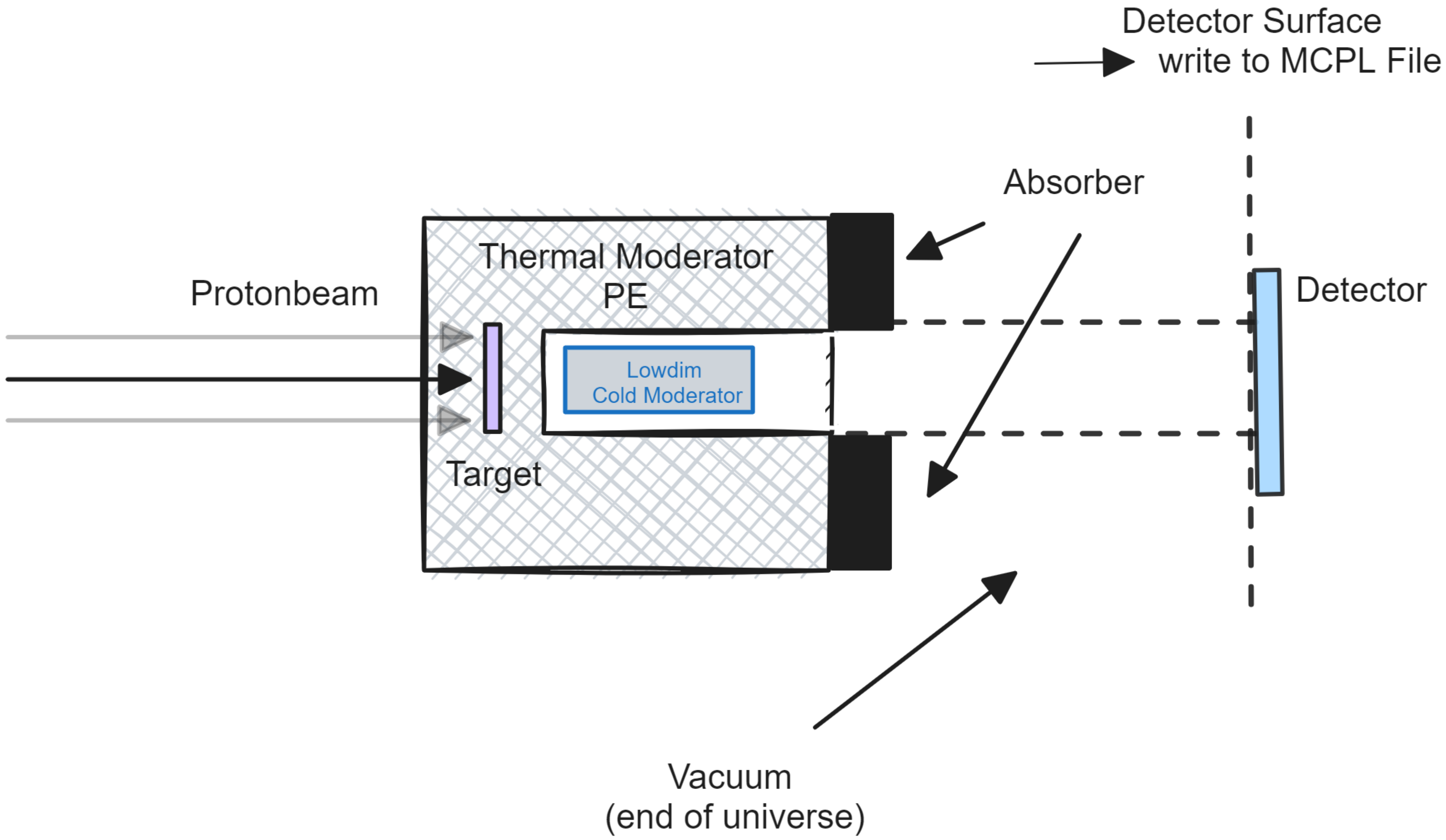


Para-Hydrogen
Singlet State



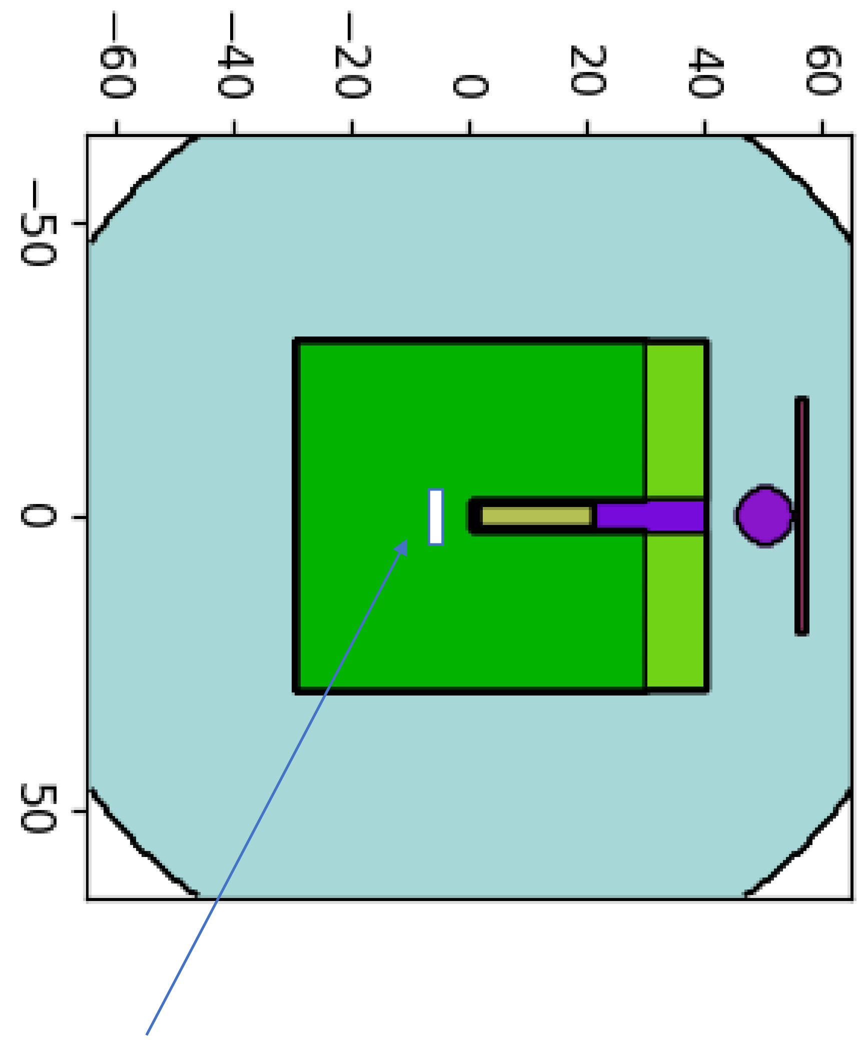
Ortho-Hydrogen
Triplet State

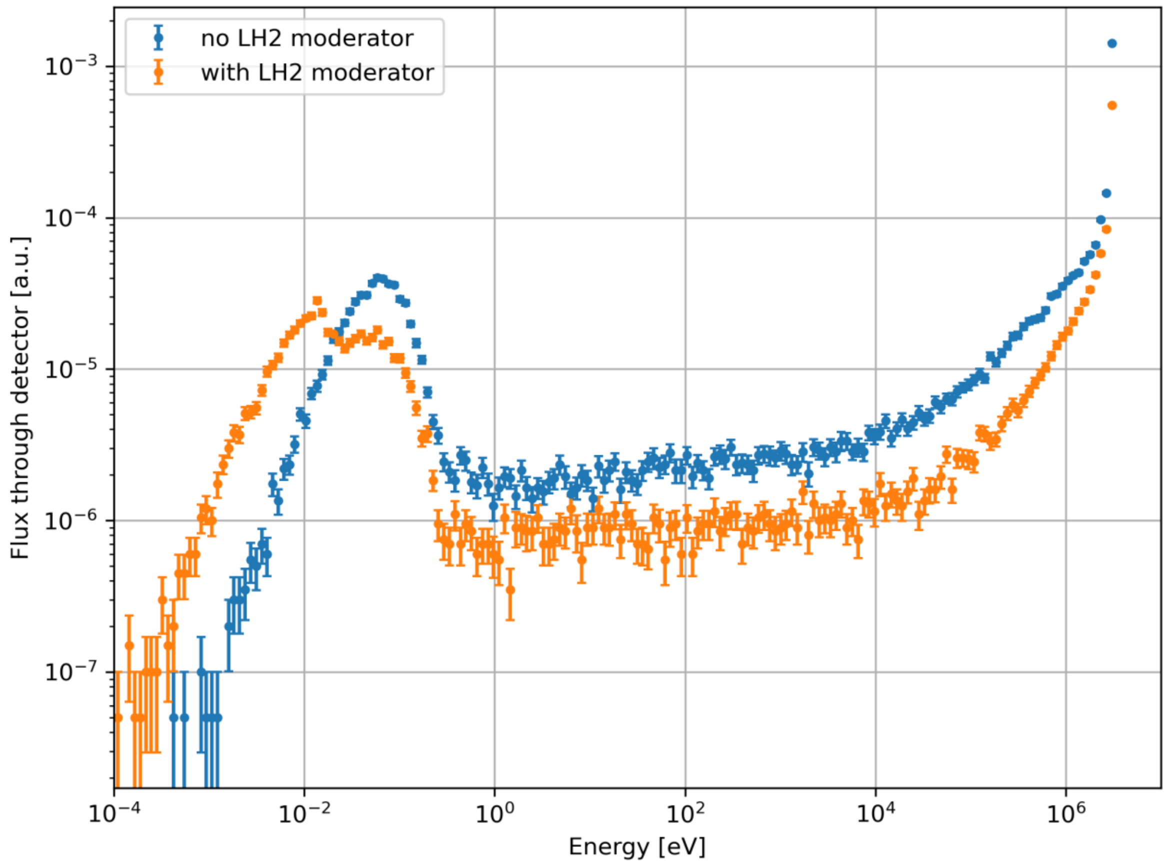
Basic Model


Detector Surface
write to MCPL File
Absorber
Thermal Moderator
PE
Protonbeam
Detector
Lowdim
Cold Moderator
Target
Vacuum
(end of universe)

Results Spectrum

- Shift in Spectrum

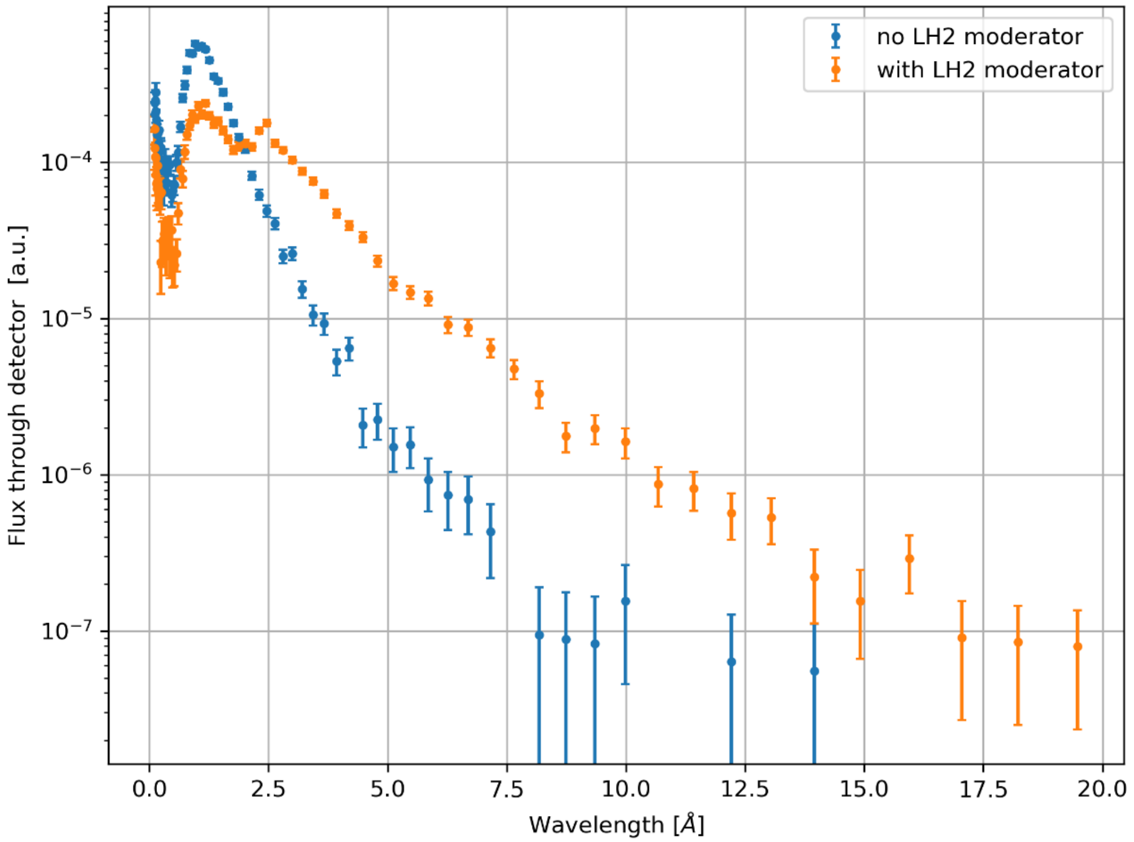


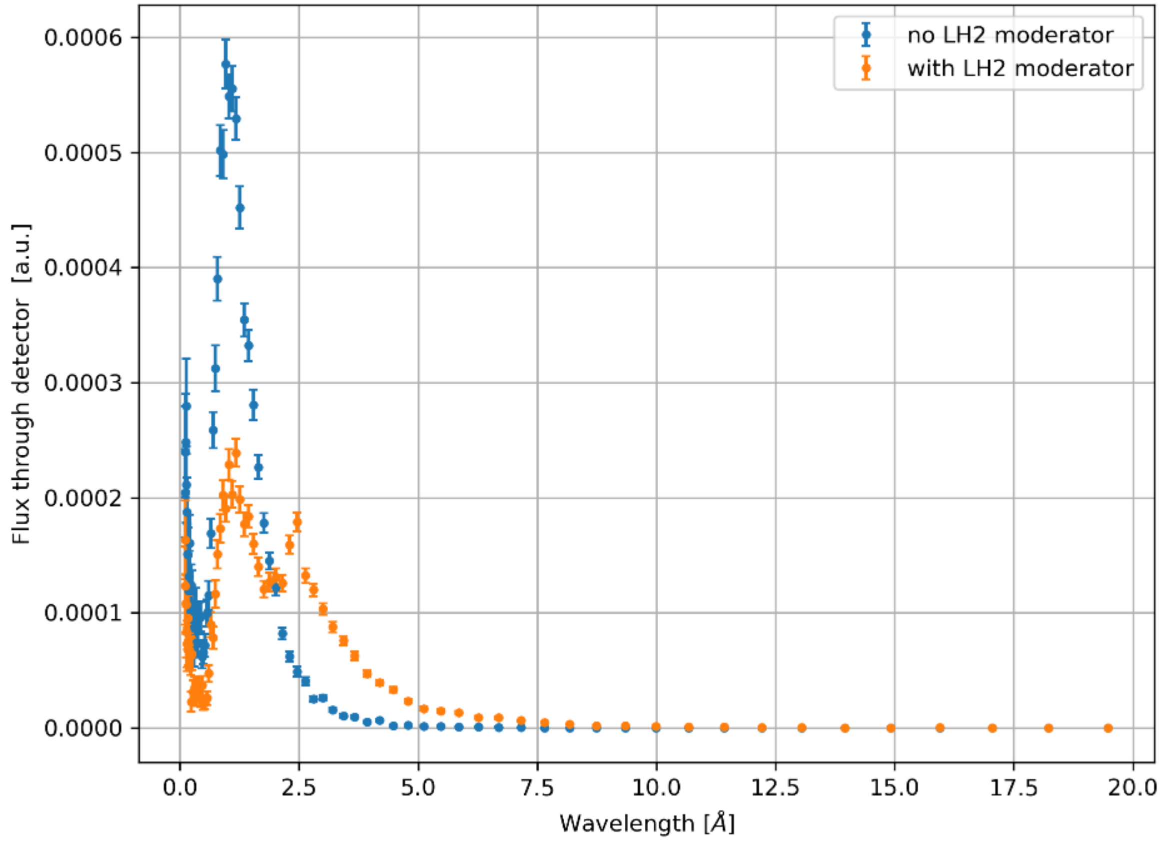


Mono-energetic Source (3MeV)

Results Spectrum

- Shift in Spectrum

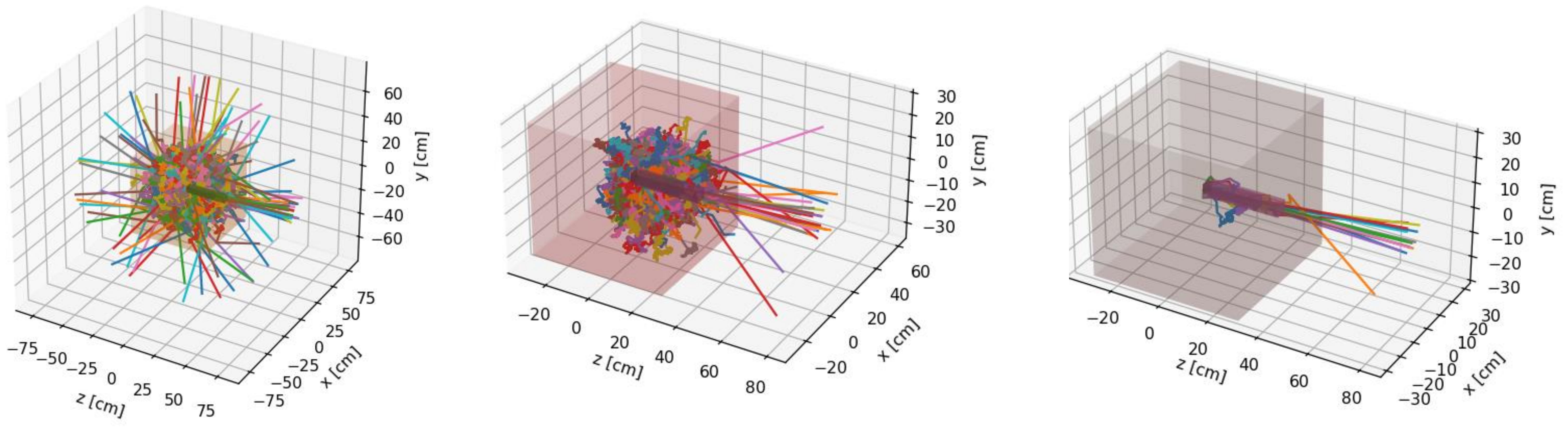




OpenMC Tracks

- Save tracks during simulations (convert to vtk-format)
    - “Visualize” the low dimensionality behavior

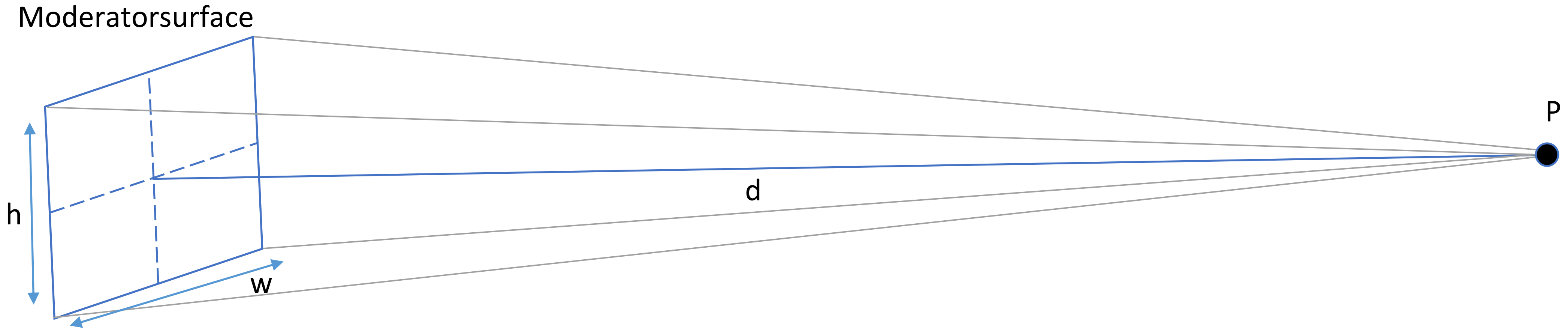
- # simulated: 15000 (filtered down to 14 (!))
    - Think of method to save only tracks that reach the detector (leave the moderator surface)



Brightness

- Quantify performance
- Figure of merit → mean brightness/brilliance of the source/moderator surface

- Brilliance: $B = \frac{neutrons}{s\ cm^2\ Å\ sr}$ sr … solid angle (Steradian)



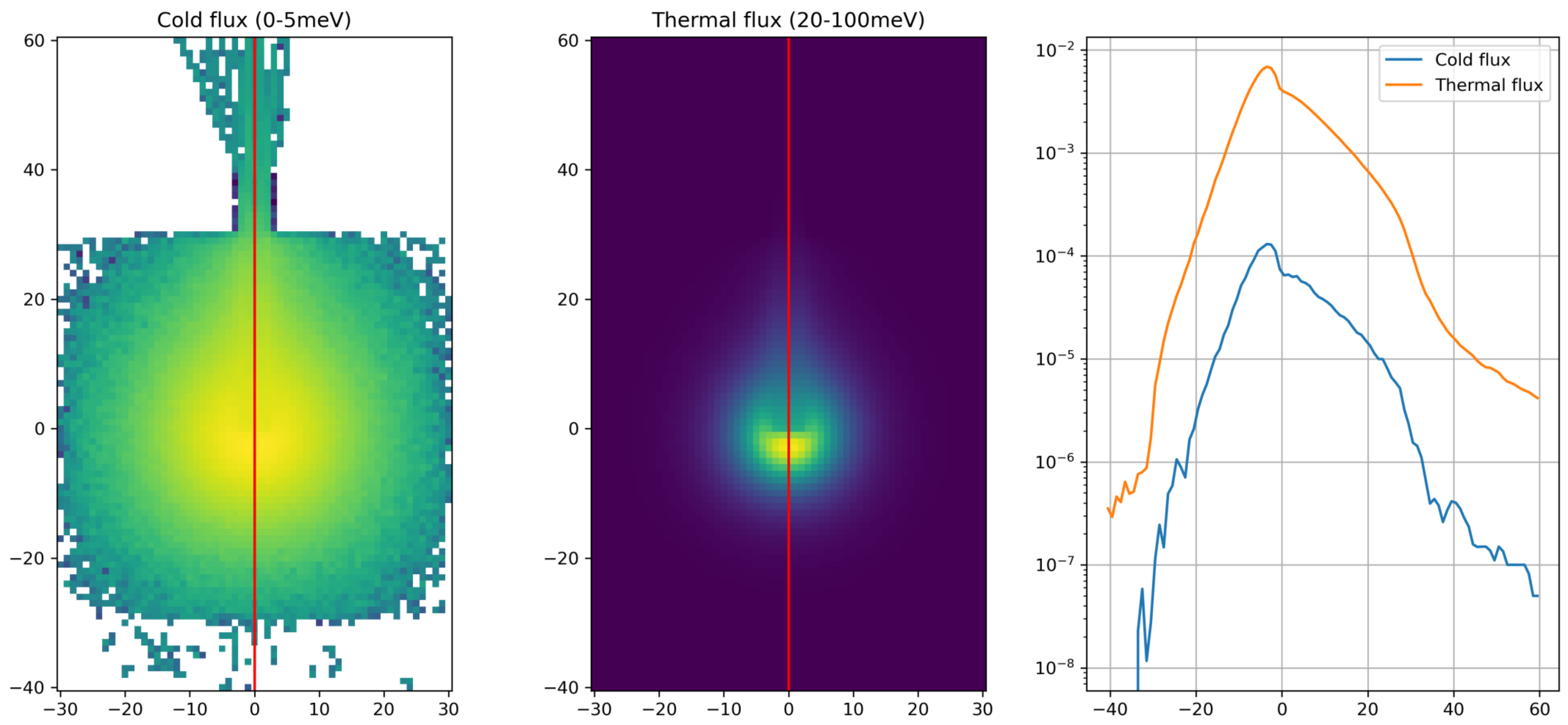
- Solid Angle: $\Omega = \frac{hw}{d^2}$ if $\mathrm{h, w} \ll d$

Accurate formula:

$$\Omega = 4 \arcsin\left(\frac{hw}{\sqrt{(h^2+4d^2)(w^2+4d^2)}}\right)$$

Flux in moderator assembly

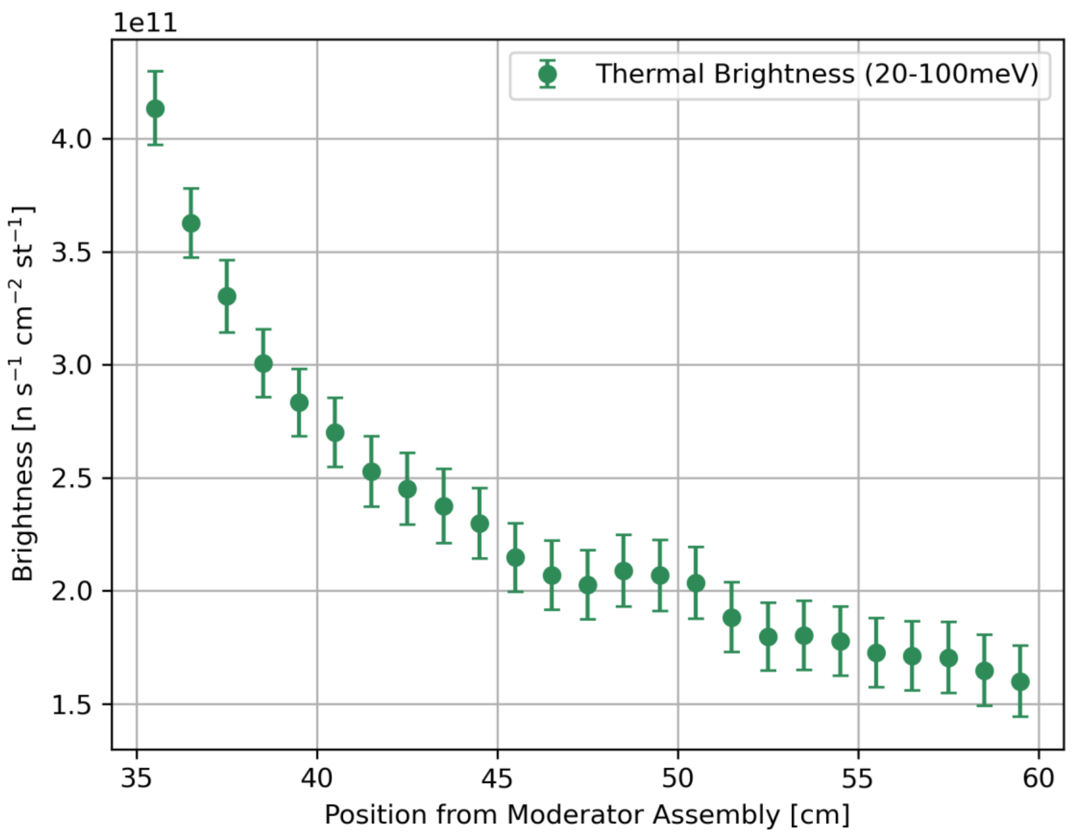
- Thermal case (No LH2 Moderator)
  - Flux-map generated with 3D Mesh (`openmc.RectilinearMesh`)
  - Energy Filter -> 4 groups ([0, 0.005, 0.010, 0.020, 0.1]) eV



Result: Brightness

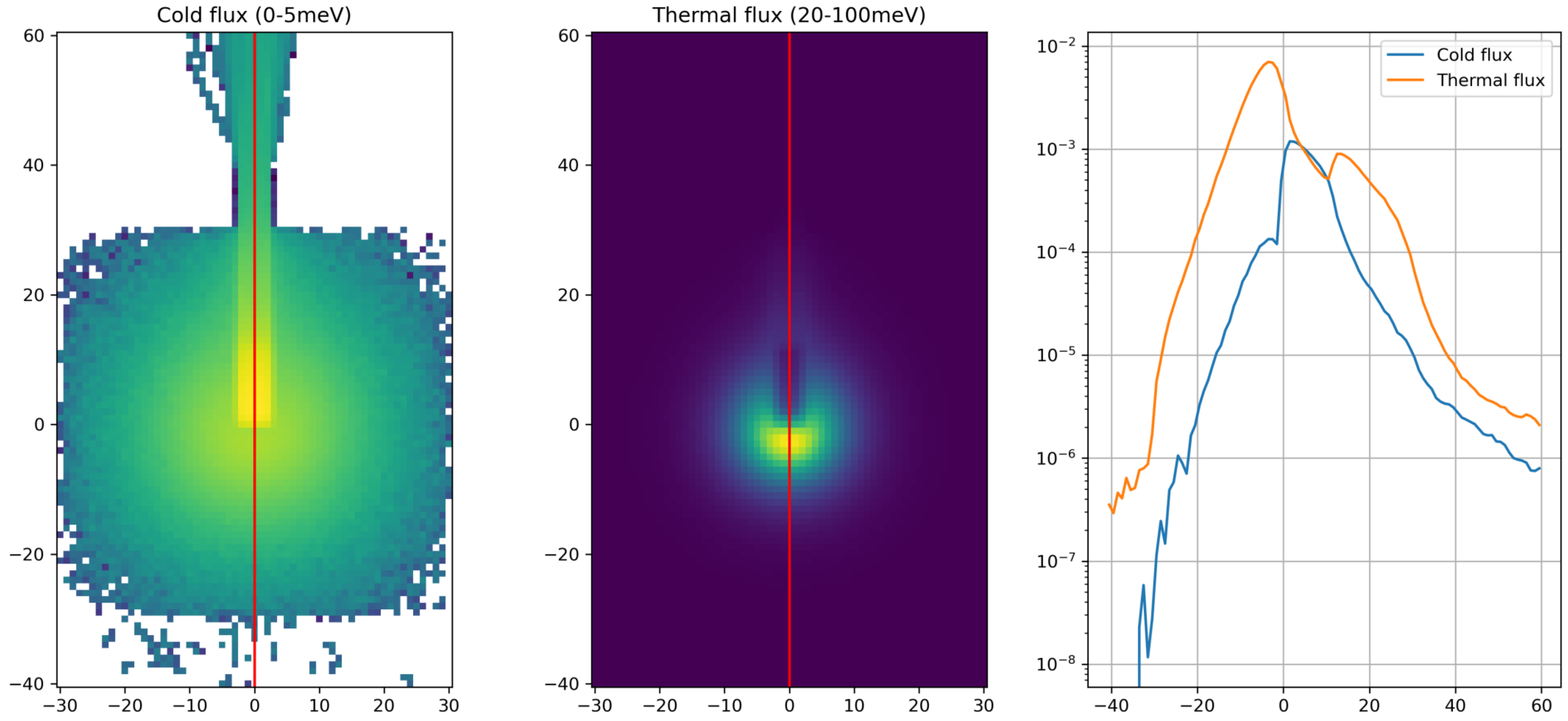
- **Thermal Case** (No LH2 Moderator)
  - Brightness [0-5meV]: **3.21e+09** +/- 2.26e+09
  - Brightness [20-100meV]: **1.73e+11** +/- 1.53e+10

Parameter for Brightness:
Yield for 13 MeV protons = 6.2e-3 n/p
Protons per sec per mA = 6.24e15
Beampower 100kW -> current ~7mA



Flux in moderator assembly

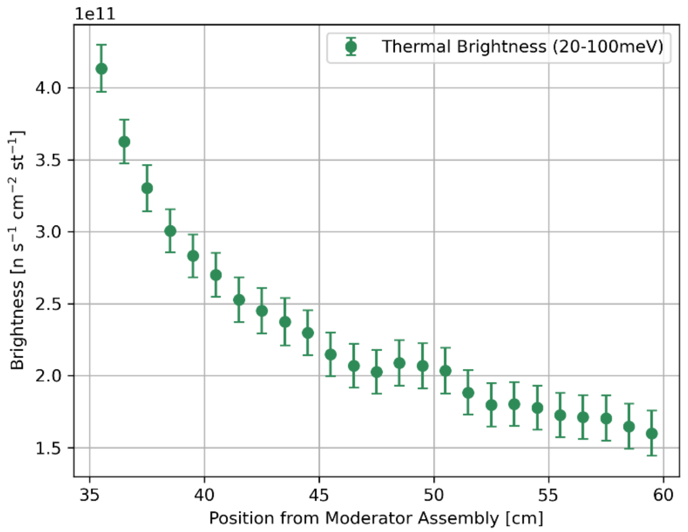
- **Cold Case** (with LH2 moderator of size 11x4x4 cm)

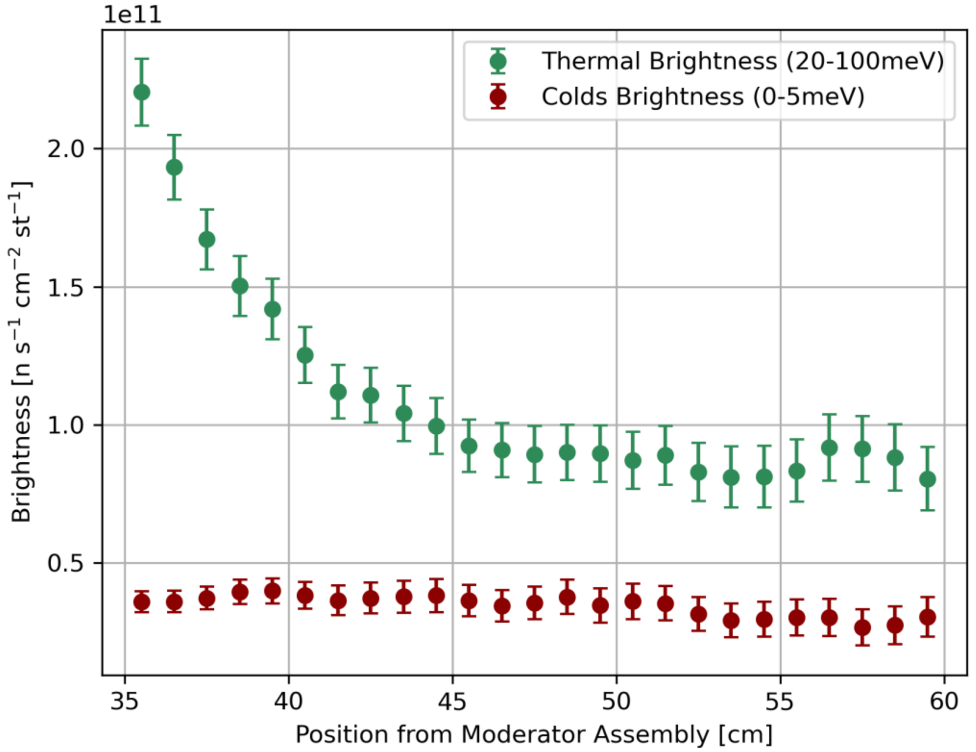


Result: Brightness

- Cold Case (with LH2 moderator)
  - Brightness [0-5meV]: **3.03e+10** +/- 6.55e+09
  - Brightness [20-100meV]: **8.34e+10** +/- 1.12e+10

- Thermal case
- Brightness [0-5meV]: 3.21e+09 +/- 2.26e+09
- Brightness [20-100meV]: 1.73e+11 +/- 1.53e+10





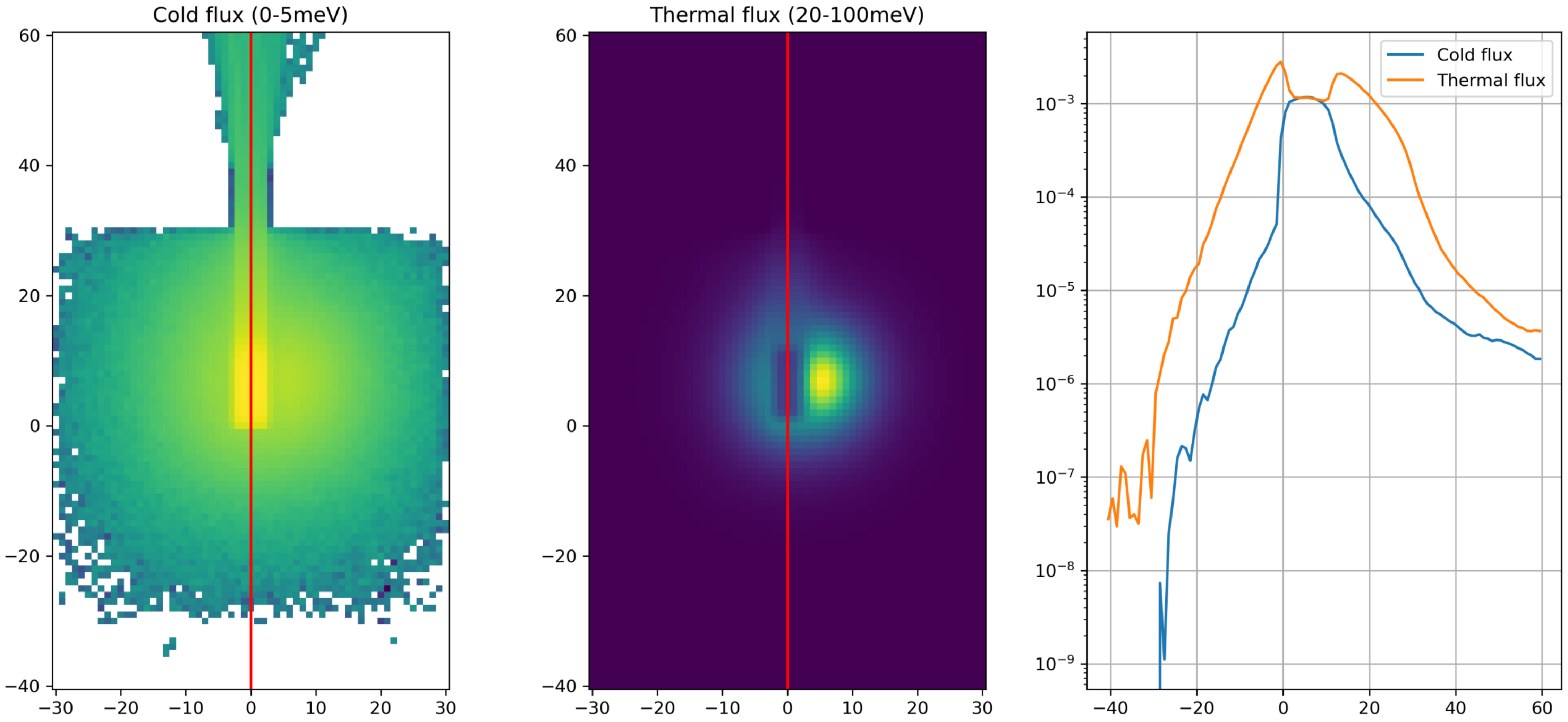
Zanini et al. (2018), “General Use of Low-Dimensional Moderators in Neutron Sources”

Thermal -> 3.3 $\times 10^{10}$ n/cm2/s/sr

Cold -> 3.2 $\times 10^{10}$ n/cm2/s/sr

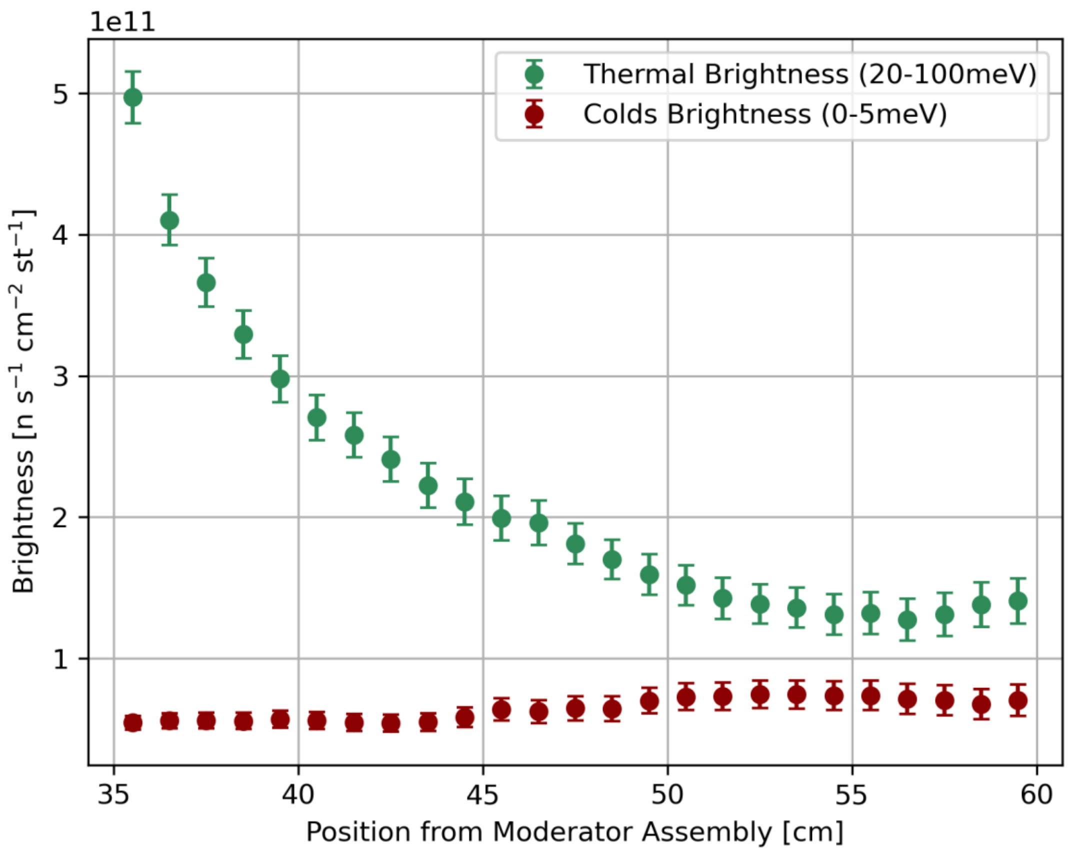
Sideward Source

- Cold Case II (with LH2 moderator of size 11x4x4 cm)
- Source placed next to long moderator side



Results for Sideward Source

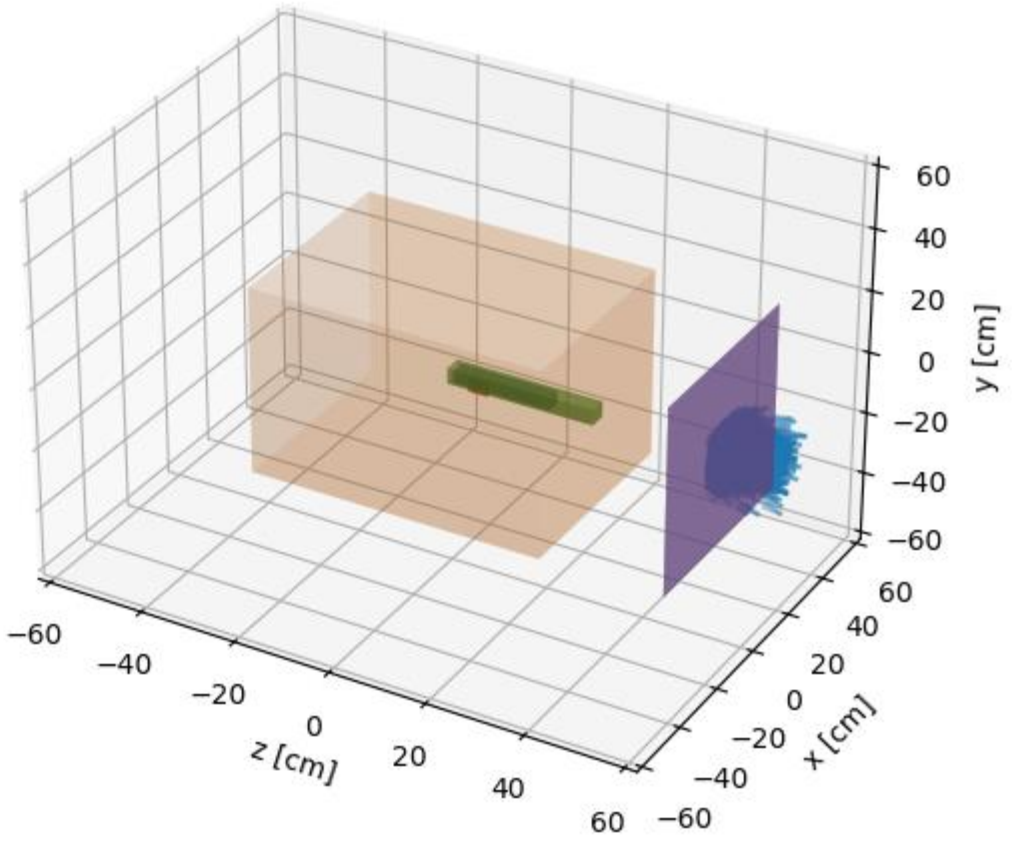
- Cold Case II (with LH2 moderator of size 11x4x4 cm)
  - Brightness [0-5meV]: **7.39e+10** +/- 1.03e+10
  - Brightness [20-100meV]: **1.32e+11** +/- 1.49e+10

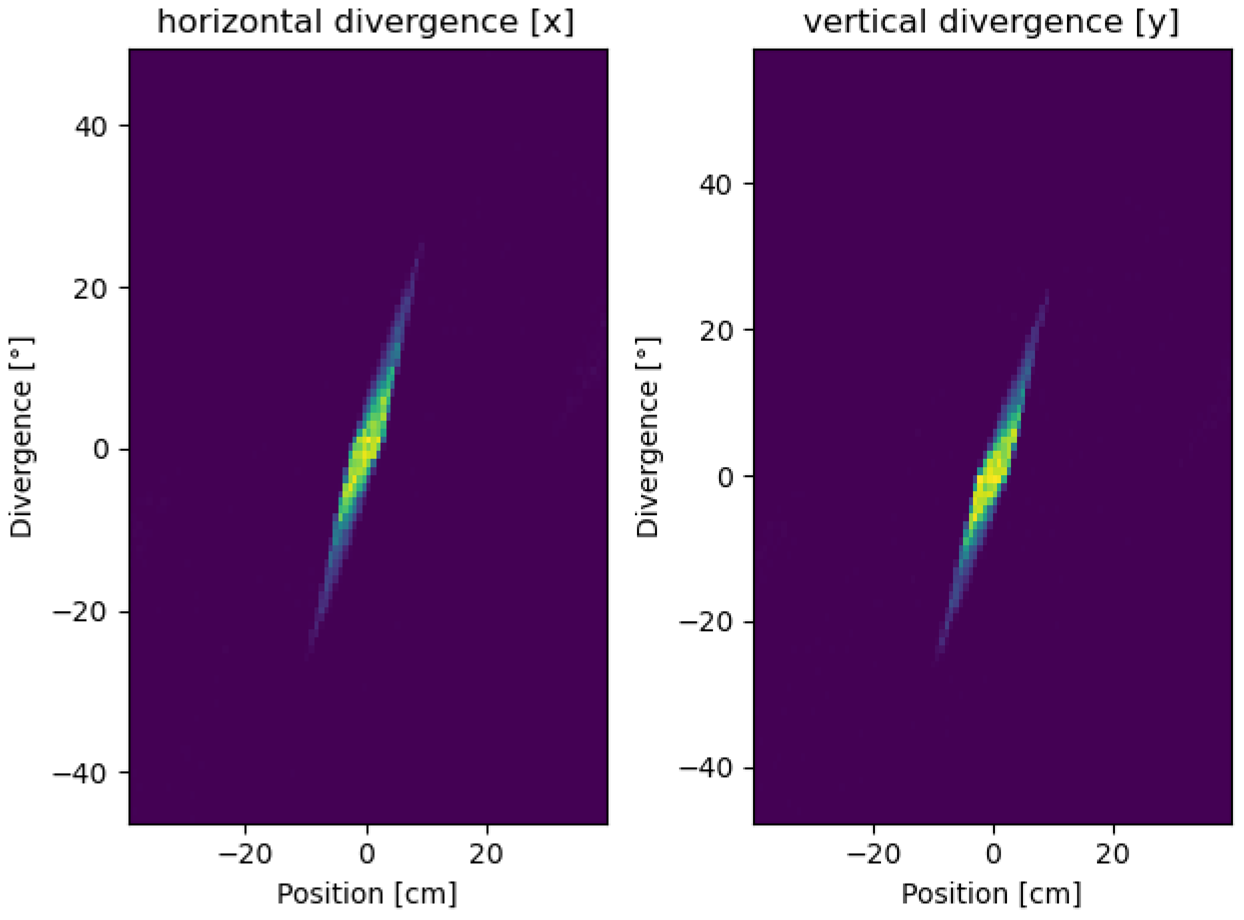


Zanini et al. (2018),
"General Use of Low-Dimensional Moderators in Neutron Sources"
Thermal -> 3.3 $\times 10^{10}$ n/cm2/s/sr
Cold -> 3.2 $\times 10^{10}$ n/cm2/s/sr

Divergence

- Use mcpl–interface - *surf_source_write()*
  - Write all particles that cross given surface to file
- Extract divergence and brightness info
- Interface to instruments (McStas)

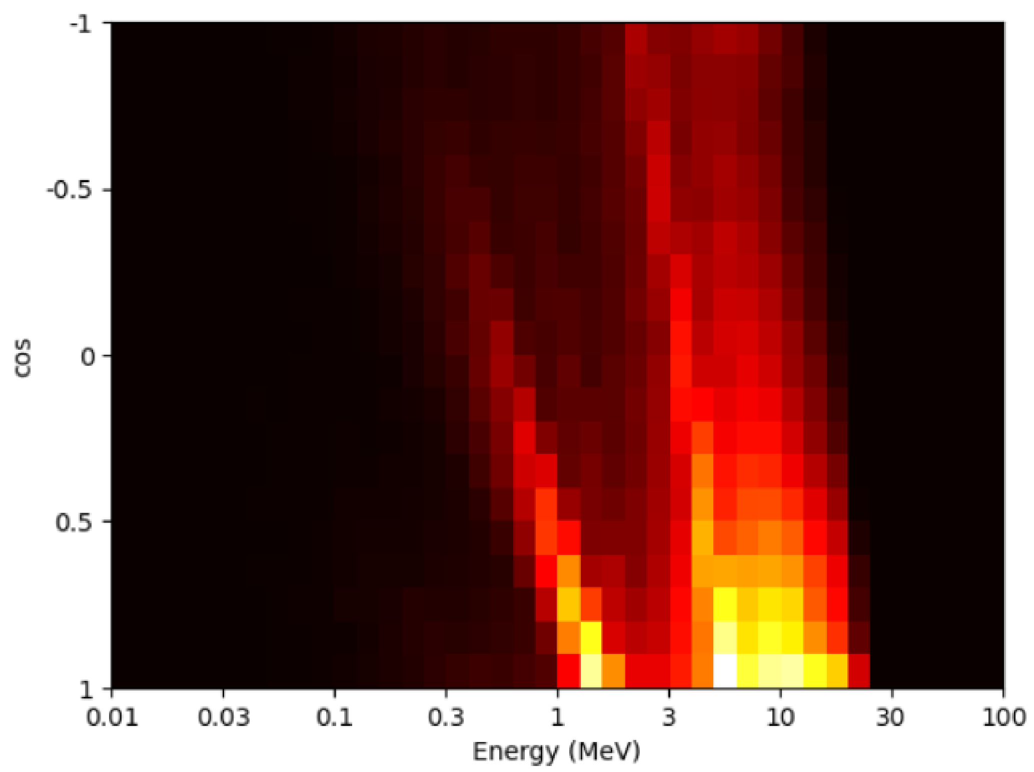




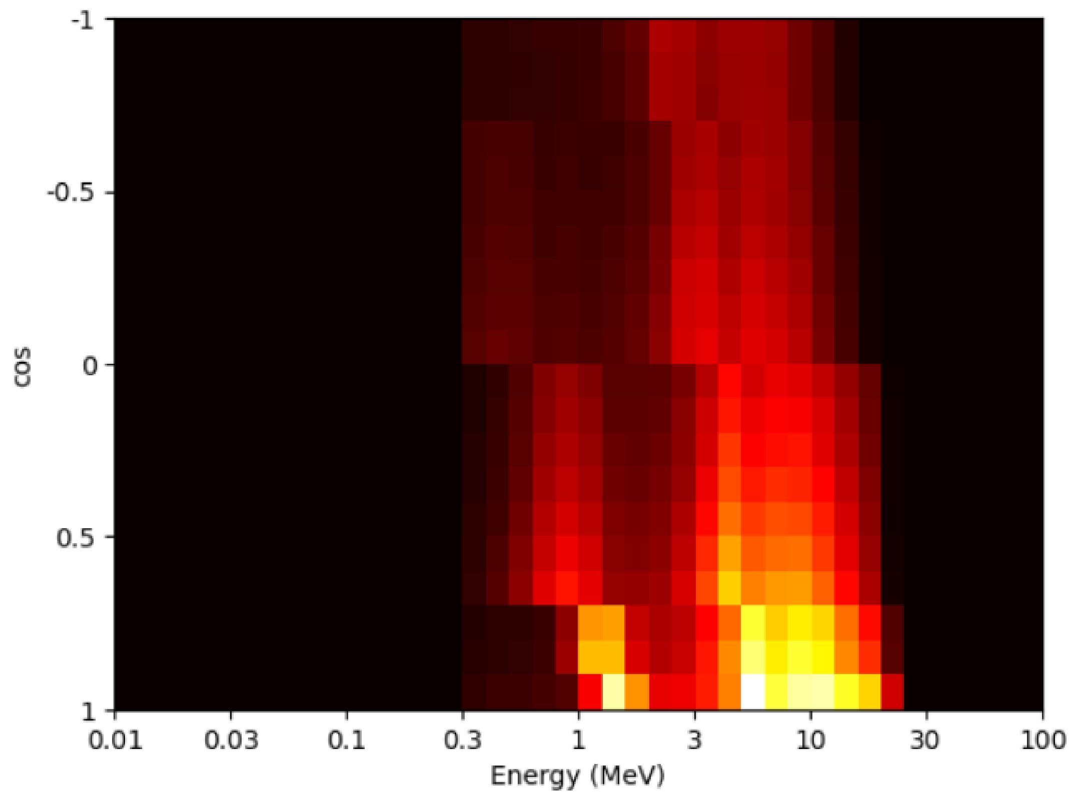
Source

- Source Model (J. DARPENTIGNY)
  - OpenMC cannot model accelerated charged particles (i.e. protons)
  - Sources modelled from MCNP Simulations
    Lookup tables (Energy and direction, cos(ϕ) = 1 is forward direction)
    for different source material and proton energies
  - Target length matched to the Bragg Peak (penetration depth) of the incoming proton (energy)

MCNP



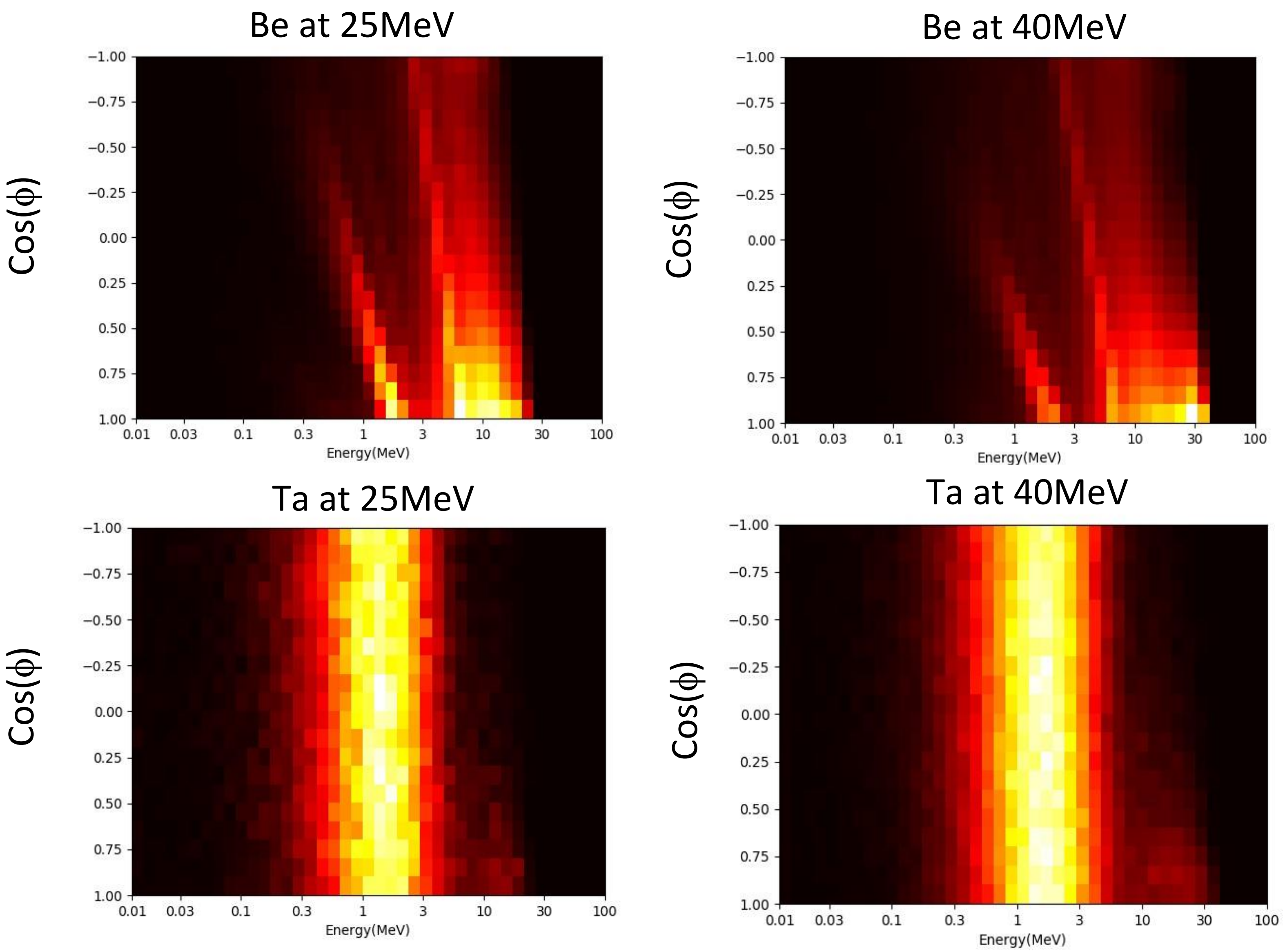
OpenMC



Example 25 MeV protons on Be

Source II

- Different Target Materials



- Energy and direction cos(ϕ) of the fast neutrons produced in Be and Ta targets at 25 and 40 MeV

- **Note**
  in case of Tantalum, the neutron production process is spallation which is essentially isotropic.

- colour scales are not normalize and cannot be compared

Conclusions and Outlook

- OpenMC seems good and capable alternative for our CONEMO development
- First results show good agreement with pervious work (Zanini (2018))

- Cold Moderator design
  - Optimize design of moderator
  - Add Engineering Details
- Simulations
  - Study impact of radiative heating
  - Activation Analysis of TMR assembly
  - Simulations with realistically modelled source (benchmark)
- Quantify the quality of the moderator output for instruments (McStas)

Acknowledgment

Thank you for your attention!

Credits: Group at LLB (CEA/IRAMIS), J. Darpentigny, X. Guillou, J.-L. Meuriot, F. Ott,