ICONE

Neutrons for Materials Sciences

A proposal for the ICONE cold neutron moderator

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UCANS 1+1

cea

cnrs

The ICONE Project

(formerly known as Sonate NEUTRONS FOR MATERIALS SCIENCE)

The **I**nnovative **CO**mpact **NE**utron facility (**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

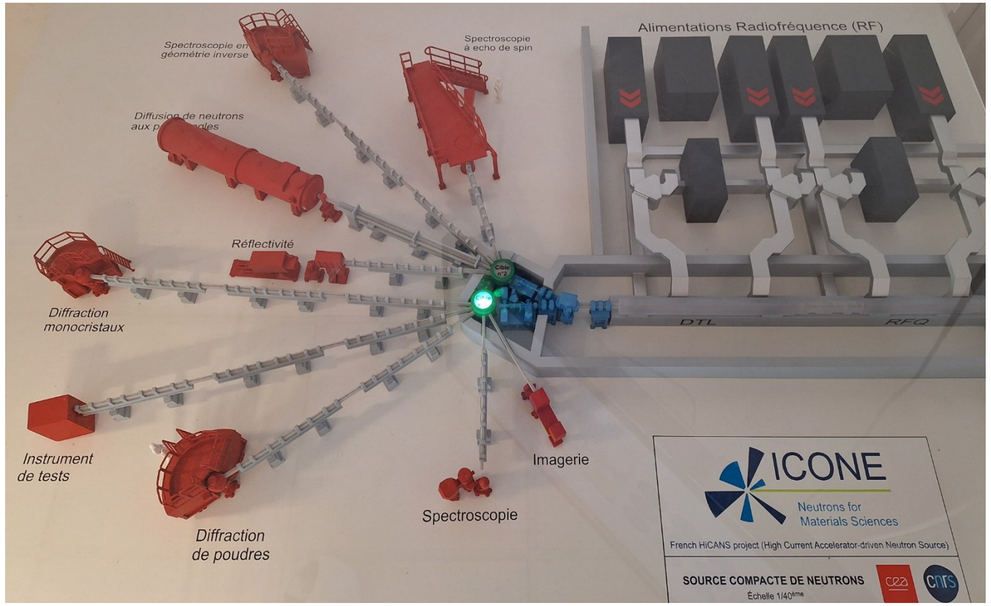
High Resolution Configuration: ~200µs@100Hz

High Flux Configuration : ~2ms@20Hz

2-3 **Targets**

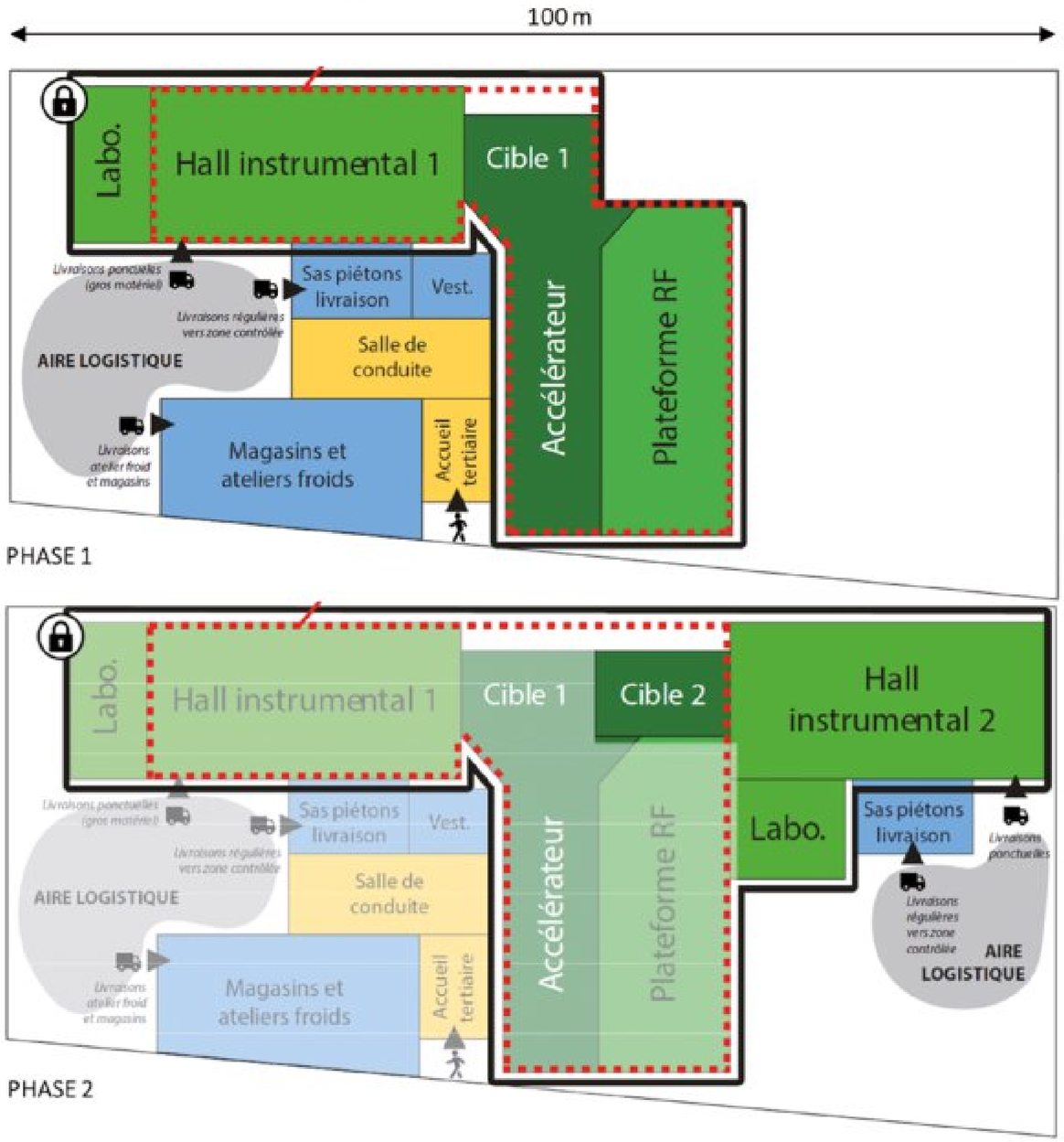
6 instruments per target

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



[ICONE White Book published 2023]

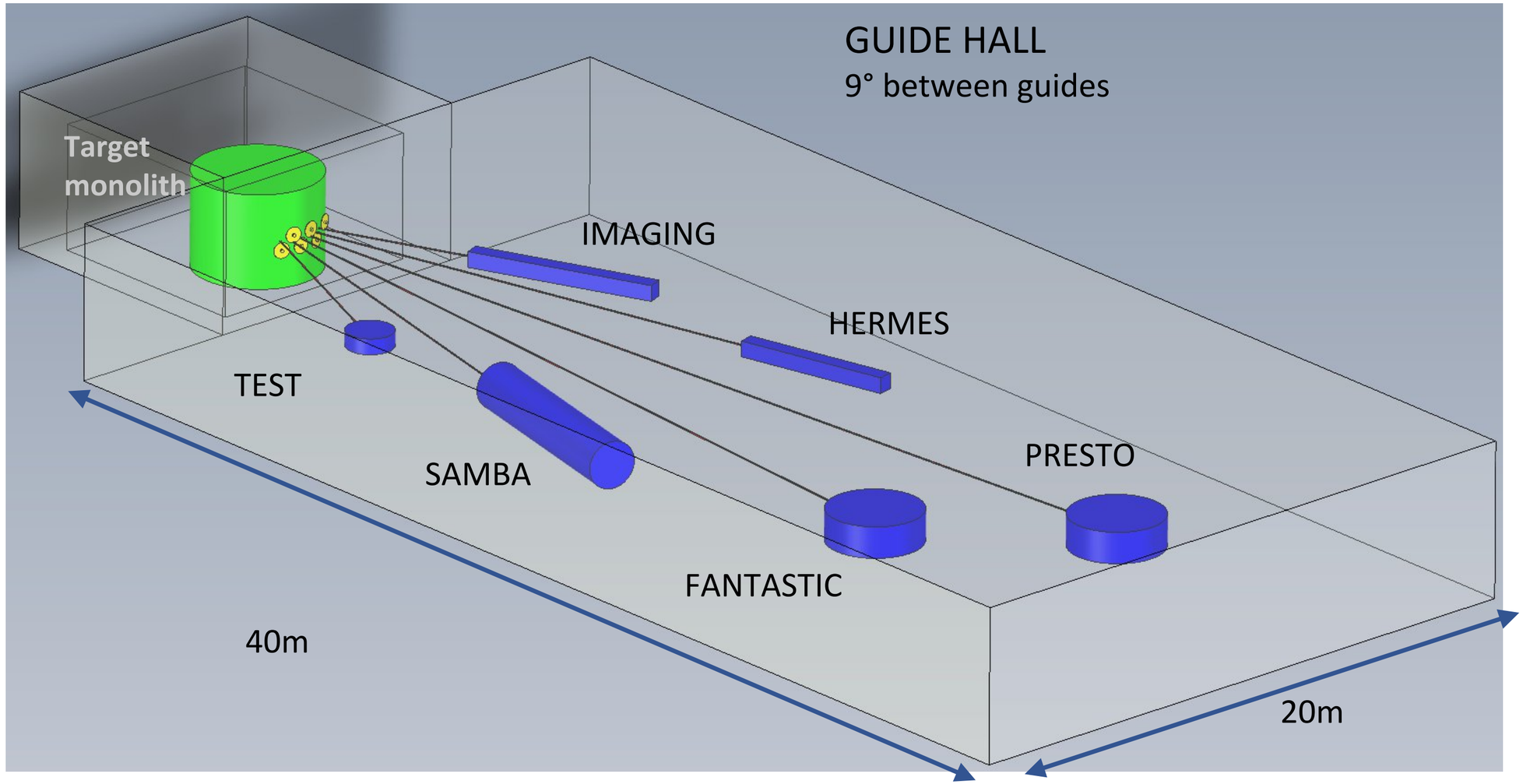
ICONE general layout



- ICONE aims to be a compact facility (should fit on a soccer field)

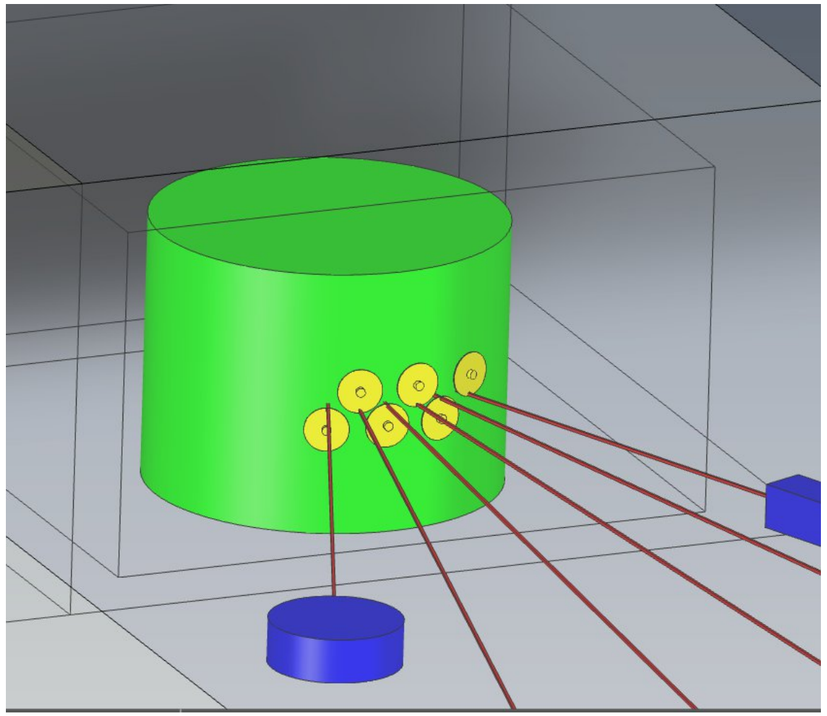
Possible layout for ICONE Phase 1

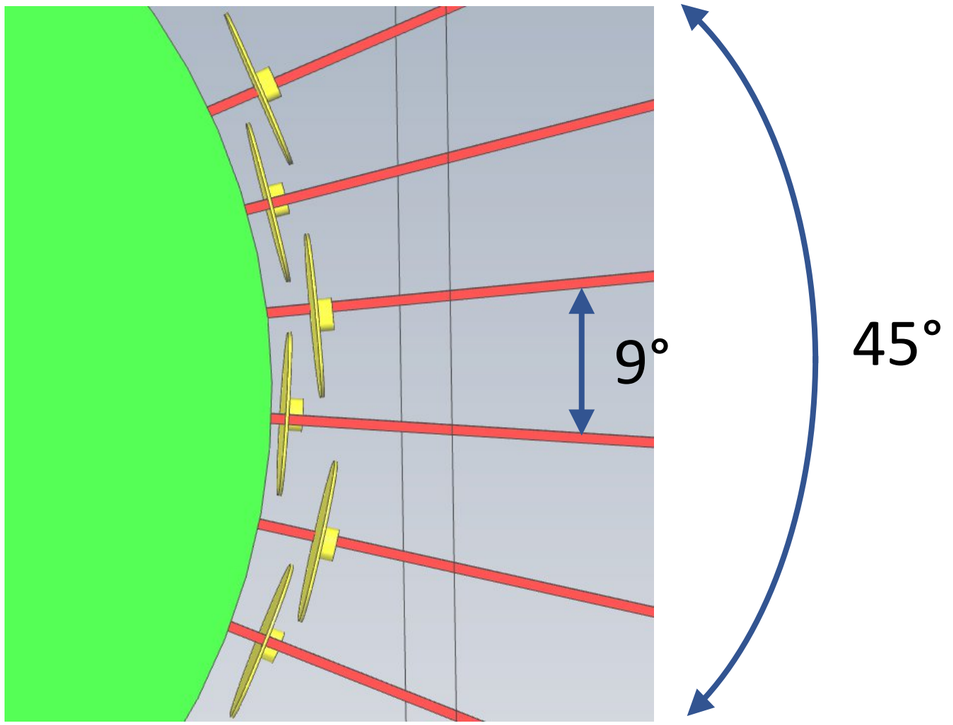
Target casemate



Chopper system

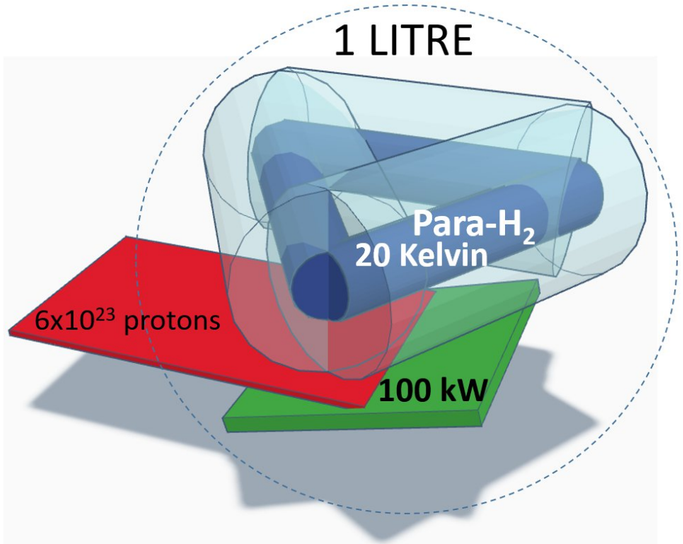
- Choppers are needed to properly shape the neutron pulse
  - The closer to the source, the more efficient they are
  - Goal : setting the choppers (D = 50 m) at about 2 meters from the source





Moderator Geometry

- **Goals**
  - maximize the brilliance
  - Reduce volume of source < 1 liter
- **Initial choice = use 1D moderators to enhance the brilliance**
  - Ideally, 1 optimized moderator per instrument
  - Very (too) complex to implement and not necessarily efficient when combined
  - Very specific
  - Fabrication and maintenance is challenging
- **New strategy : design simplicity / flexibility**
  - We accept compromises on the performances
  - We consider a « generic » design
  - Most instruments would prefer { thermal + cold neutrons }



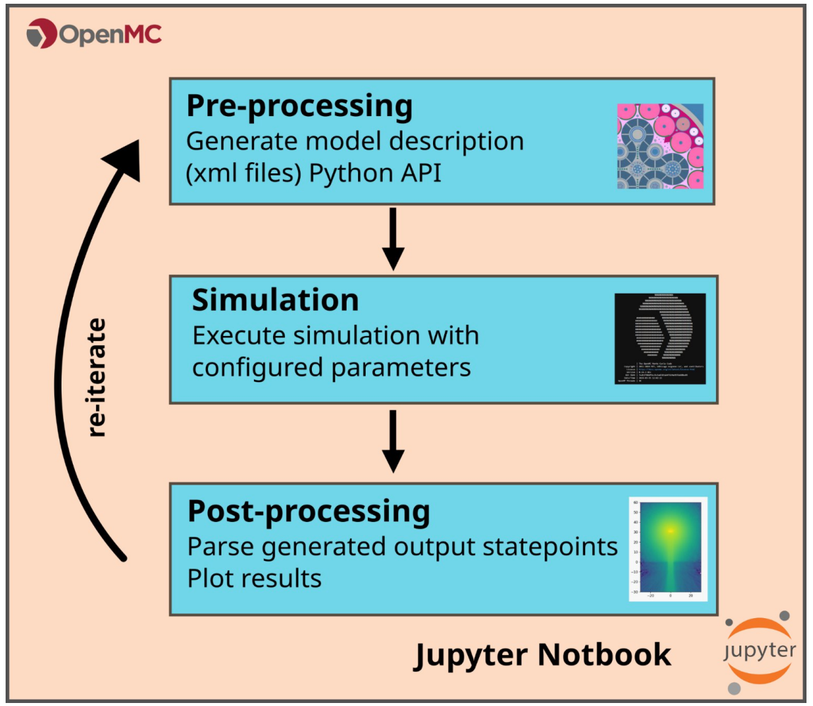
OpenMC

- 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 consistently over time; ma nyuniversities, laboratories and organizations contribute now to the development of OpenMC

- **Advantages**
  - Open Source ->
    Easy and on short term available and accessible
    (especially important with regard to the use by 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

OpenMC - https://openmc.org/

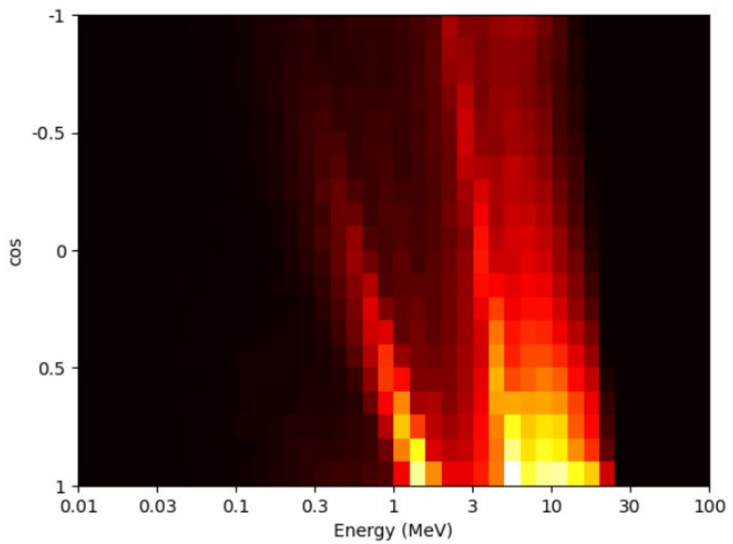
One environment



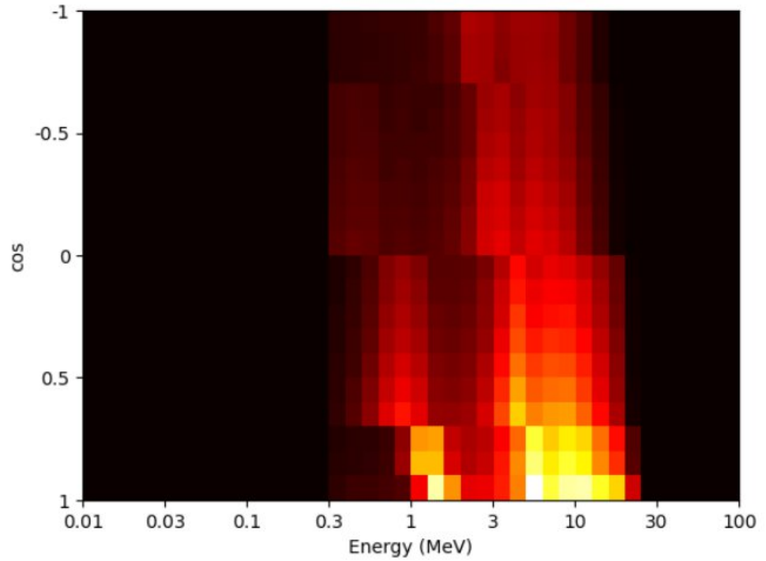
Source

- 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



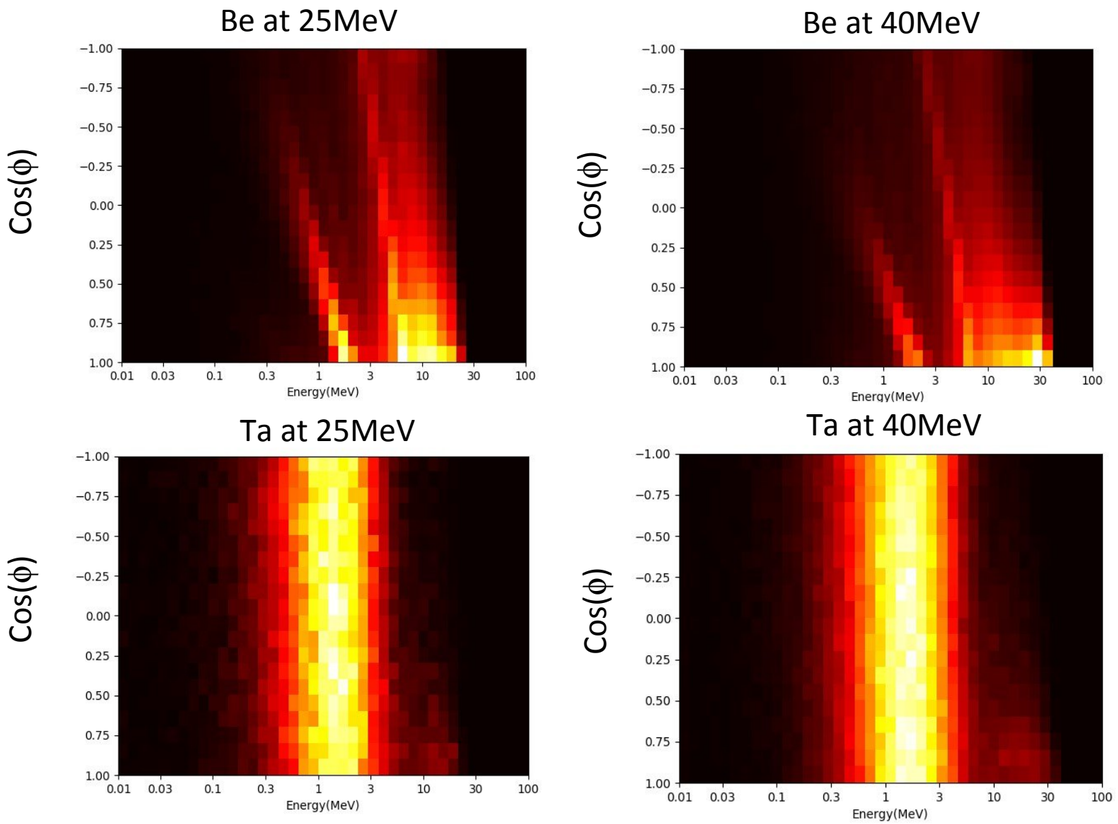
OpenMC



Example 25 MeV protons on Be

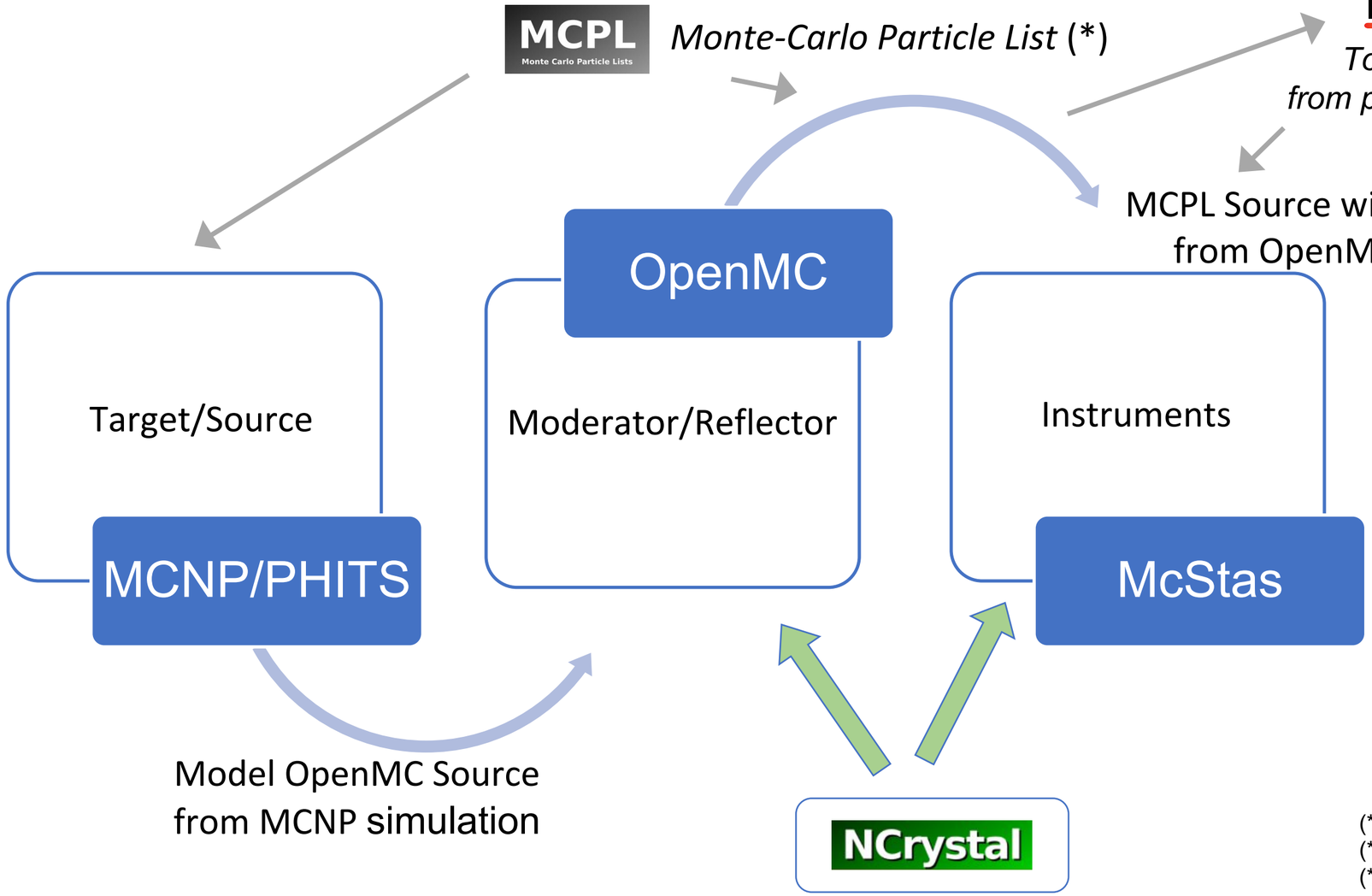
Source II

- 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 normalized and cannot be compared

Simulation Toolchain



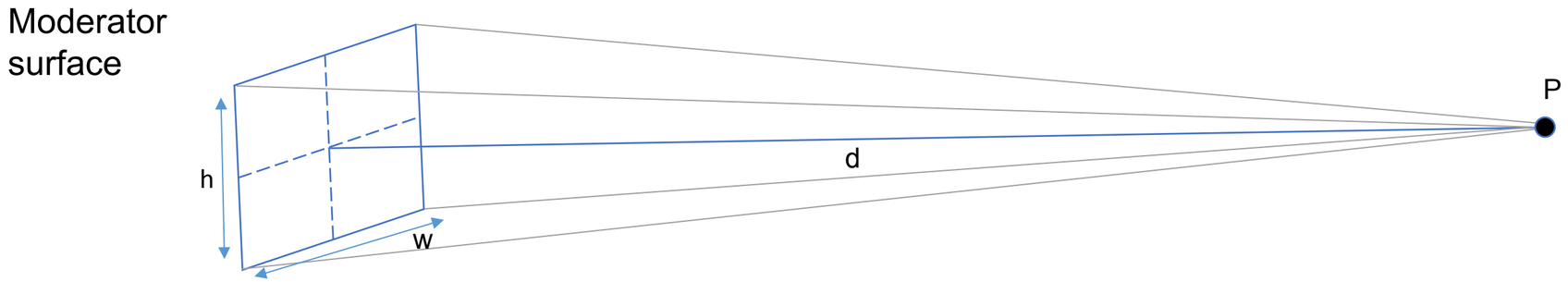
(*) https://mctools.github.io/mcpl/
(**) https://github.com/mctools/ncrystal/wiki
(***) https://github.com/KDSource

Library for thermal scattering transport (**)

Extend physics beyond limits of different
scattering library formats (e.g. reflector materials, composition of spin isomers)

Brightness

- Quantify performance of moderation
- Figure of merit (FoM): mean brightness/brilliance of the source/moderator surface
  - Brilliance: $B = \dfrac{\text{neutrons}}{\text{s cm}^2\ \text{sr}}$ sr … solid angle (Steradian)

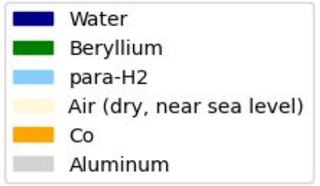


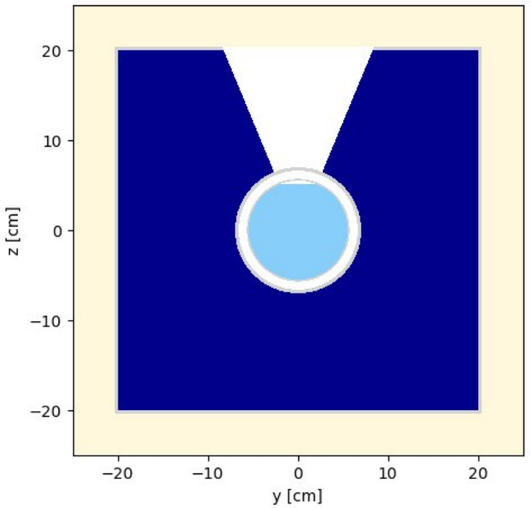
  - Solid Angle: $\Omega = \dfrac{hw}{d^2}$ if $h, w \ll d$
  - From Flux ψ in P → $B = \Psi / \Omega$

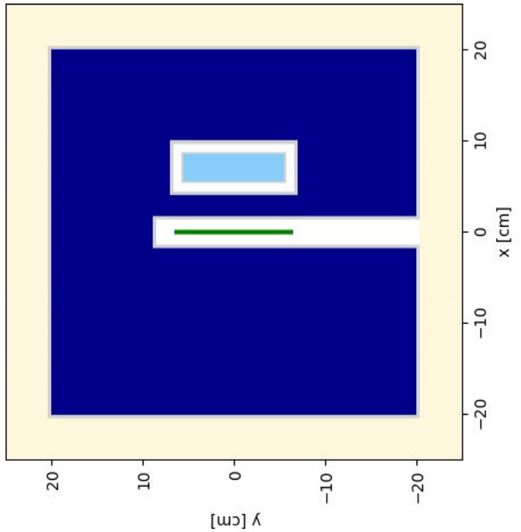
Accurate formula:

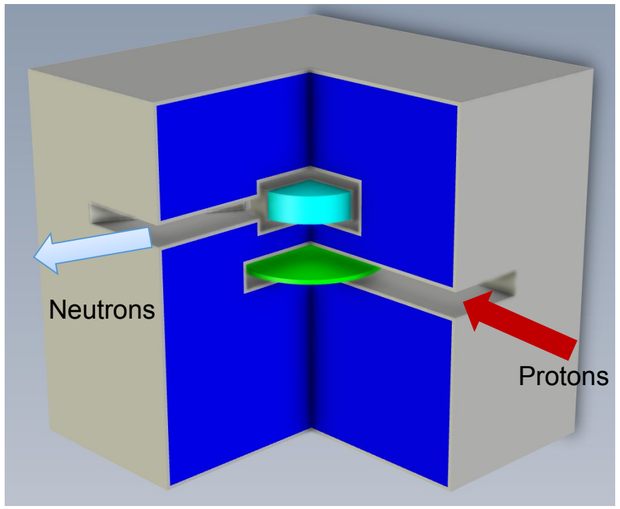
$$\Omega = 4 \arcsin\left(\frac{hw}{\sqrt{(h^2+4d^2)\,(w^2+4d^2)}}\right)$$

1st 'Baseline' Model I





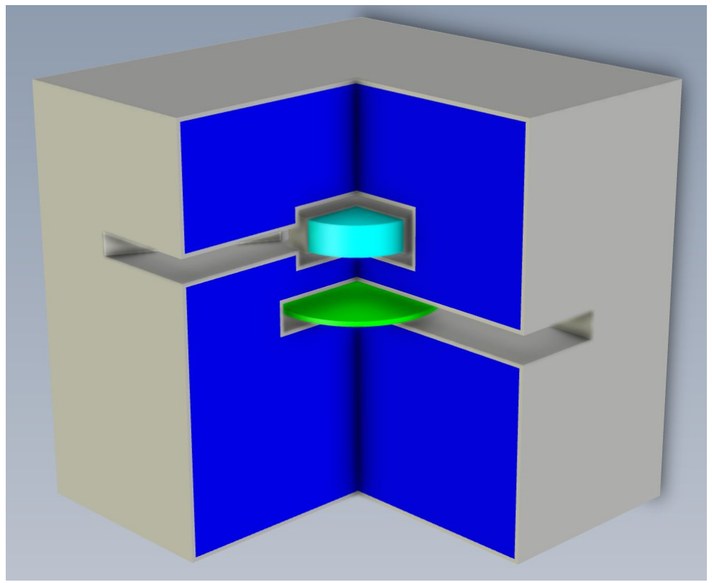


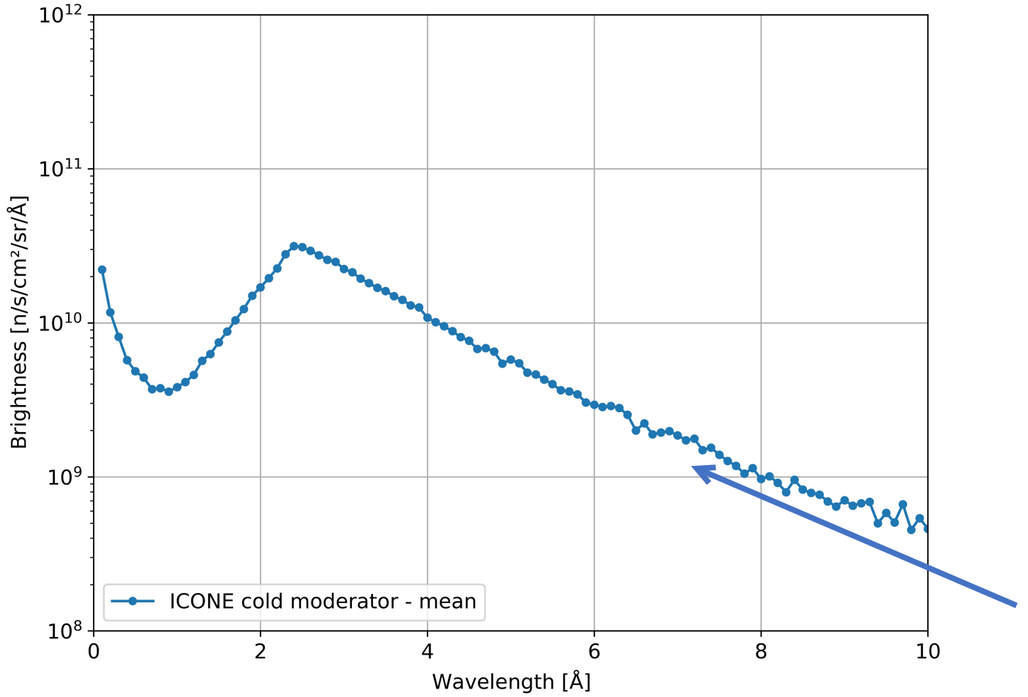


- Source:
  80kW, 25MeV Protons on Be
- Moderator exit window:
  3 x 4 cm

1st 'Baseline' Model II

- Source:
  80kW, 25MeV Protons on Be,
  mean current I = 3.2 mA
- Moderator exit window: 3 x 4 cm

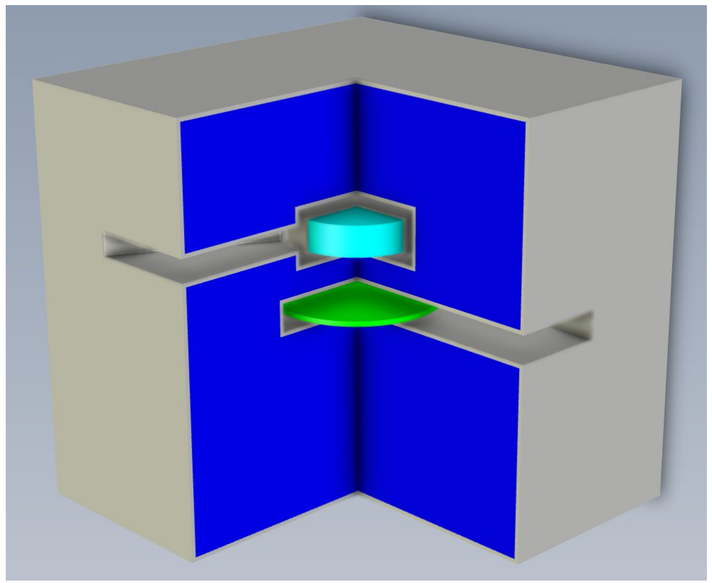




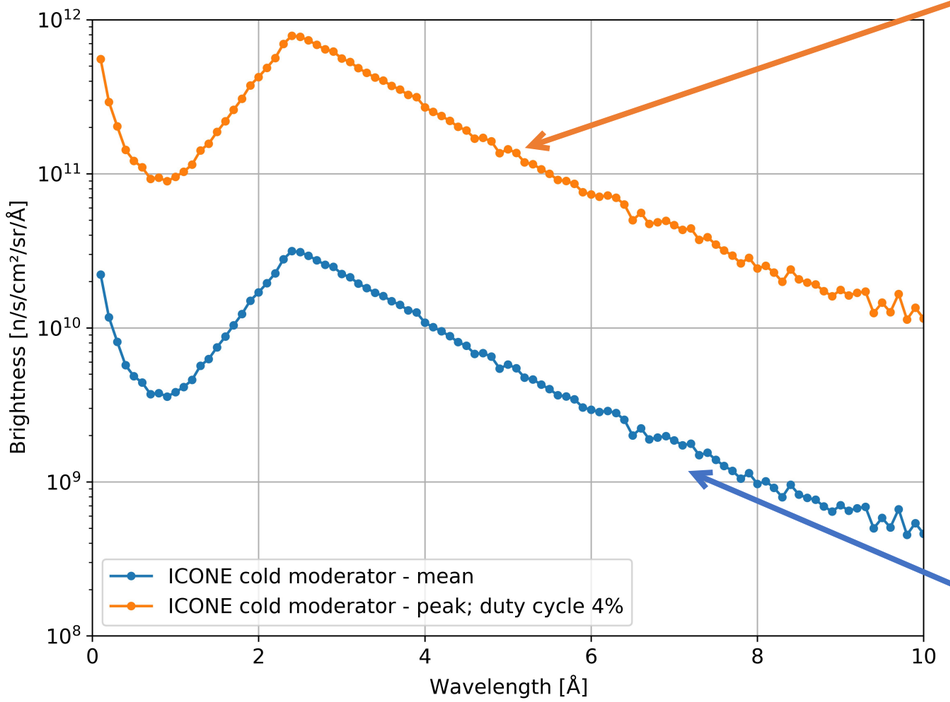
Mean Flux

1st 'Baseline' Model III

- Source:
  80kW, 25MeV Protons on Be,
  mean current I = 3.2 mA
- Moderator exit window: 3 x 4 cm



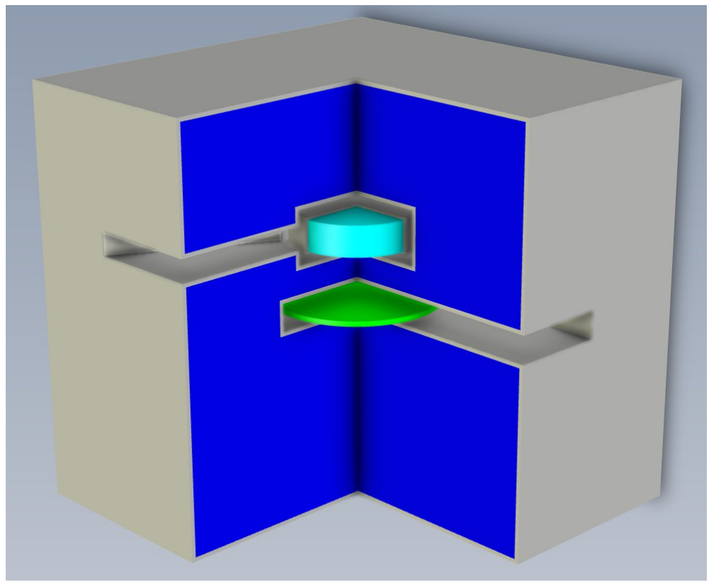
Peak Flux in the pulses (2ms@20Hz) of the source. Duty cycle of 4%



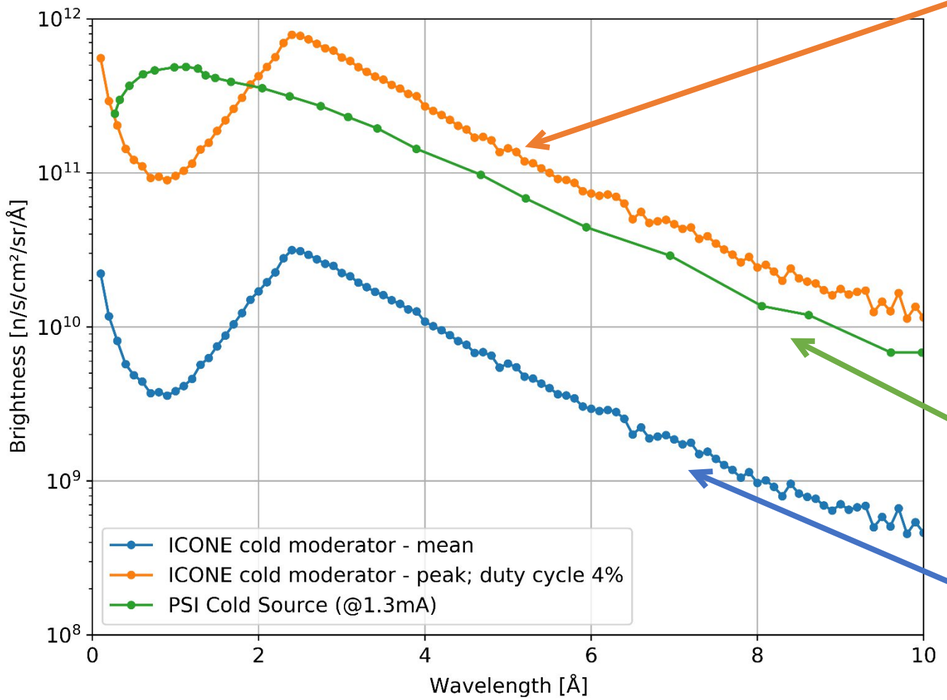
Mean Flux

1st 'Baseline' Model IV

- Source:
  80kW, 25MeV Protons on Be,
  mean current I = 3.2 mA
- Moderator exit window: 3 x 4 cm



Peak Flux in pulses (2ms@20Hz) of the source.
Duty cycle of 4%

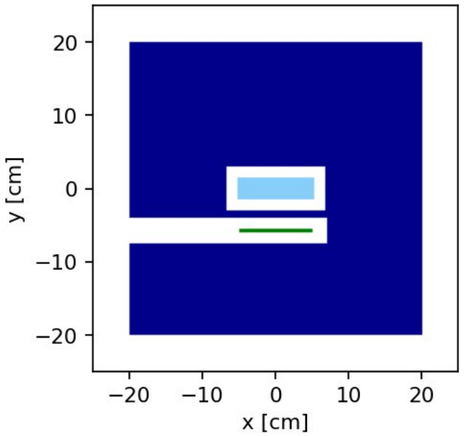


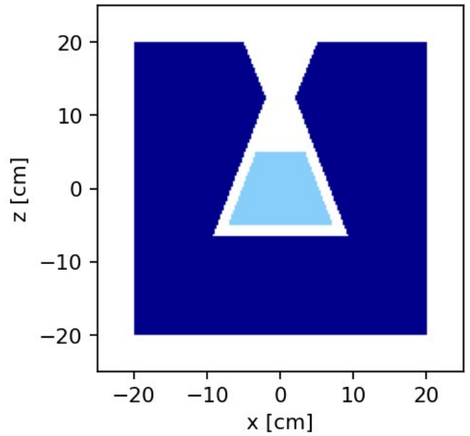
Cold Spectrum of
SINQ at PSI, Switzerland

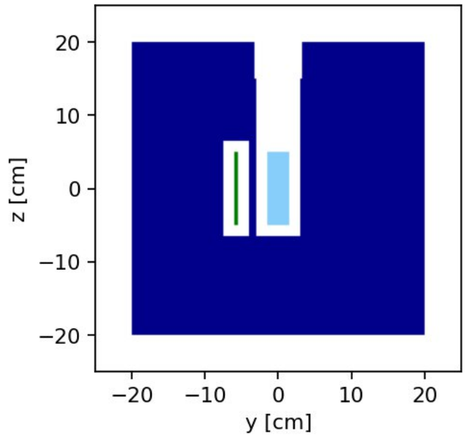
Mean Flux

PSI data from: Bergmann, R.M. *et al.* (2018)
Neutron brilliance of the liquid deuterium cold source as measured from the ICON beamline at the swiss spallation neutron source (SINQ) https://doi.org/10.1016/j.nima.2018.07.007.

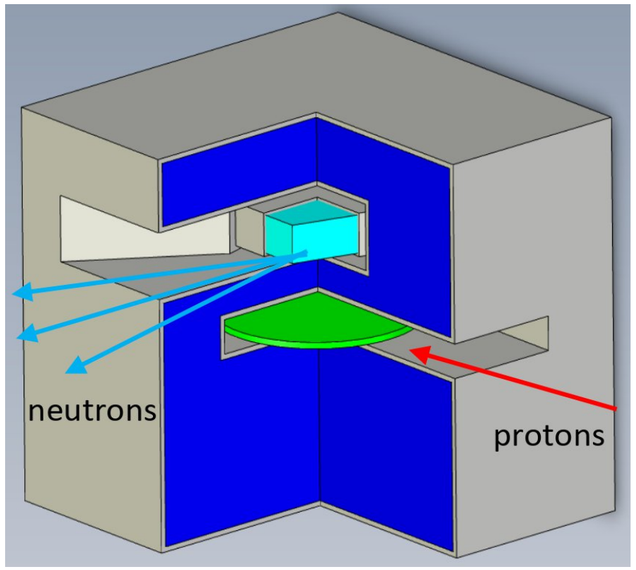
Adapted Baseline Model I





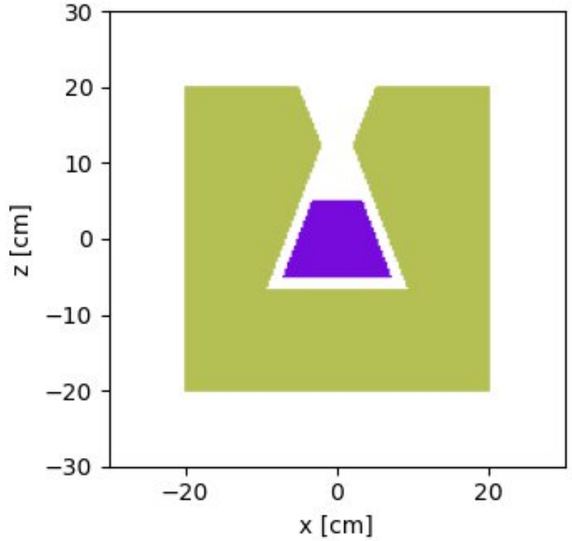


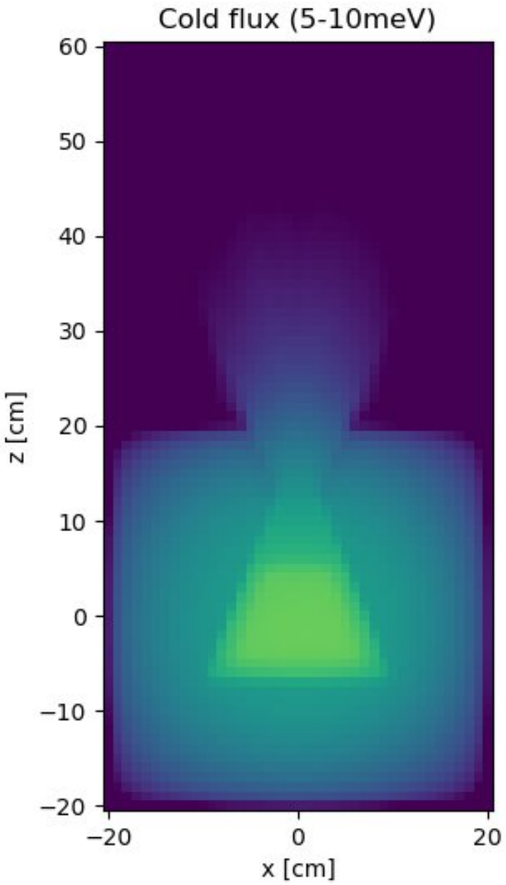
Illumination
over 45°

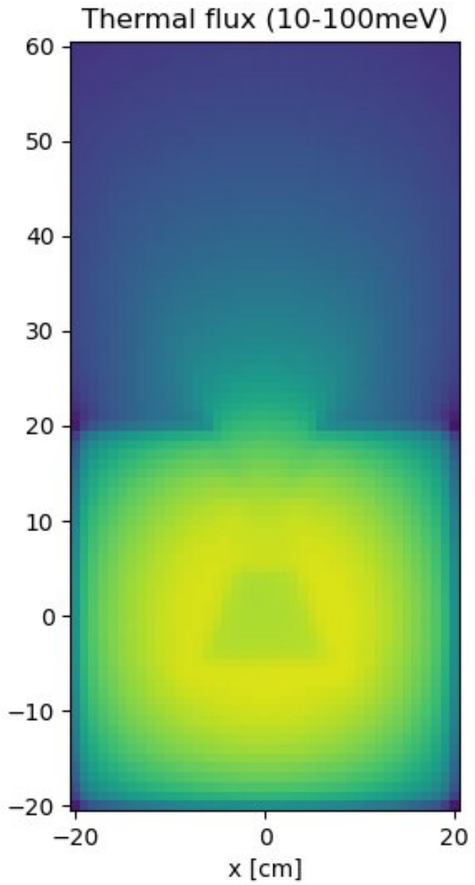


- Source:
  80kW, 25MeV Protons on Be
- Moderator exit window:
  3 x 4 cm

Flux in moderator assembly

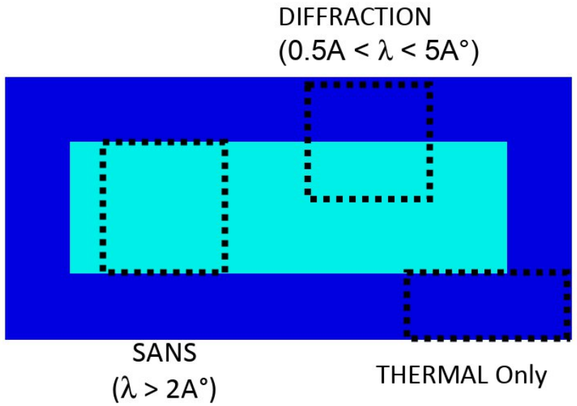




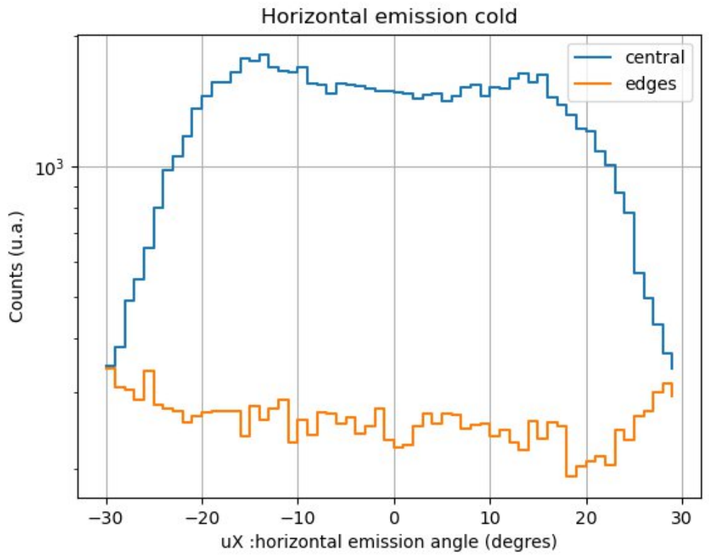


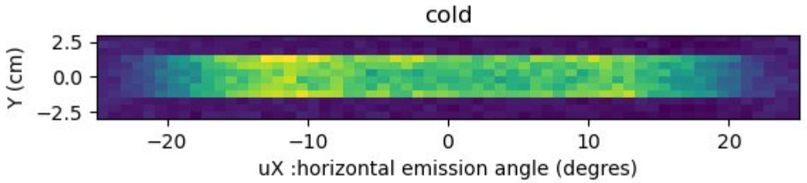
Moderator emission surface

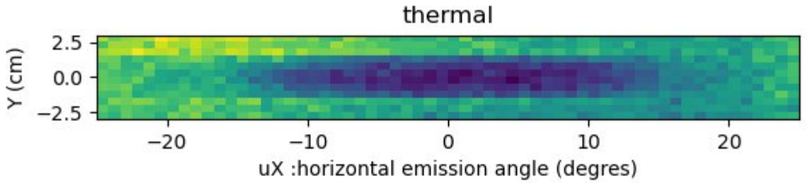
Front view



Horizontal emission divergence

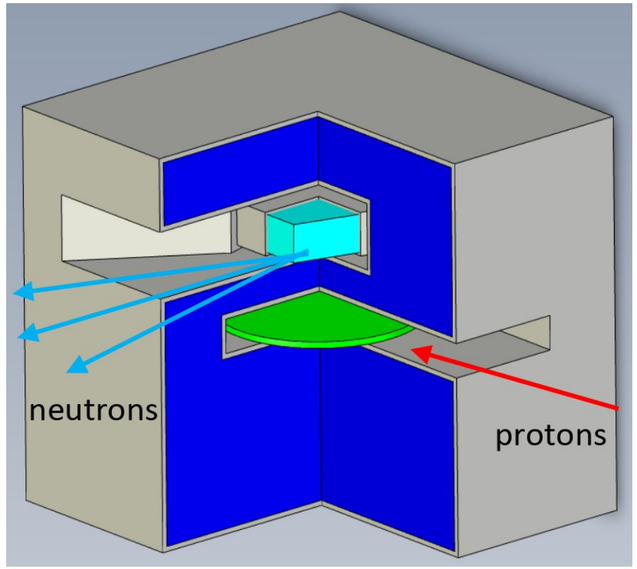


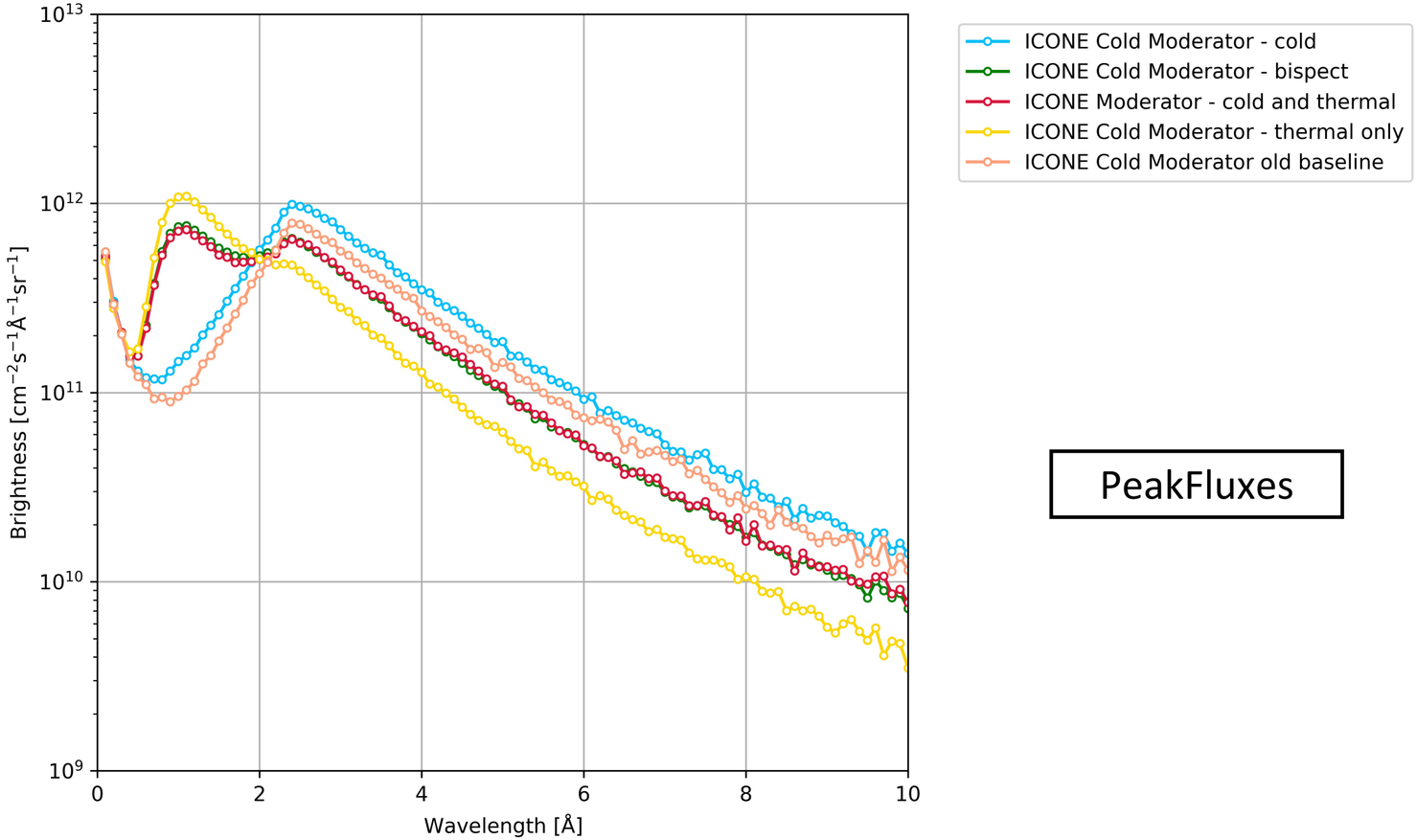




Adapted Baseline Model II

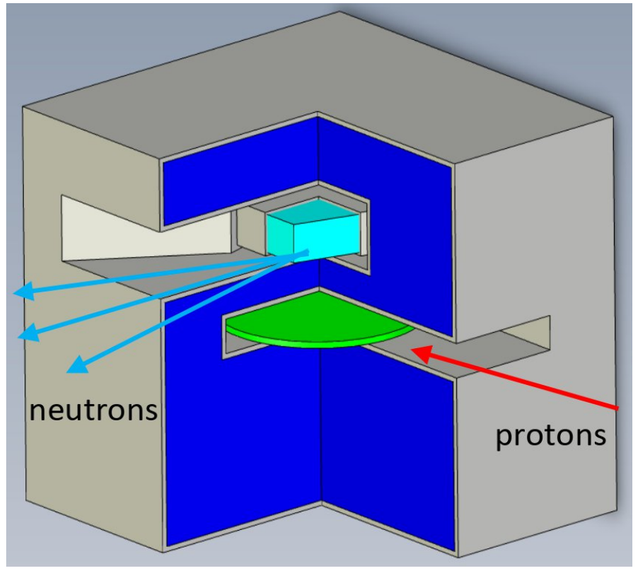
- Source:
  80kW, 25MeV Protons on Be,
  mean current I = 3.2 mA

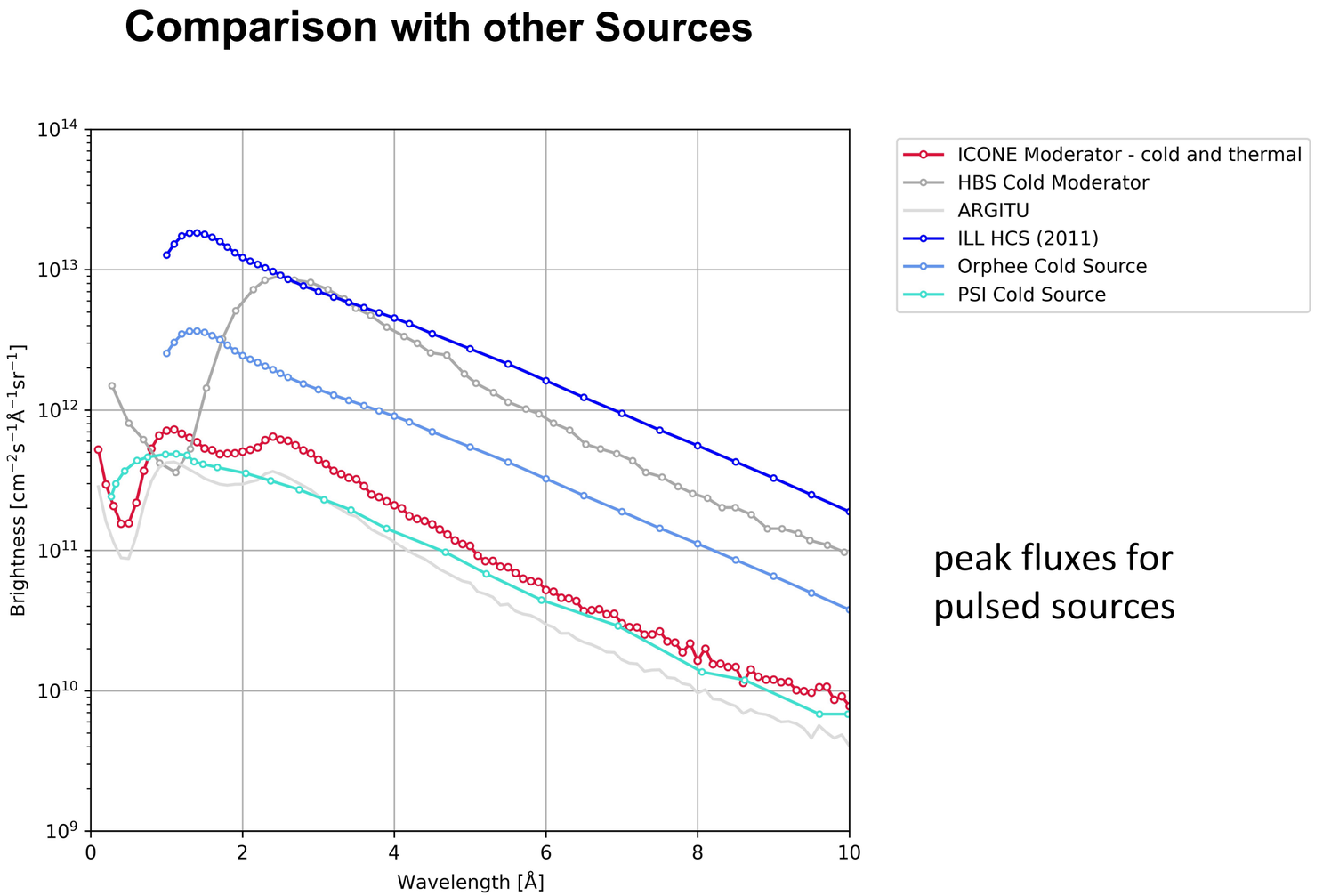




PeakFluxes

Adapted Baseline Model II

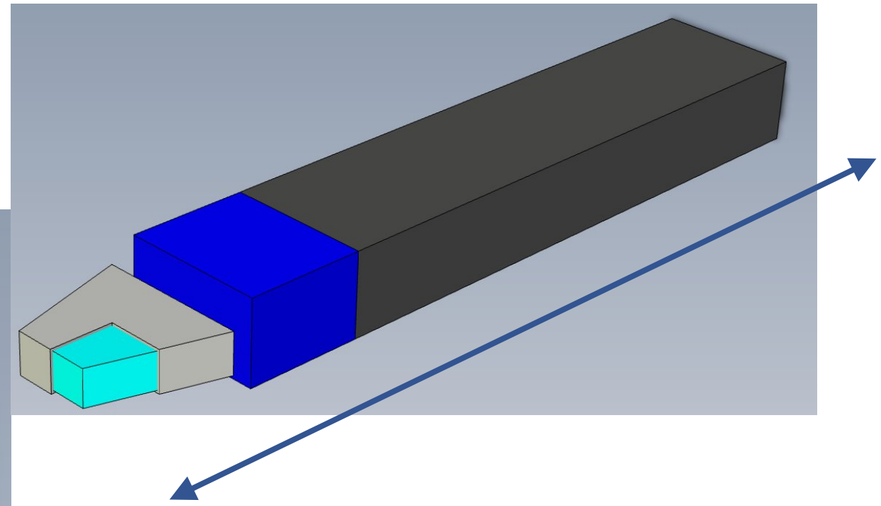


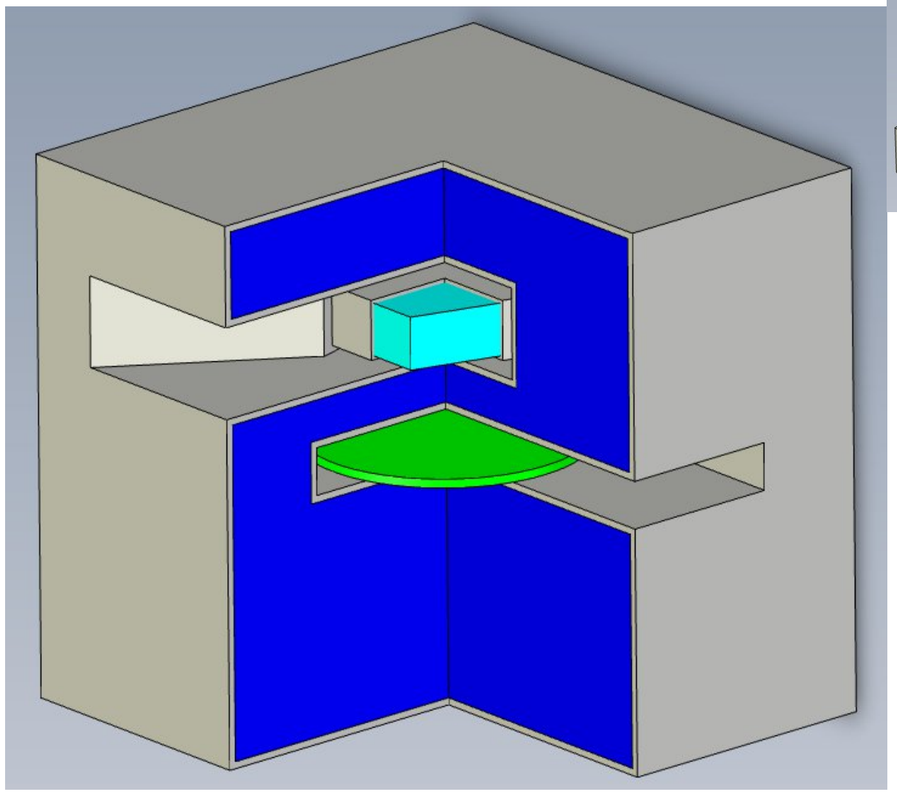


peak fluxes for pulsed sources

Maintenance

Cold cell insert





neutrons

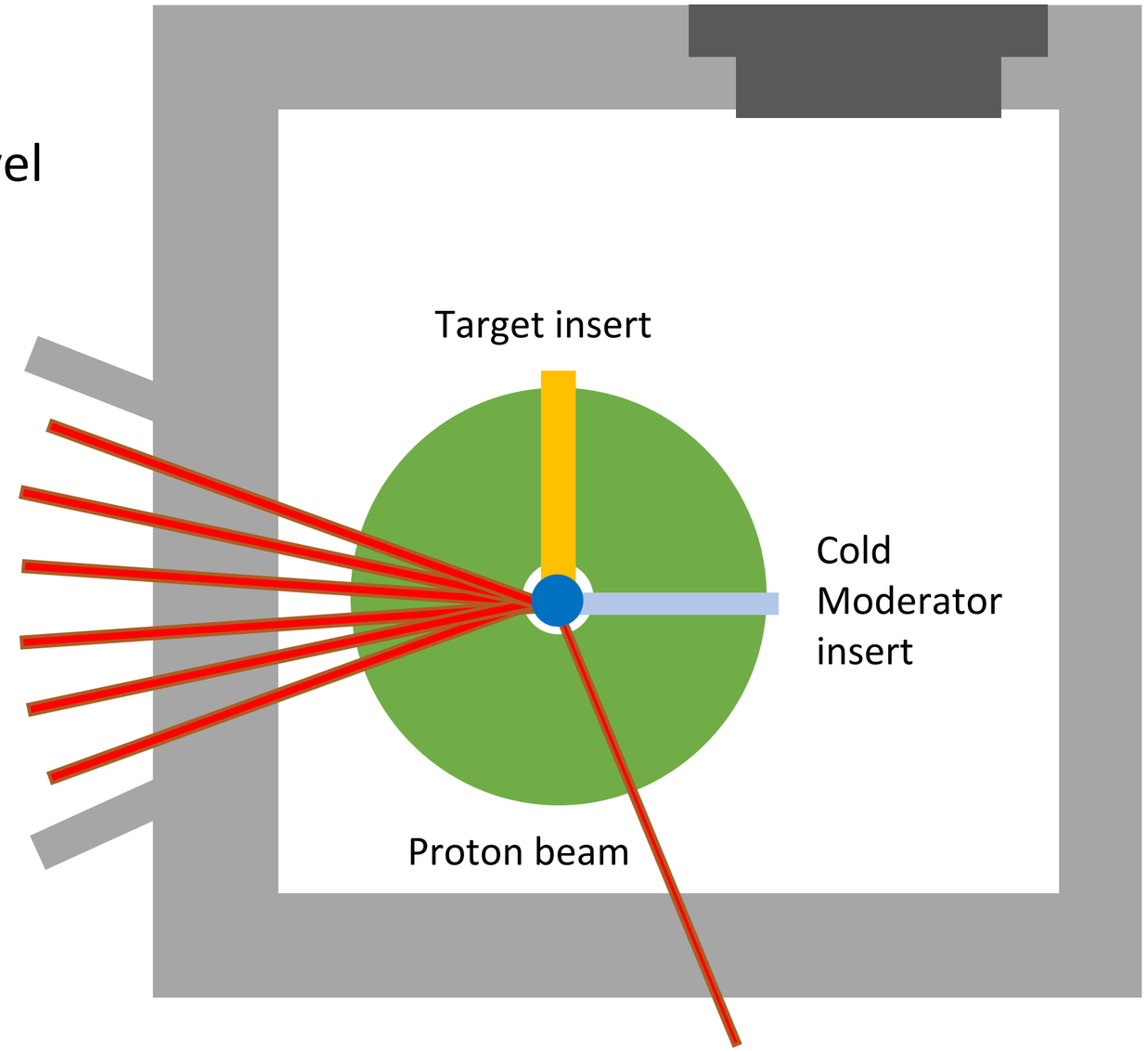
Insertion / extraction from the « back »
i.e No interference
with the guide / chopper system

Maintenance

Possible layout

- Maintenance mainly at the ground level
- No need to open the TMR

Neutrons
to guide hall



Conclusions and Outlook

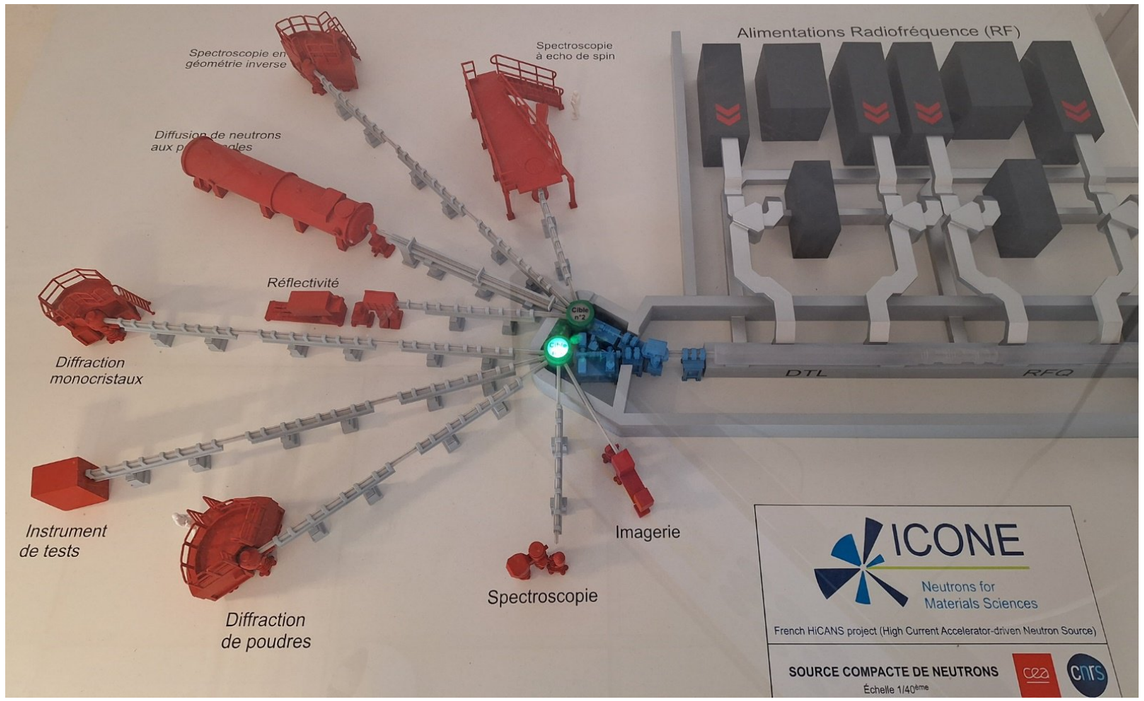
- **OpenMC Simulations**
  - Good and capable option for our ICONE development

- **Optimizations and Enhancements**
  - have still to be made, but improvements will expected to be in the order of 50% at best.
  - TMR Assembly Geometry optimization (particularly introduction of a reflector)
  - Moderator optimizations (e.g. re-entrant hole)

- **Further lines of work**
  - Detailed study bi-spectral emission: thermal + cold
  - Study time dependence and pulse shape
  - Address „second-order problem“: (i) “long” pulses + (ii) pulse shaping with choppers
  - Overcome limitations on computing power for our simulations
    - Agreement to use the Paris-Saclay “La RUCHE” mesocenter
    - (there are still a few technical difficulties to overcome before we can take advantage of this resource).

Acknowledgments

Thank you for your attention!

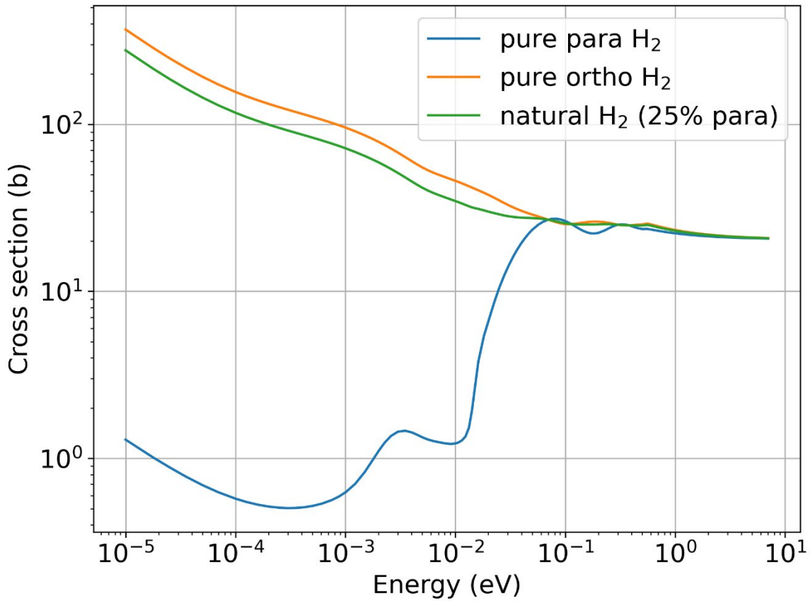


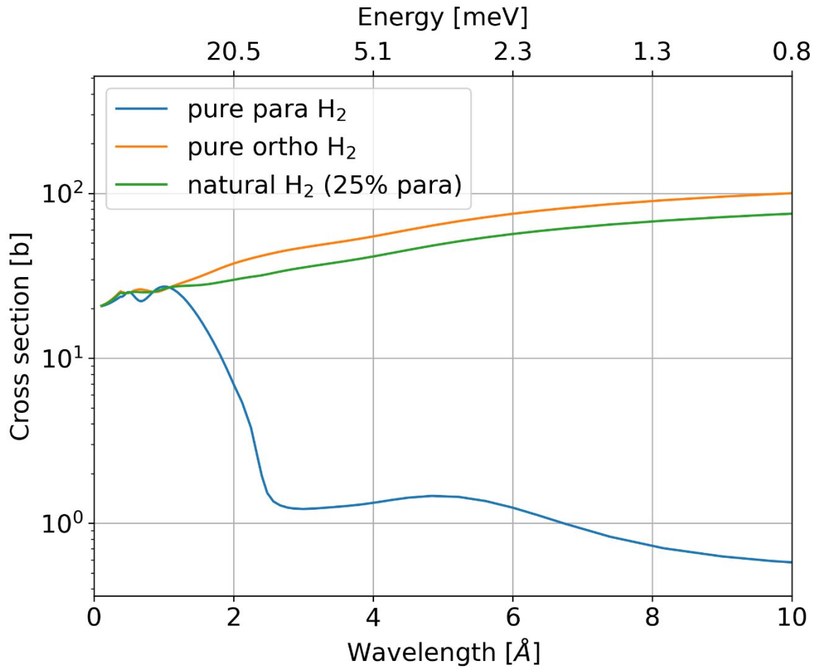
Credits: LLB (CEA/IRAMIS): J. Darpentigny, X. Fabreges, X. Guillou, A. Menelle, J.-L. Meuriot, F. Ott

Backup Slides

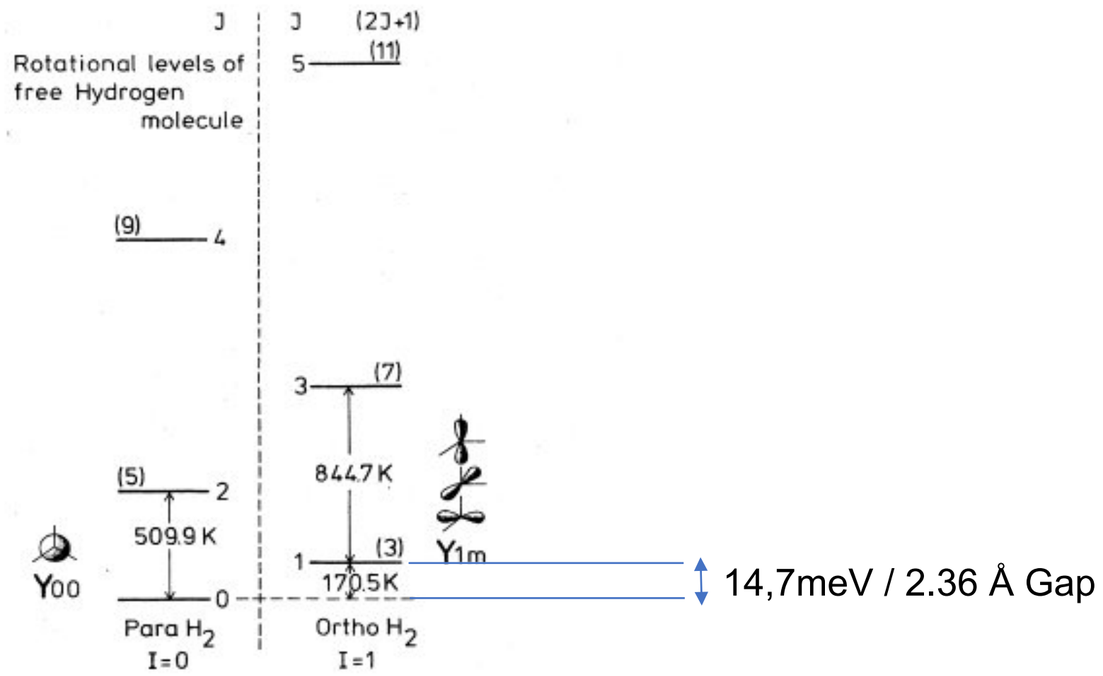
Para- and Ortho-Hydrogen

Cross Section

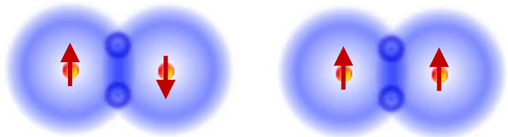




Para- and Ortho-Hydrogen



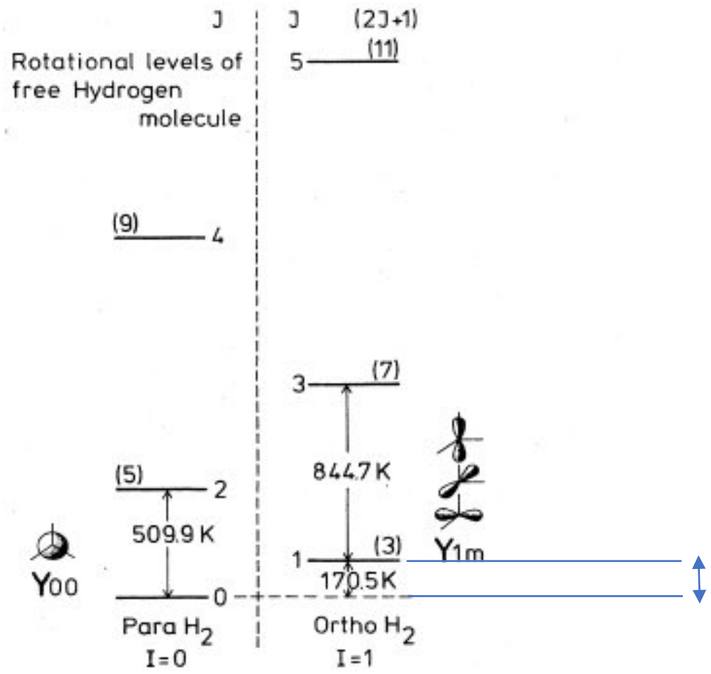
Singlet State



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.

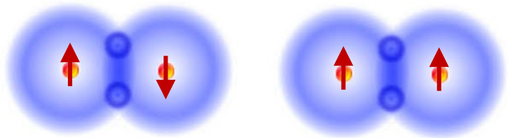
Para- and Ortho-Hydrogen



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

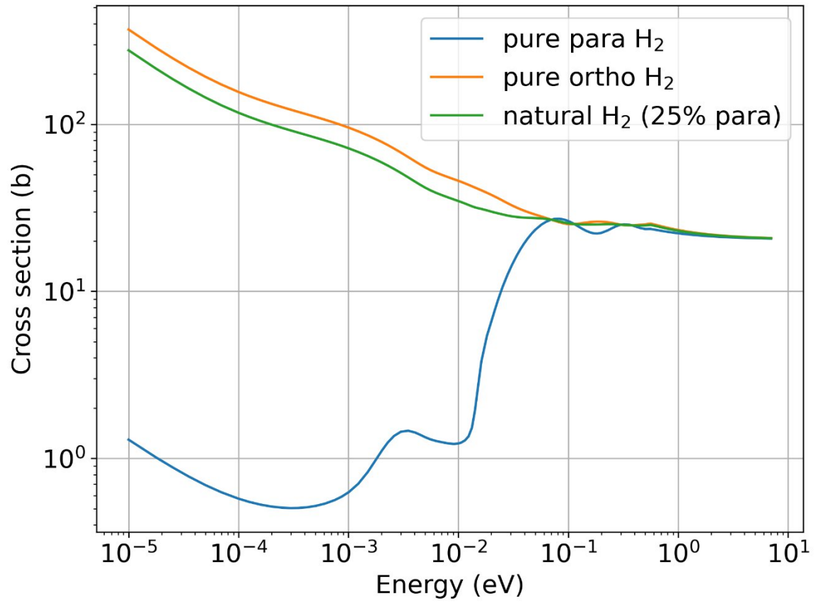


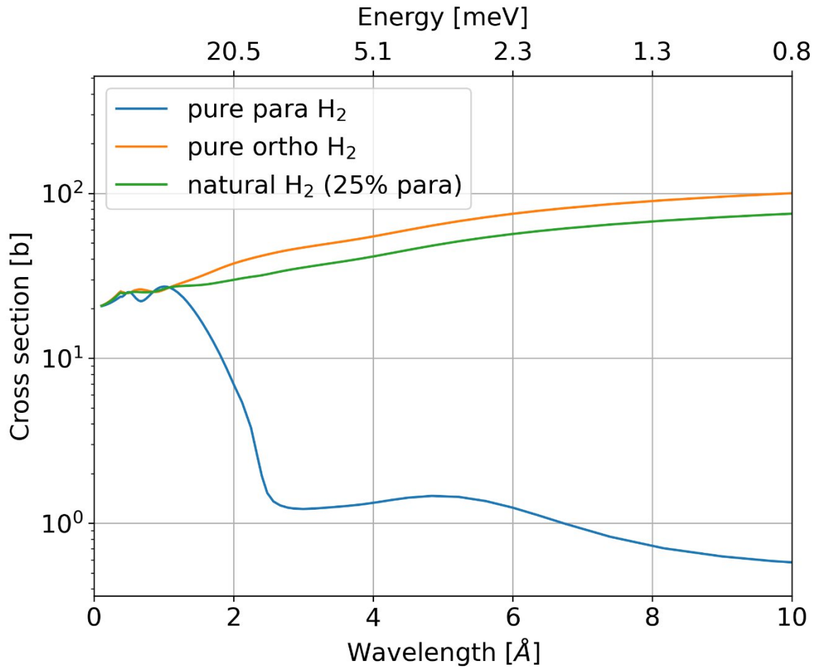
Triplet State

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.

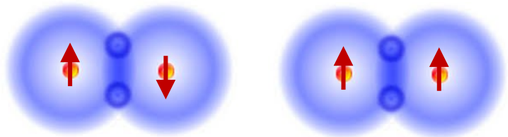
Para- and Ortho-Hydrogen

Cross Section



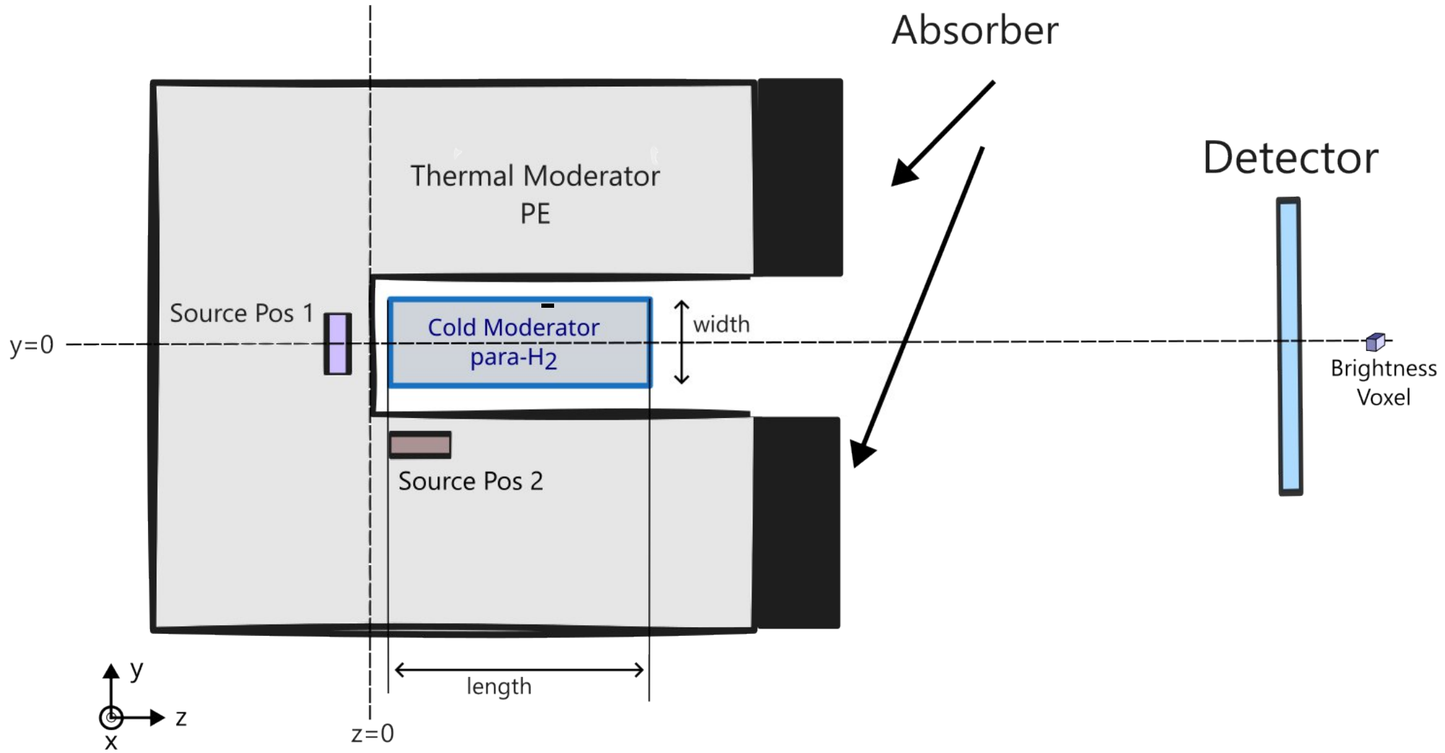


Para-Hydrogen
Singlet State



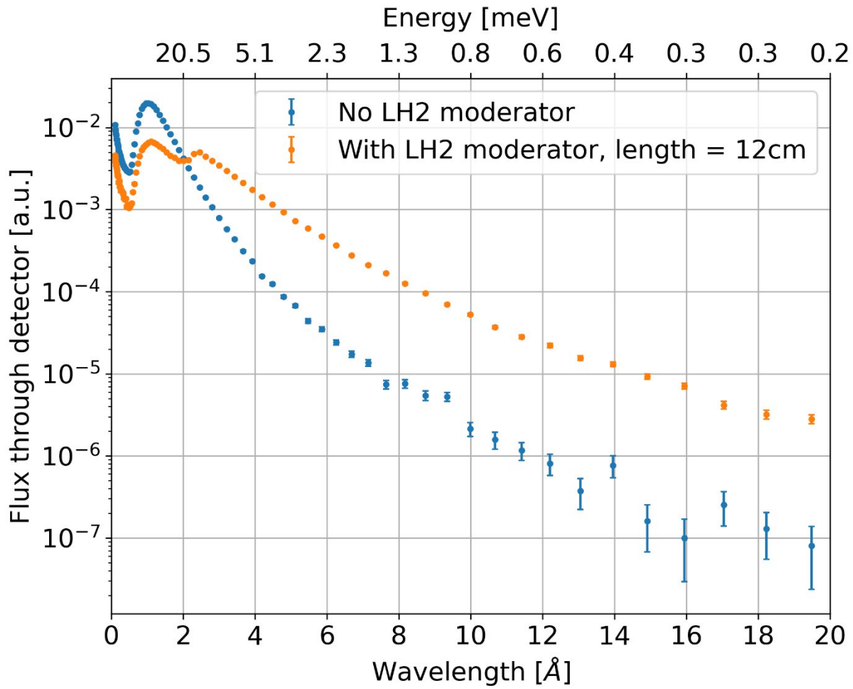
Ortho-Hydrogen
Triplet State

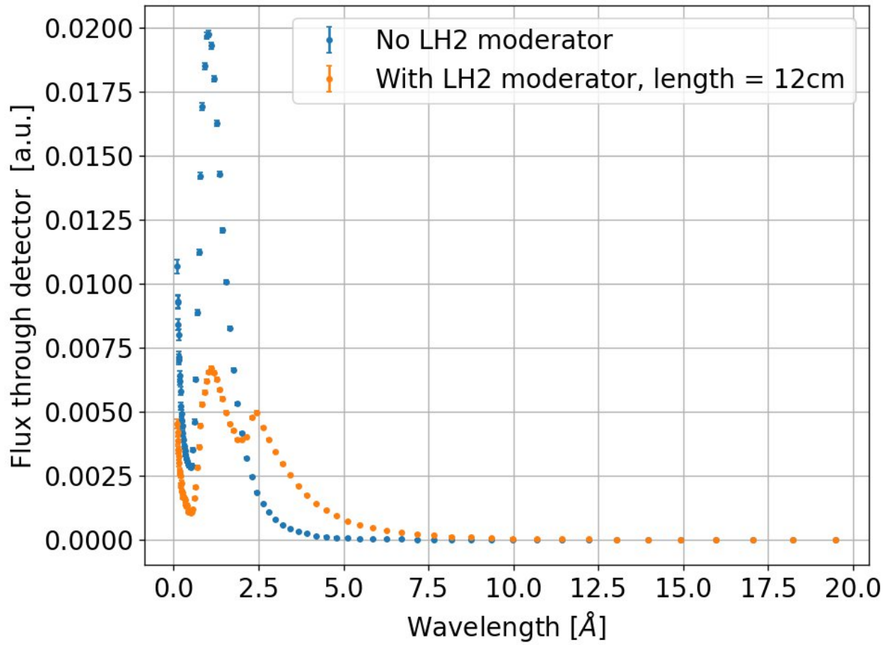
Simple Model



Results Spectrum

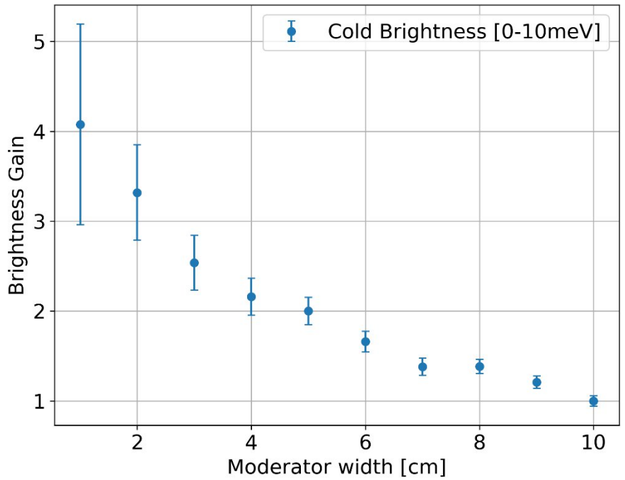
- Shift in Spectrum



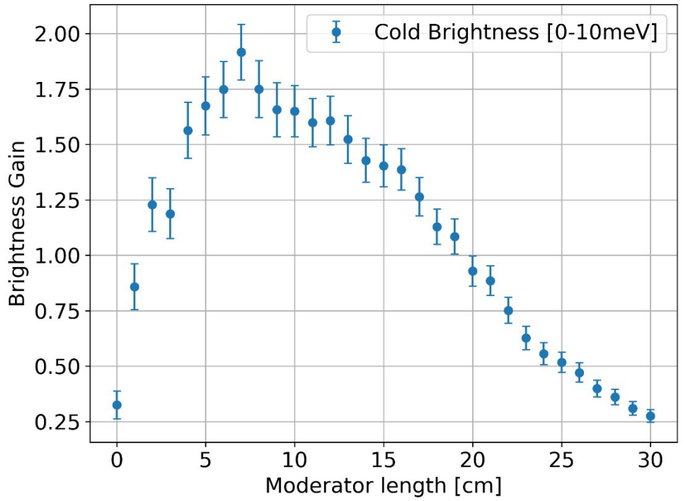


Result: Brightness Gain

- Change with area of emission surface
- Gain over Moderator with surface area: 10 × 10 cm²



- 6 × 6 cm2 surface area length scan
- Gain over Moderator (10 × 10 cm², l=10cm)



- Caveat:
  Gain comes at the expense of intensity with which (several numbers of) guides/instruments can be fee