GEANT4 simulation of the n_TOF lead spallation target: a benchmark study

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ENSAR2 workshop: GEANT4 in nuclear physics

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Outline

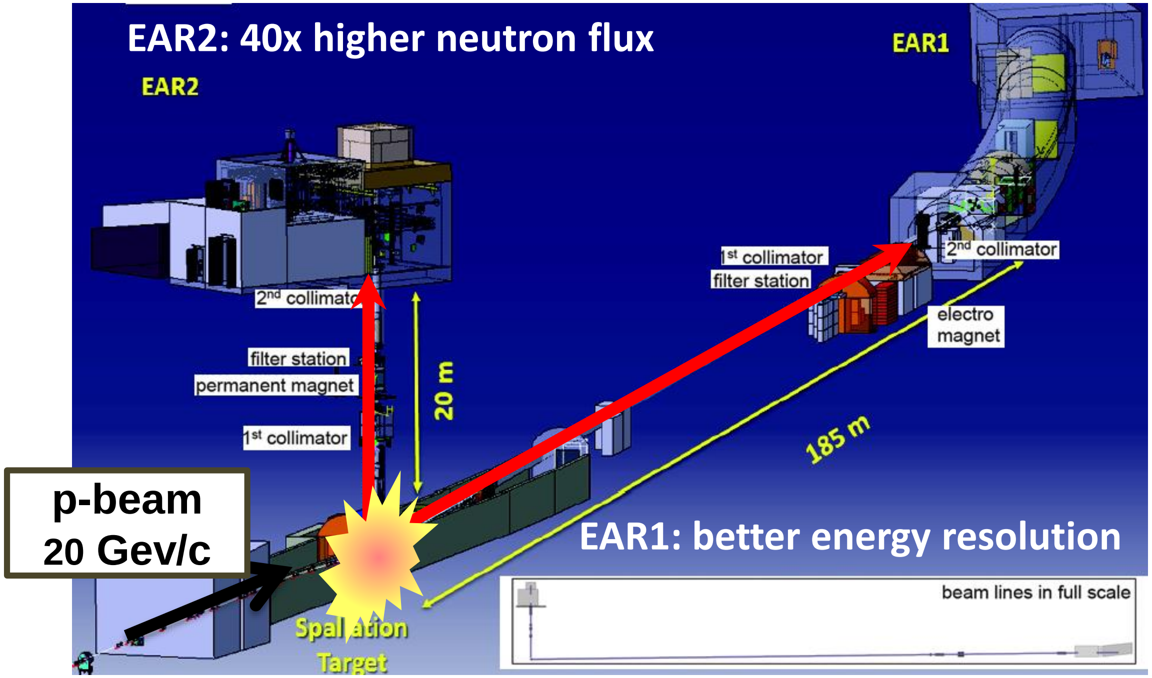
- Introduction: The n_TOF lead spallation target
- Geant4 simulations & transport to Exp. Areas
- Status of this work and recent updates
- Results Geant4 v10.5.0: Comparison of PLs
- Comparison Geant4 v10.5.0 vs v10.2.2
- Summary and conclusions

Introduction:
The n_TOF lead spallation target

The n_TOF facility at CERN

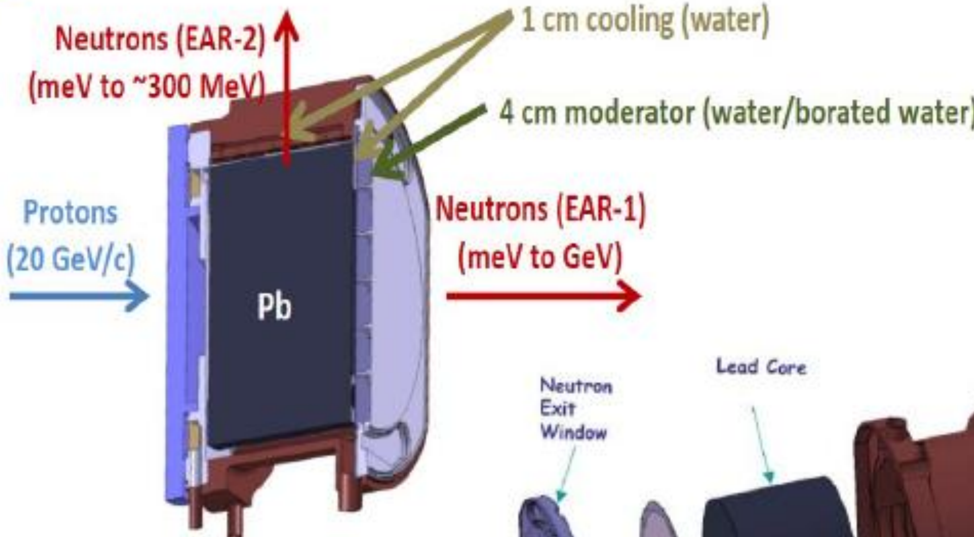
- High resolution neutron cross section measurements
  - Pulsed beam + Time-of-flight (TOF) Technique
  - Spallation 20 GeV/c protons + Pb: neutron spectrum from **thermal to few GeV**
  - **EAR1 (185m):** High energy resolution ($\Delta E/E$ @1keV : $\sim 3\cdot 10^{-4}$)
  - **EAR2 (20m):** High flux ($\sim 7.5\cdot 10^{6}$ n/cm^2/pulse)

- Applications:
  - Nuclear Technologies
    - ADS, fast reactors
  - Astrophysics
    - s-process
  - Basic Nuclear Physics

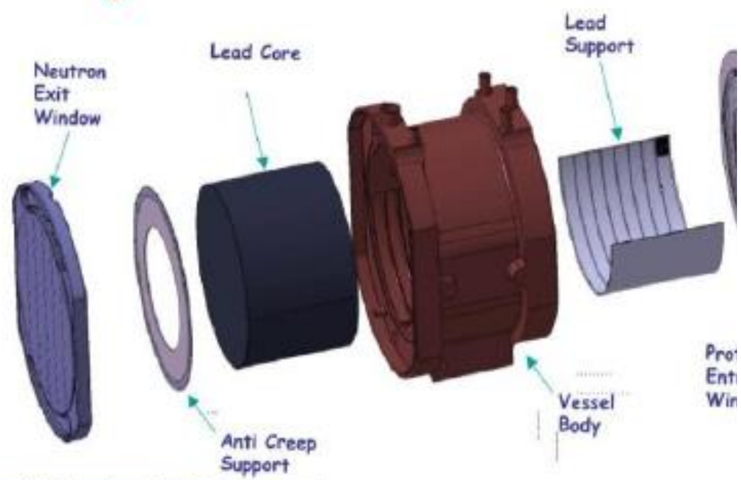


nTOF Universidad de Sevilla Geant 4

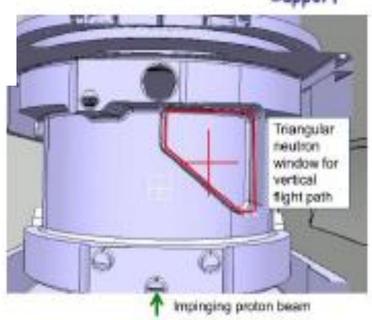
Pb Spallation Target – Technical Details



- Water-cooled lead target
- 60cmΦ, 40 cm length
- 400 neutrons/proton (MeV-GeV)



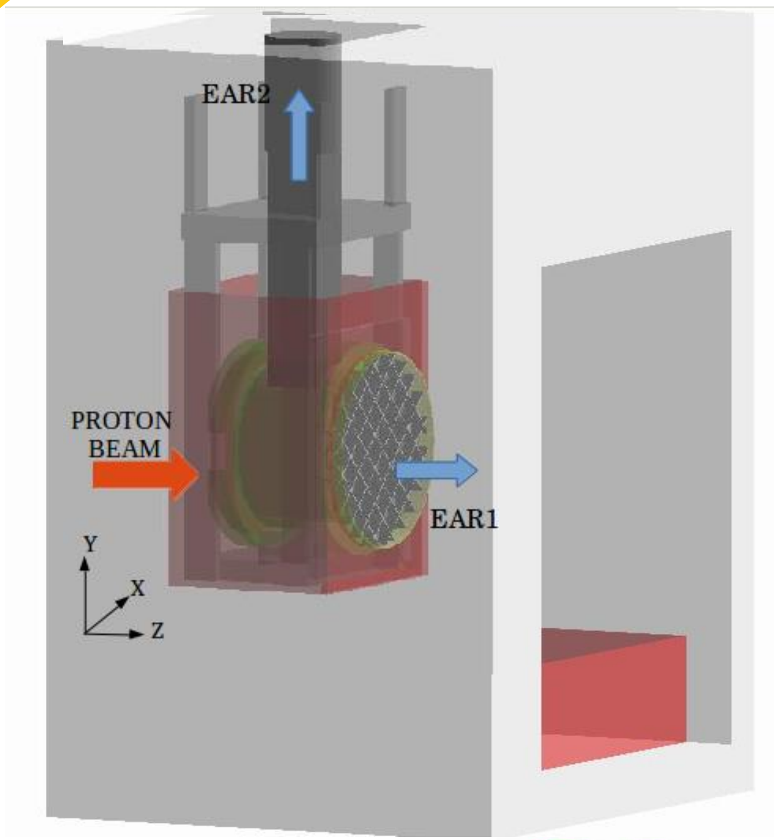
- **EAR1:** 1cm Water+4cm Borated Water (1.28% of H_3BO_3) before beam pipe.
- **EAR2**: "triangular" shape entrance to beam line. NO Boron, just water.



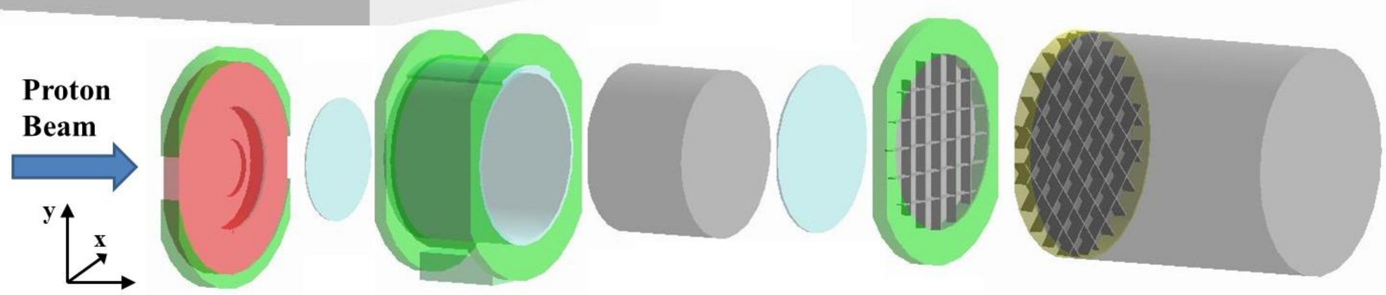
Aluminum vessel and support structures from the CAD drawings

Geant4 simulations and transport along beamlines

Geometry model

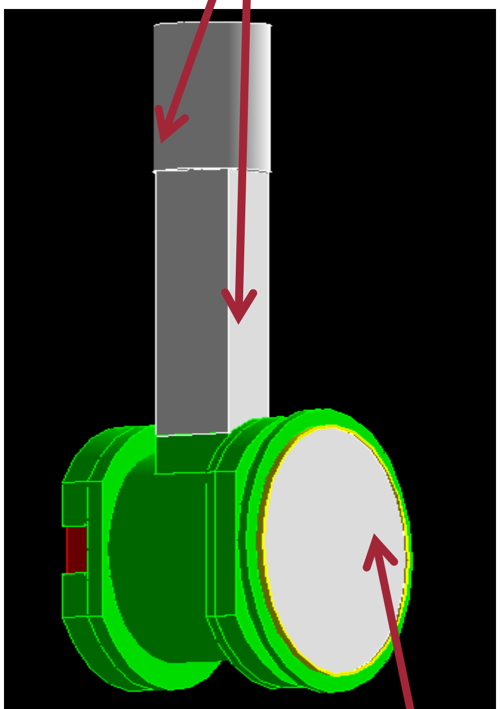


- **Primary particles:** 20 GeV/c protons, with an incidence angle of 10 deg + Gaussian profile beam (FWHM=3.53cm).
- **Spallation target:**
- Precise implementation of the cooling and moderation layers.
- All the surrounding structures **following the technical drawings.**
- **Special care** in the **composition** of the lead block and the target vessel.



Geant4 scoring @ target exit + transport code

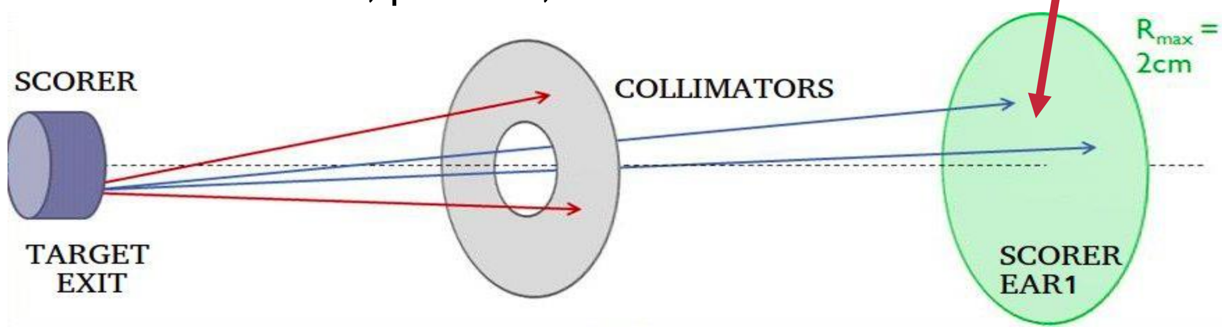
EAR2 : Detailed 3D scorer, beam line shape



EAR1: 2D scorer @ entrance of beam line

- **Scoring surfaces** defined as in **previous simulations** at n_TOF (FLUKA).
- Angular acceptance limited to 4 deg ↔ isotropic spectra within this solid angle.
- **Collected information at scorer:** Particle, position, time and momentum

Measured @ Exp. area



- **Geometric transport required:** CPU time limitation
- **Resample ~1000 times each particle** towards a 2cm scorer in the EAR + collimation system
- If collimator hit: neutron discarded **(no interaction)**

Status of this work and recent updates

Publications/applications related to this work

- **Validation/benchmark** with neutron flux @ **EAR1** (2015)

EPJ A

Hadrons and Nuclei

Eur. Phys. J. A (2015) 51: 160

EPJ.org your physics journal

GEANT4 simulations of the n_TOF spallation source and their benchmarking

S. Lo Meo, M.A. Cortés-Giraldo, C. Massimi, J. Lerendegui-Marco, M. Barbagallo, N. Colonna, C. Guerrero, D. Mancusi, F. Mingrone, J.M. Quesada, M. Sabate-Gilarte, G. Vannini, V. Vlachoudis and The n_TOF Collaboration

- **Characteristics and prospects** of the new n_TOF-**EAR2** (2016)

Geant4 simulation of the n_TOF-EAR2 neutron beam: characteristics and prospects

J. Lerendegui-Marco[1], S. Lo Meo[2,3], C. Guerrero[1], M. A. Cortés-Giraldo[1], C. Massimi[3,4], J. M. Quesada[1], M. Barbagallo[5], N. Colonna[5], D. Mancusi[6], F. Mingrone[3], M. Sabaté-Gilarte[1,6], G. Vannini[3,4], V. Vlachoudis[6], The n_TOF Collaboration[7],

- Follow-up of this work**: Role of secondary pions in spallation targets**

  Mancusi, D., Lo Meo, S., Colonna, N. et al. Eur. Phys. J. A (2017) 53: 80

- Application**: initial design phase** for the future n_TOF target (n_TOF Target #3)
  - **Goal:** validate/check the results of the main simulation team at CERN-n_TOF (FLUKA)

  J. Lerendegui-Marco, Collaboration Board meeting - Target # 3 Design
  https://indico.cern.ch/event/544449/

Geant4 v10.1.1

nTOF Geant 4

Updates to new Geant4 releases

- **September 2016:**
  - M.A. Cortés-Giraldo, Geant4 Collab. Meeting in Ferrara
  - Update to Geant4 10.2.2 + corrections in the optical transport code
  - Preliminary comparison @ EAR2 (not yet published)
  - Include in the comparison QBBC and FTFP_BERP Physics lists

- **This contribution:**
  - Update the results to Geant4 v10.5.0
  - Benchmark Geant4 10.5.0 with the experimental neutron fluxes @ EAR1 and EAR2
  - Use the same geometry (simplified materials) & collimation input transport code than in 2016 → Direct comparison between v10.2.2 and v10.5.0

Simulations with Geant4 10.5.0

- Geant4 **v10.5.0 + different Physics Lists (PLs)** (including QBBC, FTFP_BERP)
- **HPT:** Using neutron High Precision (**HP**) transport models and XS below **20 MeV**. ElasticThermalScattering (**En < 4 eV**) activated for available materials
- **Different neutron libraries:** native & from IAEA web site (released by CIEMAT group) **(*)**
- **Evaluated neutron flux @ EAR1 and EAR2** used to benchmark Geant4**(**)**
- **"Optical" transport to experimental areas** with the geometric transport code **(***)**

(*) E. Mendoza et al., IEEE-TNS 61: 2357 (2014)

(**) M. Barbagallo et al., EPJ A 49: 27 (2013)
M. Sabaté-Gilarte et al., Eur. Phys. J. A 53: 210 (2017)

(***) Thanks to Vasilis Vlachoudis (n_TOF/CERN)

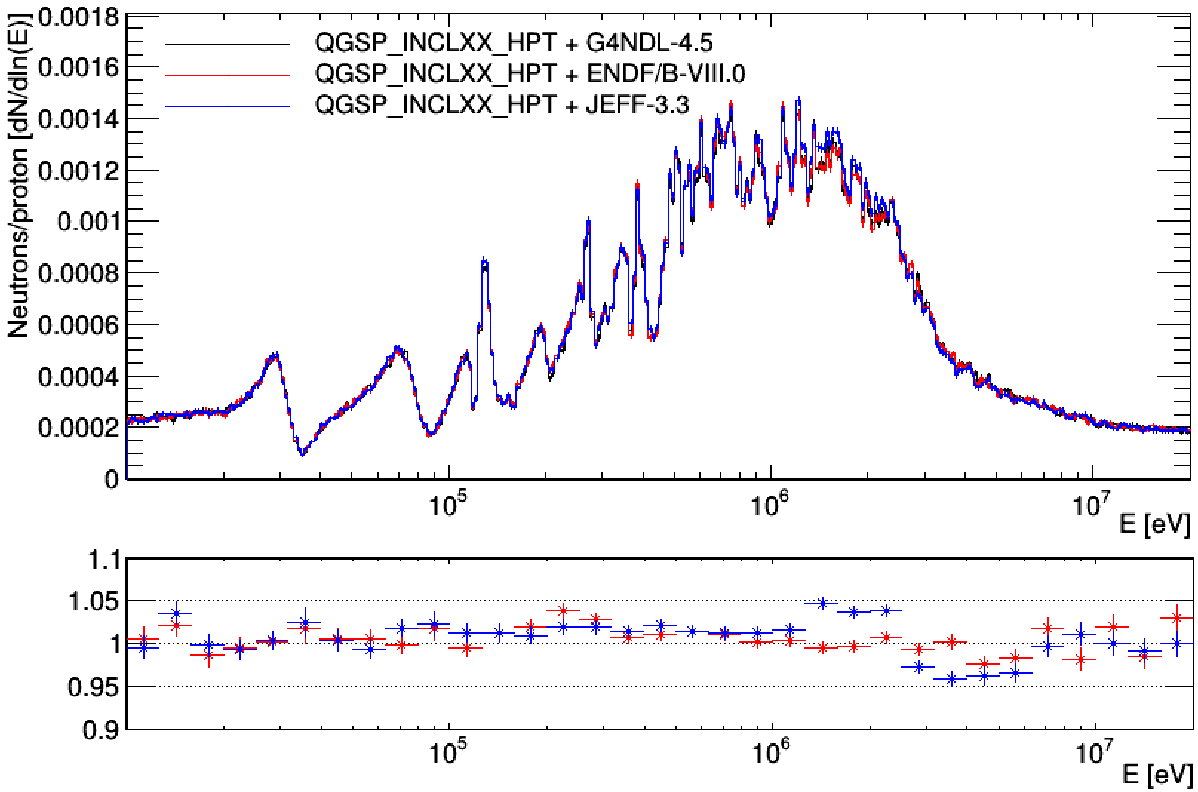
Upcoming results: PLs will omit the _**HPT:** (Neutron**HP** below 20MeV + **T**hermal Scattering below 4eV)

nTOF Geant 4

Results Geant4 v10.5.0:
Impact of the choice of neutron library

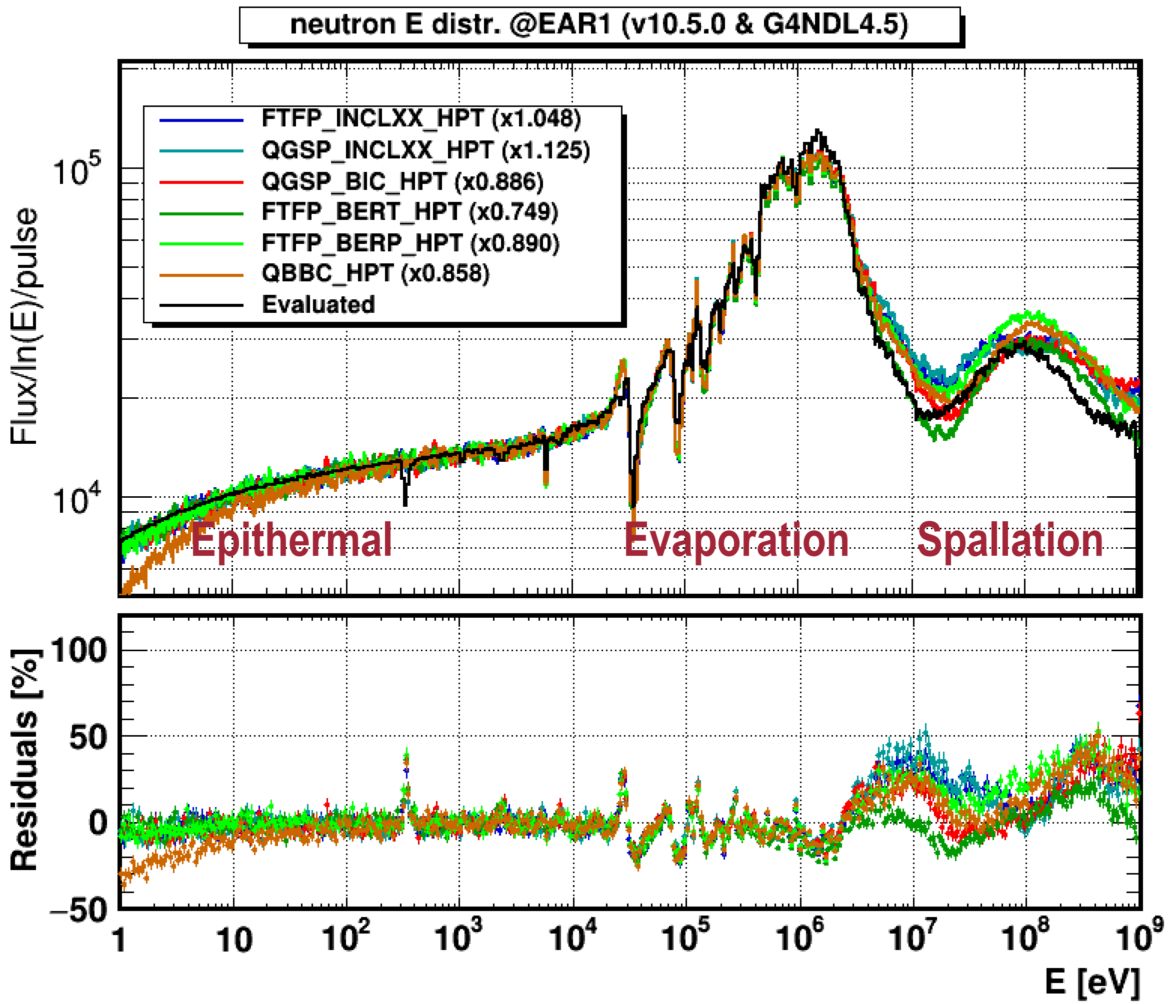
Neutron Energy Distribution @ EAR1 scorer

- G4NeutronHP + **G4NDL-4.5**, **ENDF/B-VIII.0** and **JEFF-3.3**
- All the neutron libraries **agree within 2%** in most of the energy range.
- **Largest differences (4%) in the dips** of the evaporation peak
- **Final choice for the simulations**: G4NDL-4.5



Results Geant4 v10.5.0:
Flux at EAR1

Neutron Energy Distribution @ EAR1 (v10.5.0)



Normalization factors calculated using flux integral in **1-10 keV**:

***_INCLXX_HPT** physics lists provide the best normalization factors

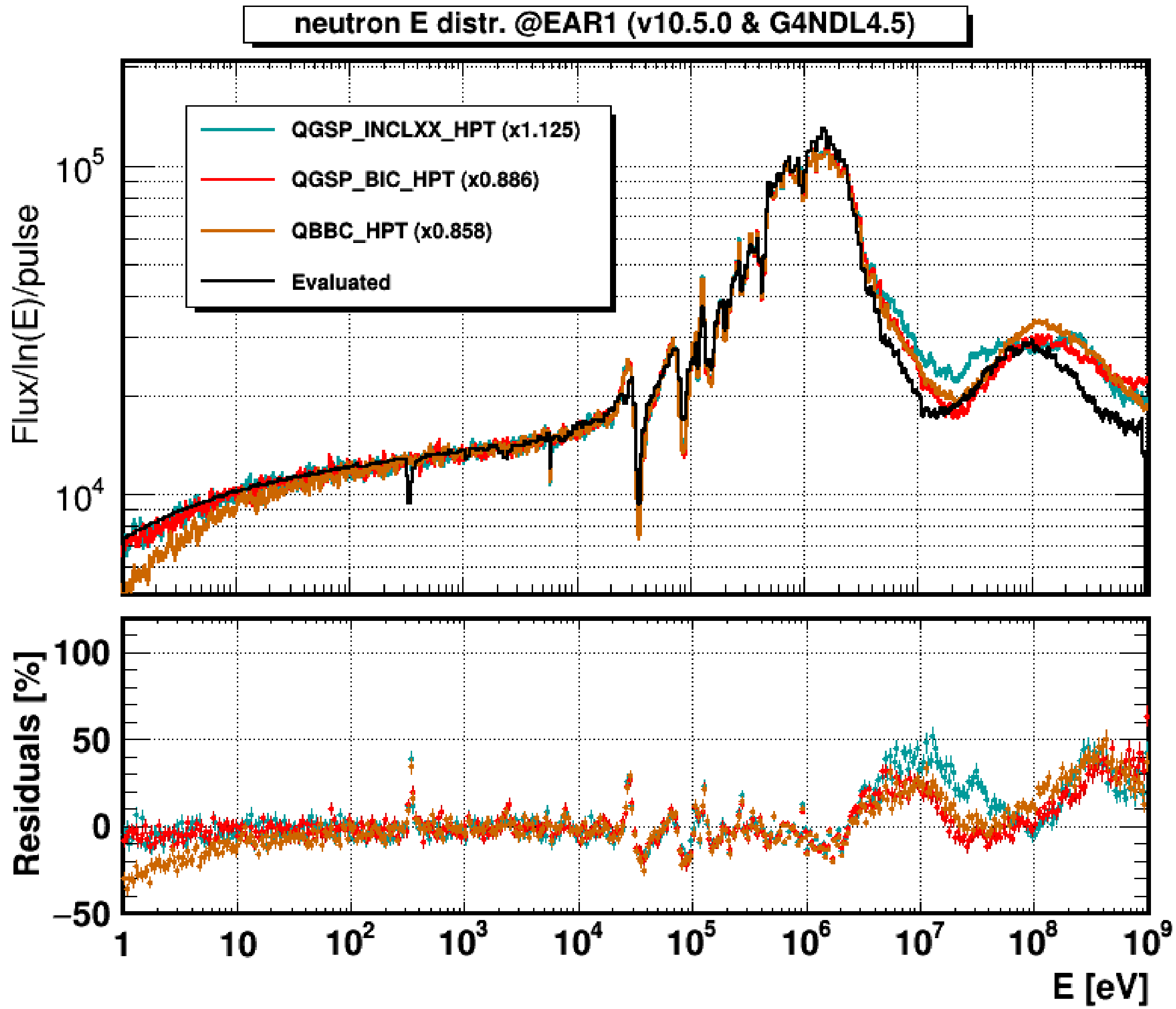
Once normalized: General overestimation above 5 MeV

FTFP_BERT_HPT follows better the **spallation** part of the spectrum

- **Absolute Deviations**: -12% (epithermal, QGSP_INCL) +60% (Spallation, FTFP_* & QBBC)

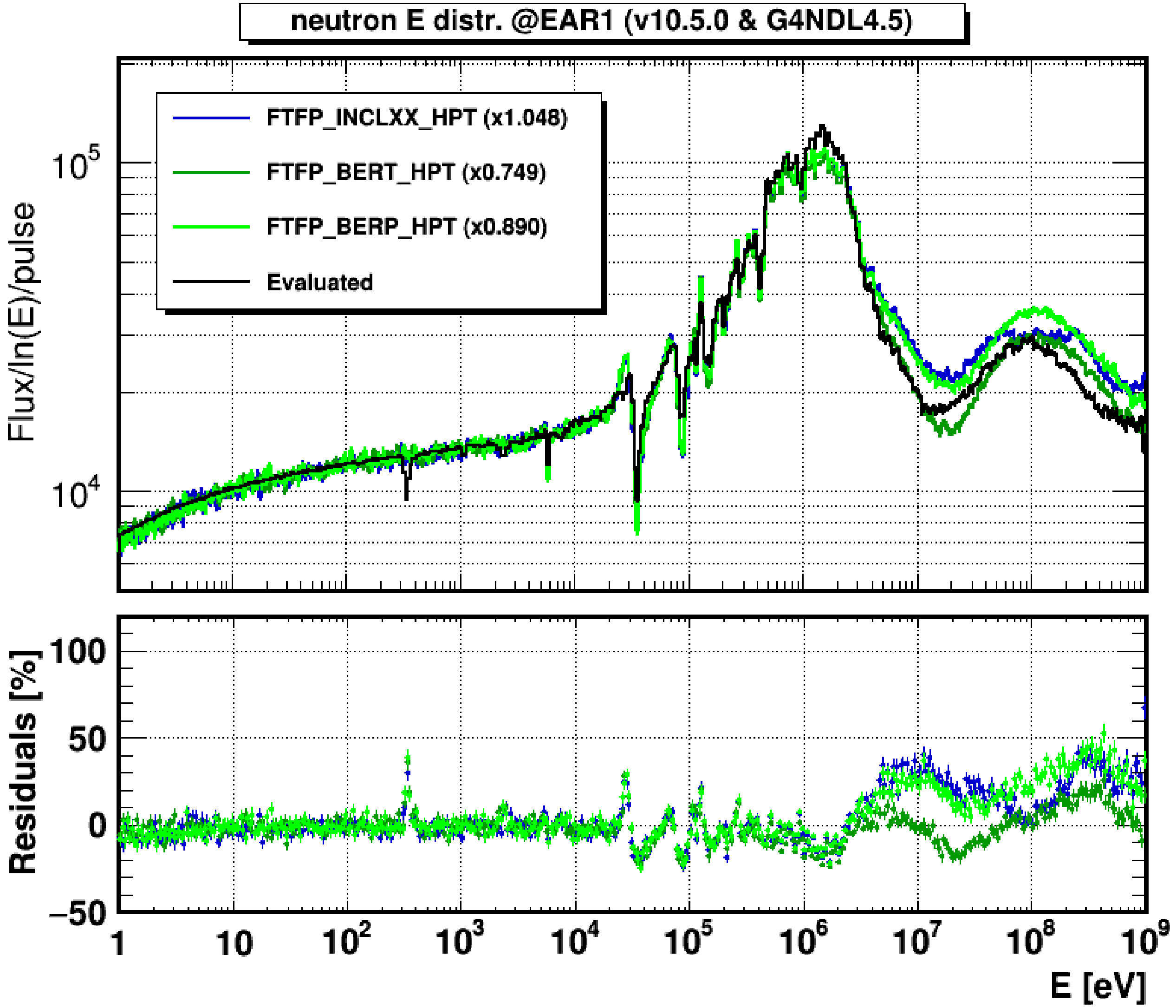
Neutron Energy Distribution @ EAR1 (v10.5.0)

- **QGS-based PLs:**
- **Best agreement** neutron flux: **INCLXX (1.12) and BIC (0.89)**
- **Largest overestimation** neutron flux: **QBBC**
- **QBBC (+HPT module)** does **not reproduce** the flux **below 100 eV**



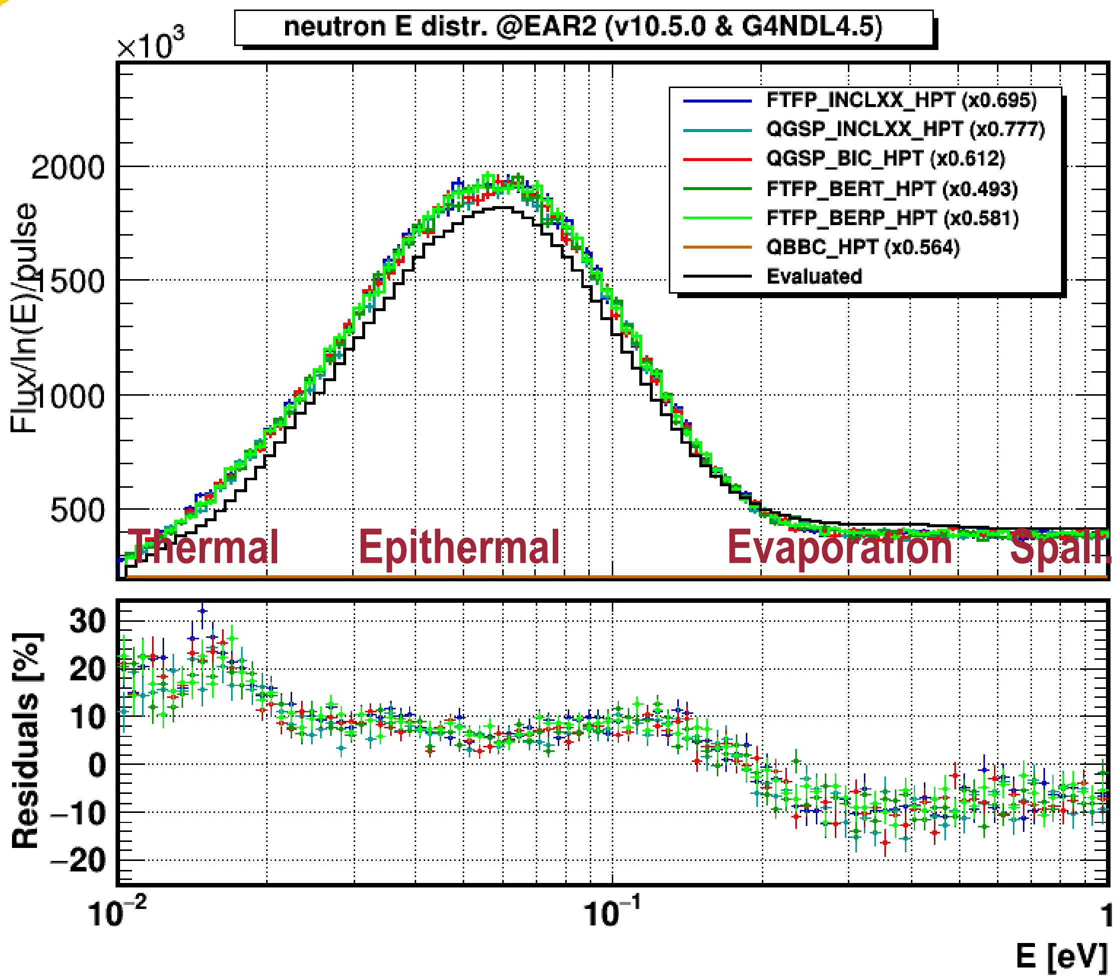
Neutron Energy Distribution @ EAR1 (v10.5.0)

- **FTFP-based PLs:**
- **Best agreement** neutron flux: **INCLXX (1.05)**
- **BERP closer to experimental** flux than **BERT**
- **But** in **spallation** region: **BERT better than BERP**



Results Geant4 v10.5.0: Flux at EAR2

Neutron Energy Distribution @ EAR2 (v10.5.0)



Normalization factors integral in **1-10 keV**:

EAR2: all PLs clearly overestimate flux but not in EAR1: Transport code, geometry or Geant4?

After normalizing to epithermal: evaporation and spallation underestimated

Thermal peak shape not well reproduced

Comparison between PLs similar to EAR1: Back-up

- **Absolute Deviations**: +120% (thermal, FTFP_BERT) -20% (Spallation,QGSP_BIC)

Results v10.2.2 vs v10.5.0

Geant4 v.10.5 vs 10.2.2: Qualitative

FTFP_BERT @ EAR1

QGSP_INCLXX @ EAR2

- **Normalization factors increase:**

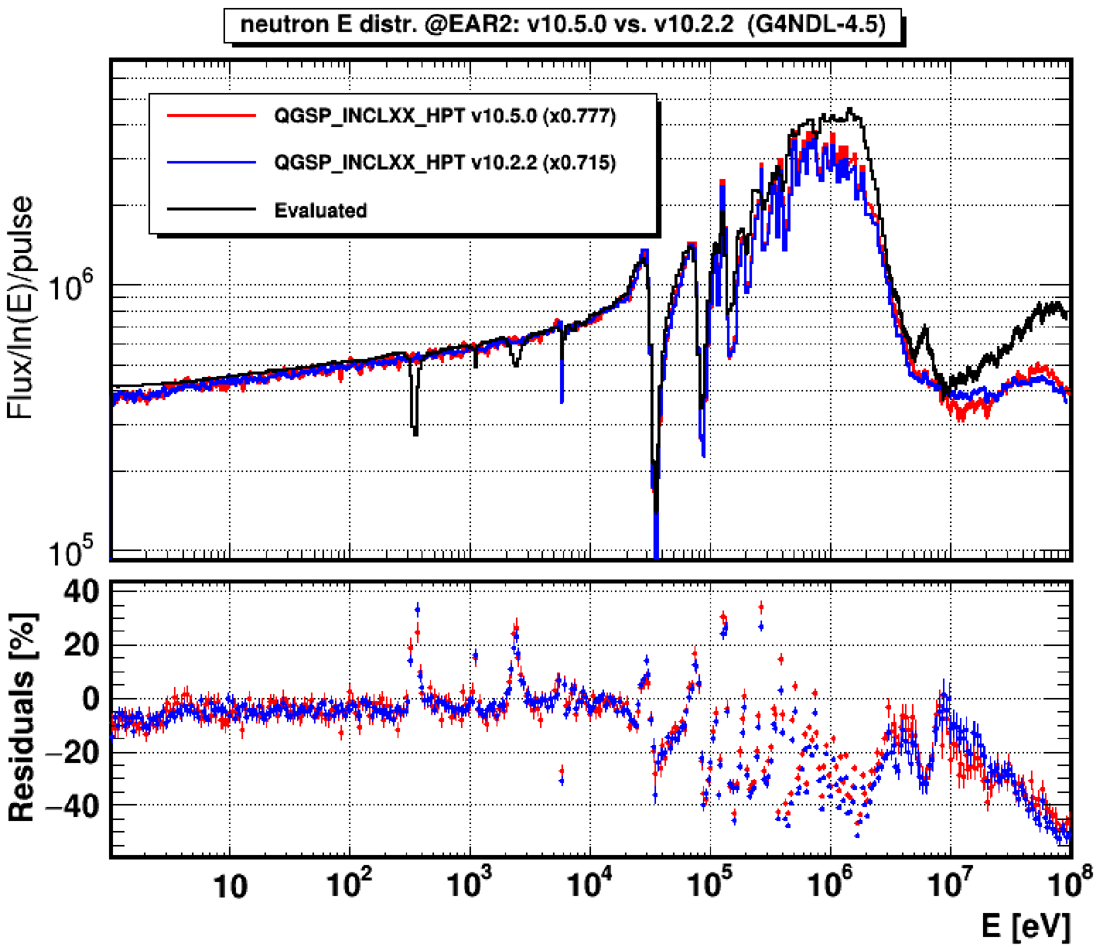
FTFP_BERT: 0.664 →0.749

QGPS_INCLXX: 0.715→0.777

- **Shape above 1 MeV presents changes:**

FTFP_BERT: Improves agreement in evaporation peak

QGPS_INCLXX: Slightly better agreement in spallation



Geant4 v.10.5 vs 10.2.2: Quantitative Change in normalization factors

Normalization factors: match the integral of experimental flux at **1-10 keV**

- **General trend:** Normalization factors increase → Closer to the experimental measurement
- Largest relative improvements: **FTFP_BERP** and **QBBC**
- Smallest change: **QGSP_INCLXX**
- **Remarkable difference** between the agreement in EAR1 and the overestimation in EAR2

EAR1			
Physics list	**v10.5.0**	**v10.2.2**	**Variation**
FTFP_INCLXX_HPT	1,048	0,950	10%
FTFP_BERT_HPT	0,749	0,664	13%
FTFP_BERP_HPT	0,890	0,755	18%
QGSP_INCLXX_HPT	1,125	1,033	9%
QGSP_BIC_HPT	0,886	0,788	12%
QBBC_HPT	0,858	0,713	20%

EAR2			
Physics list	**v10.5.0**	**v10.2.2**	**Variation**
FTFP_INCLXX_HPT	0,695	0,627	11%
FTFP_BERT_HPT	0,493	0,439	12%
FTFP_BERP_HPT	0,581	0,496	17%
QGSP_INCLXX_HPT	0,777	0,715	9%
QGSP_BIC_HPT	0,612	0,541	13%
QBBC_HPT	0,564	0,477	18%

Geant4 v.10.5 vs previous: CPU performance

- Extended to **v10.5.0** the preliminary comparison of the Ferrara 2016 Meeting **(M.A. Cortés-Giraldo)** between **v10.1.1** and **v10.2.2**

Physics List	V10.1.1	V10.2.2	V10.5.0
QBBC	45	40	40
FTFP_BERT	67	55	46
FTFP_INCLXX	233	230	330
QGSP_BIC_HPT	233	**540**	**192**
FTFP_BERT_HPT	278	**600**	**220**
FTFP_INCLXX_HPT	233	**465**	**208**

CPU time (min)
5000 protons

- Simulations with **G4NeutronHP** cutting neutrons En<1 eV + simplified material compositions
- Approximate average CPU time using typical total load of real simulations

- HP Neutron transport increases the CPU time in a factor 3-4 (exception FTPF_INCLXX)
- **V10.2.2:** Time penalty was reported for *_HP PLs in 2016 compared to previous versions.
- **v10.5.0**: PLs with HP similar or improved CPU times wrt **v10.1.1**

Summary and conclusions

Summary and conclusions

- The geometry of the **target assembly** has been **implemented as much detailed as possible** and neutrons have been transported and scored @ EAR1 & EAR2 pipes entrances.

- The **initial goals of this work** were to **benchmark** Geant4 with the evaluated flux of **EAR1** and then **extract relevant features of the new EAR2** beam.

- We have **updated the results with the latest Geant4 version (10.5.0) and confirmed that the performance of Geant4** to reproduce the neutron production has improved for al the studied PLs with respect to version v10.2.2:

- **FTFP_INCLXX_HPT** gives the best overall results in terms of neutron yield in EAR1: -4% and **QGSP_INCLXX_HPT** in EAR2: +23%.

- **After normalized to the measured flux in the 1-10 keV region, Geant4:**
  -Reproduces the energy spectrum shape below 1 MeV (some issues thermal peak)
  - Overestimates (in general) the high energy region @ EAR1, Best shape: **FTFP_BERT_HPT**
  - Underestimates by 20-50% the flux above 1MeV @ EAR2.

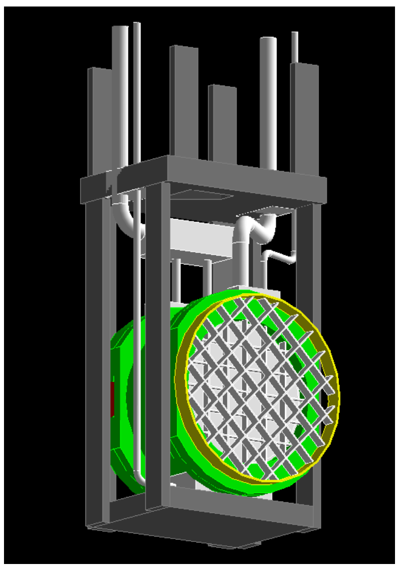
- **Large differences (of up to 40%) are found between the PLs**, following similar trends in neutron production in both experimental areas.

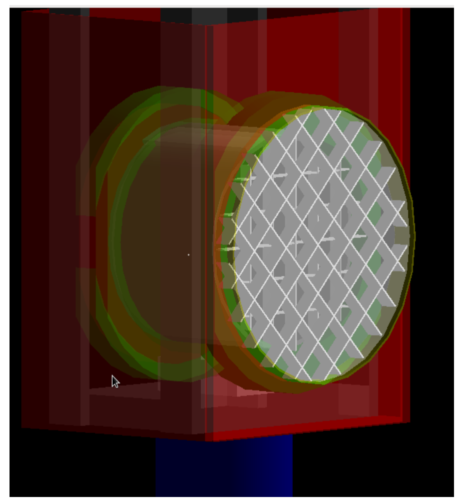
Strengths and limitations of Geant4 in this work

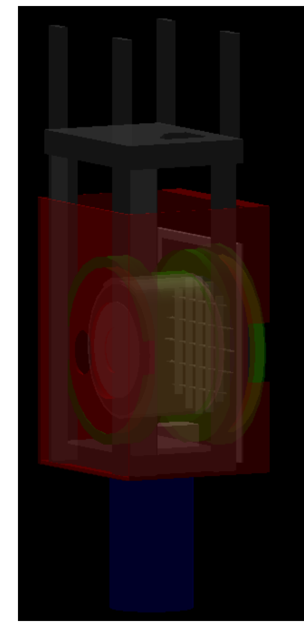
- **Strengths/advantages:**
  - After G4NeutronHP: Geant4 is capable of simulating low E neutrons considering nuclear data libraries
  - Flexible choice of high-energy hadronic models (PLs) for each application
  - Information can be extracted at any step of the simulation (e.g. particles involved in neutron/gamma production) and coupled to ROOT
  - PL improve agreement with experimental neutron flux in latest version

- **Limitations:**
  - Large deviations between PL → Choice of PL critical for similar applications
  - None of the PLs reproduces epithermal flux + shape of high energy region
  - Still "slow" computation with G4NeutronHP (G4ParticleHP)
  - Deviations for EAR1 and EAR2 not comparable → Related to Geant4?
  - Shape of thermal peak not perfectly reproduced: Thermal scattering?
  - Suggestion: Manual for G4NeutronHP and G4PHP environment variables

¡Gracias por su atención!





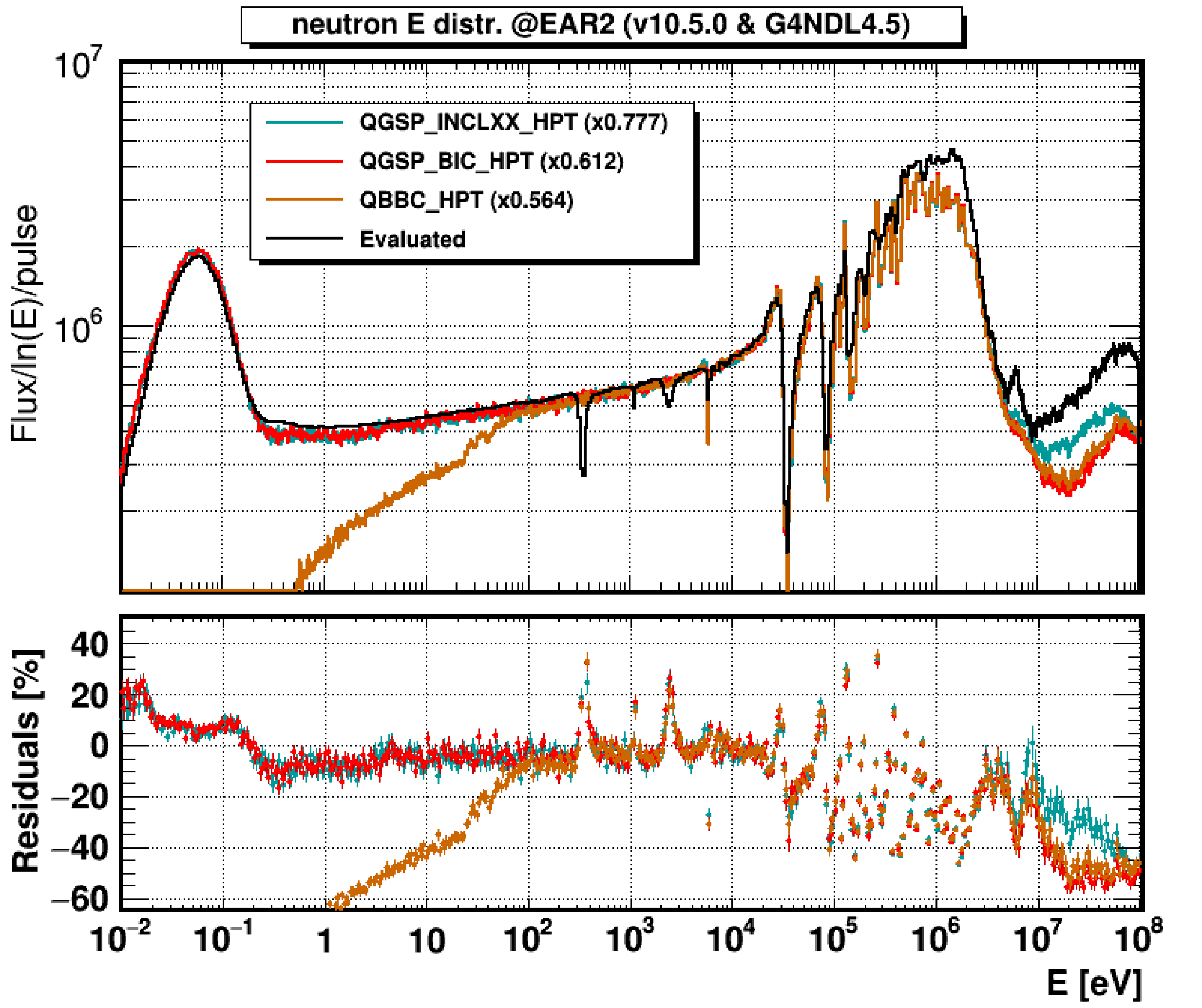


Thanks for your attention!

Backup slides

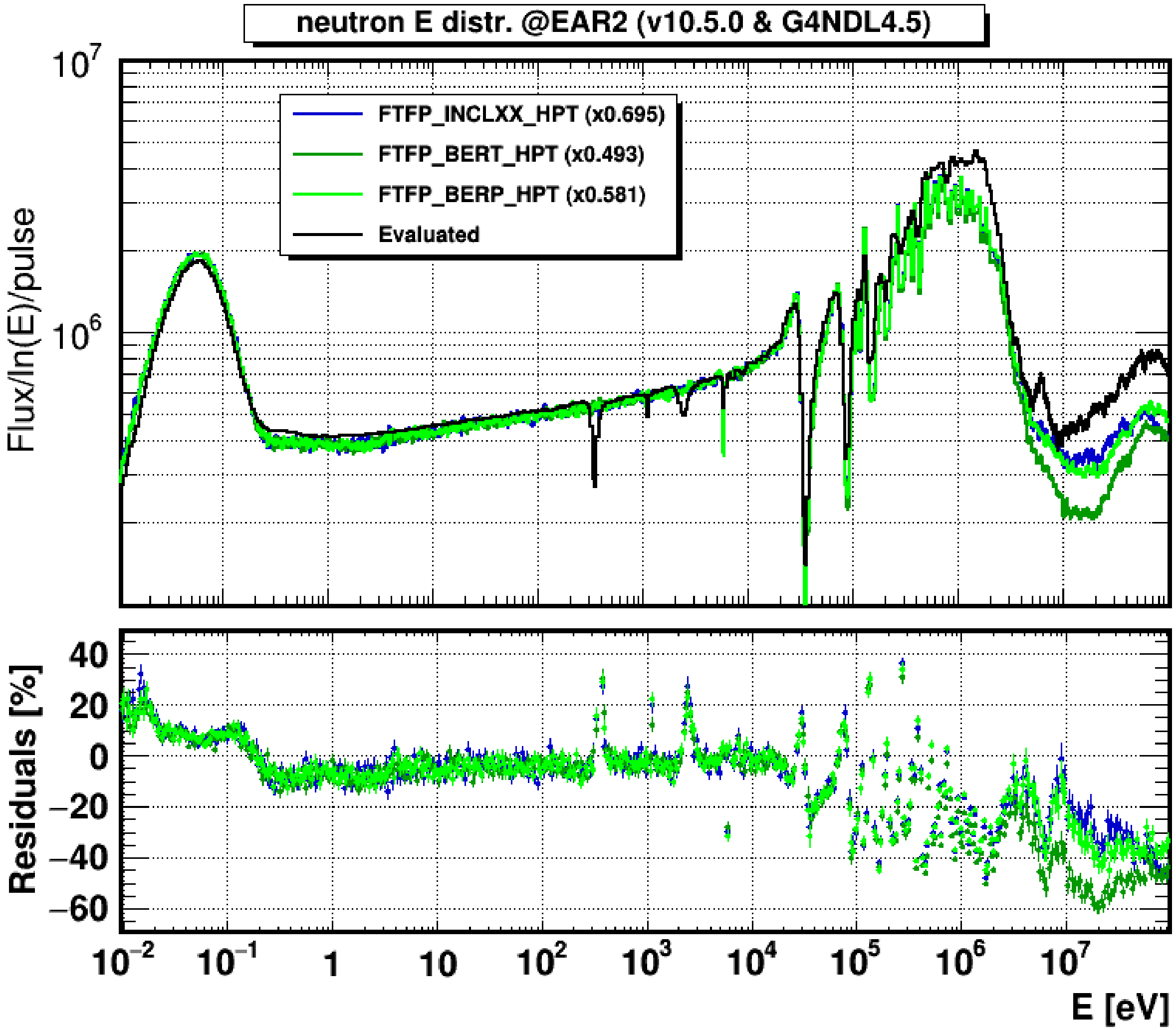
Neutron Energy Distribution @ EAR2 (v10.5.0)

- **QGS-based PLs:**
  - **Closest** to experiment **INCLXX (0.77) & largest overestimation** neutron flux: **QBBC (0.56)**
  - **QBBC (+HPT module)** does **not reproduce** the flux **below 100 eV**
  - **QBBC** and **BIC** largest **underestimation 10-100 MeV** region



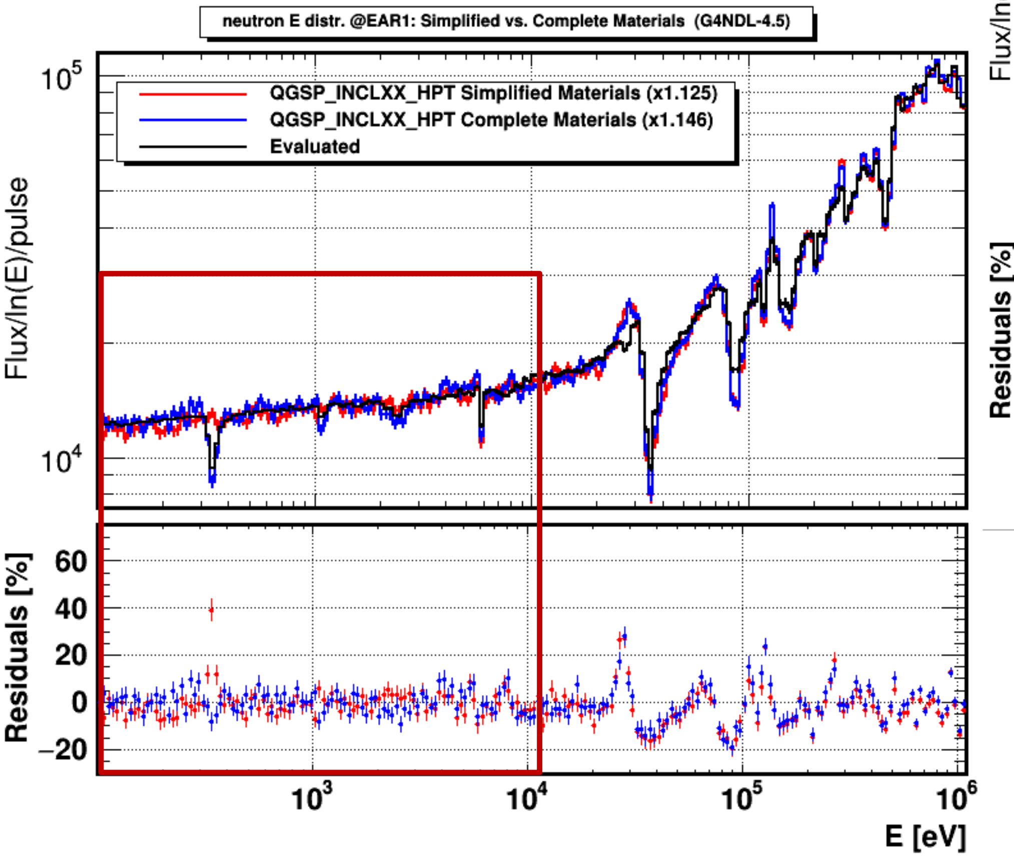
Neutron Energy Distribution @ EAR2 (v10.5.0)

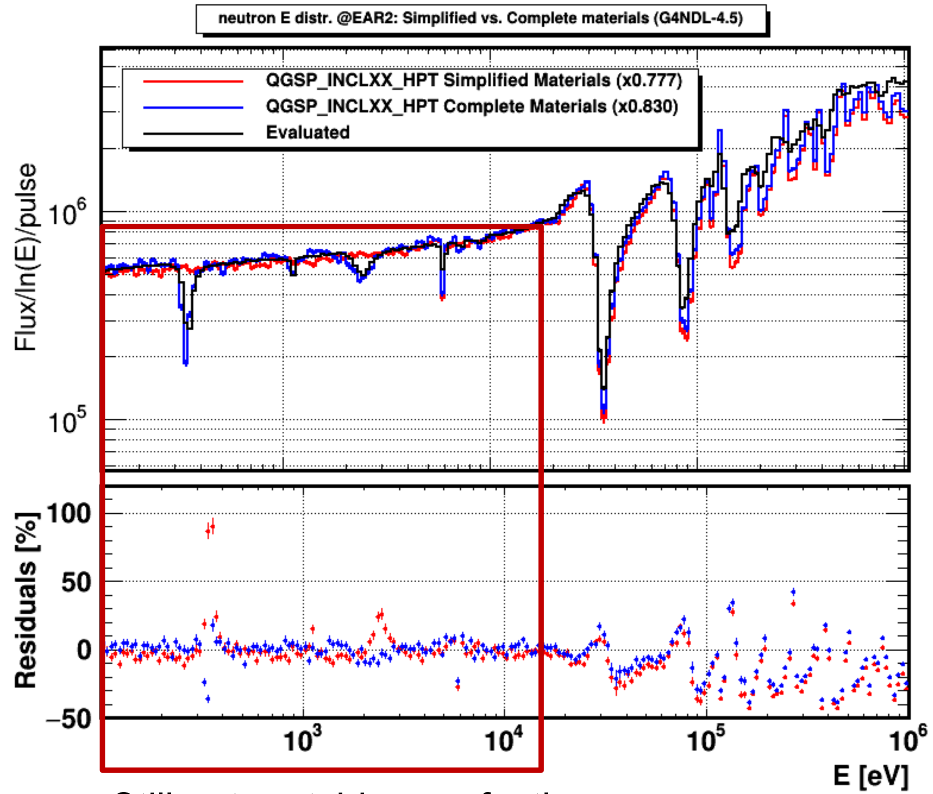
- **FTFP-based PLs:**
  - **Best agreement neutron flux: INCLXX (0.70)**
  - **Neutron flux overestimation significantly reduced in BERP wrt BERT**
  - **Largest underestimation in the spallation** relative to epithermal: **BERT**



Simulations with complete materials: QGSP_INCLXX_HPT

- Simplified materials to speed-up neutron transport (40-50% speed penalty)
- Elements Al alloys missing → DIPS

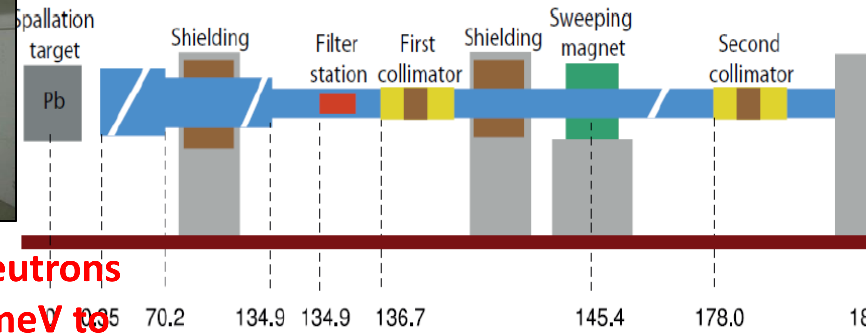


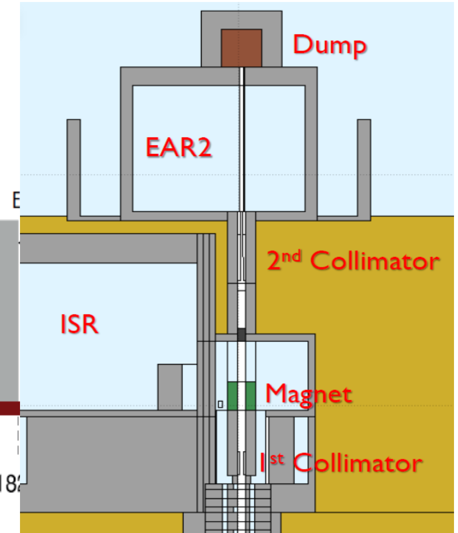


- Still not matching perfectly:
- Doppler broadening neglected (x2-2.5 speed penalty)
- Evaluated flux uncertain (~5%) at dips

n_TOF: neutron source and beamlines

BEAM LINE EAR1

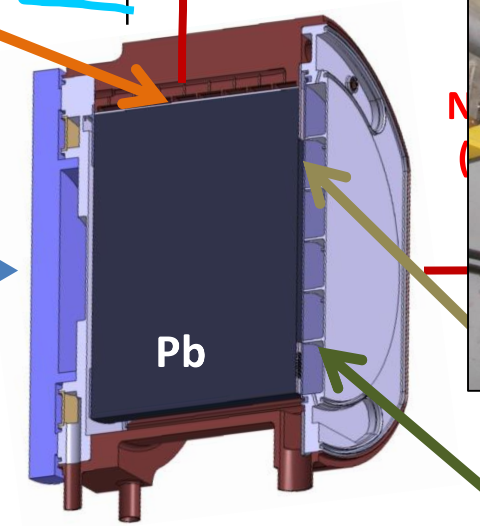




Neutrons (meV to ~100 MeV)

1+3 cm cooling & moderator (water)

PS Protons (20 GeV/c)



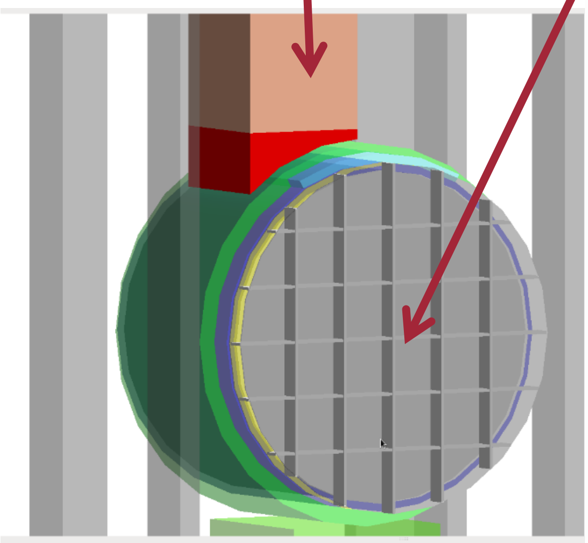
1 cm cooling (water)

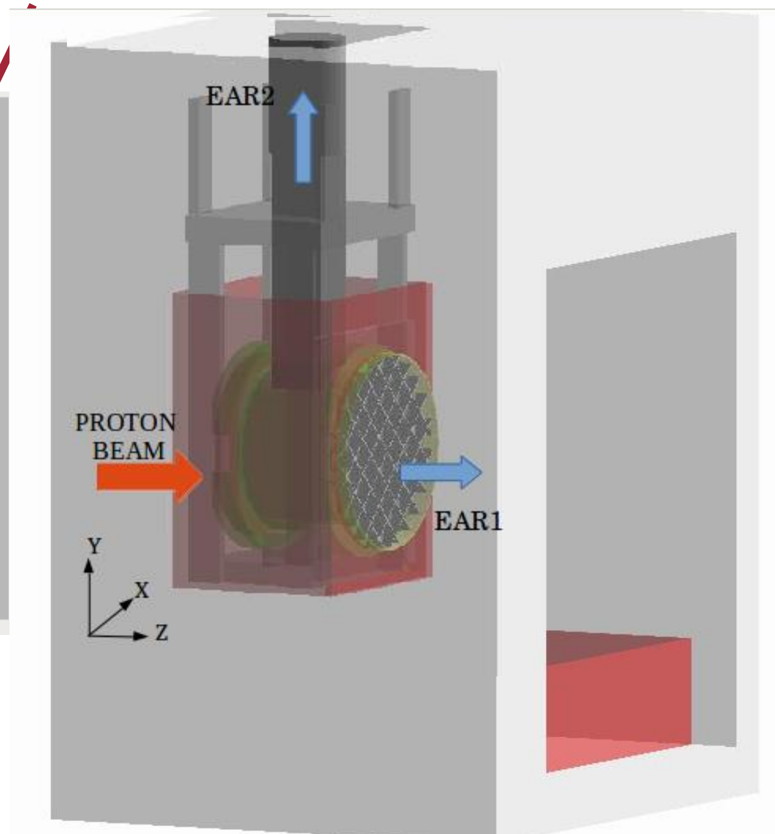
4 cm moderator (borated water)

Better Energy Resolution

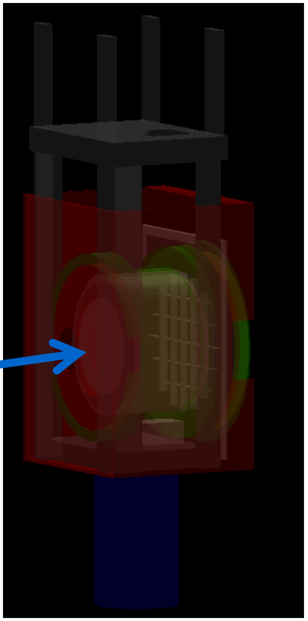
Geometry Model - Details

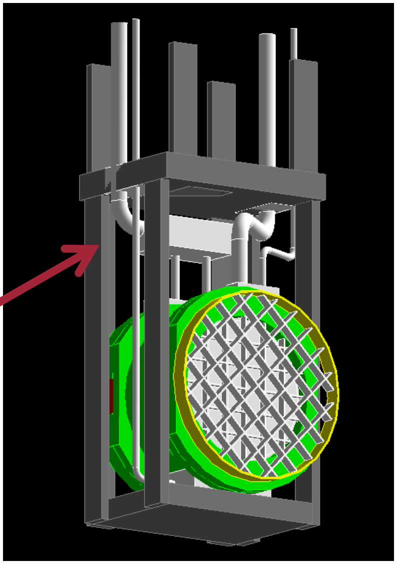
Exit toward EAR2 and Moderator layer with aluminum Support grid





Proton beam



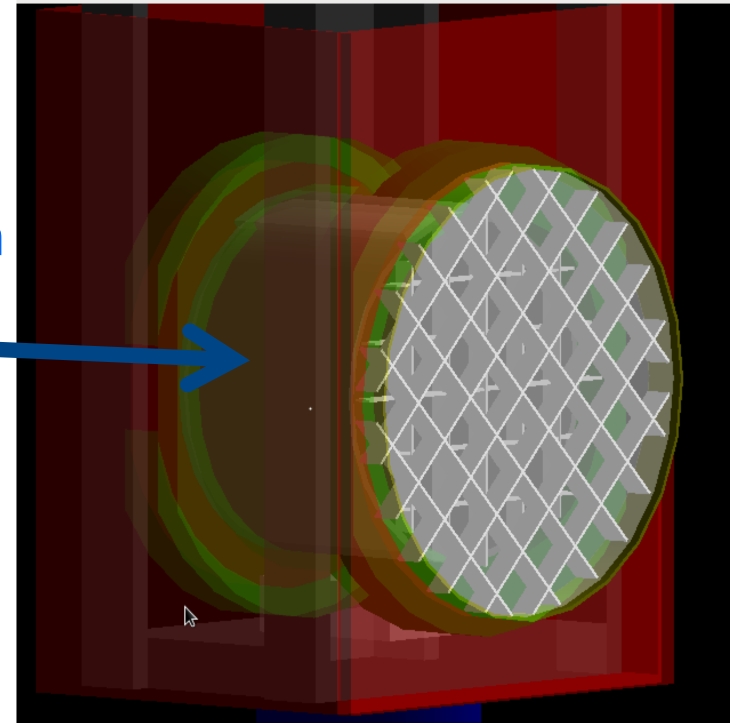


Target support structures, concrete container, cooling circuits,

Geometry Model – Details

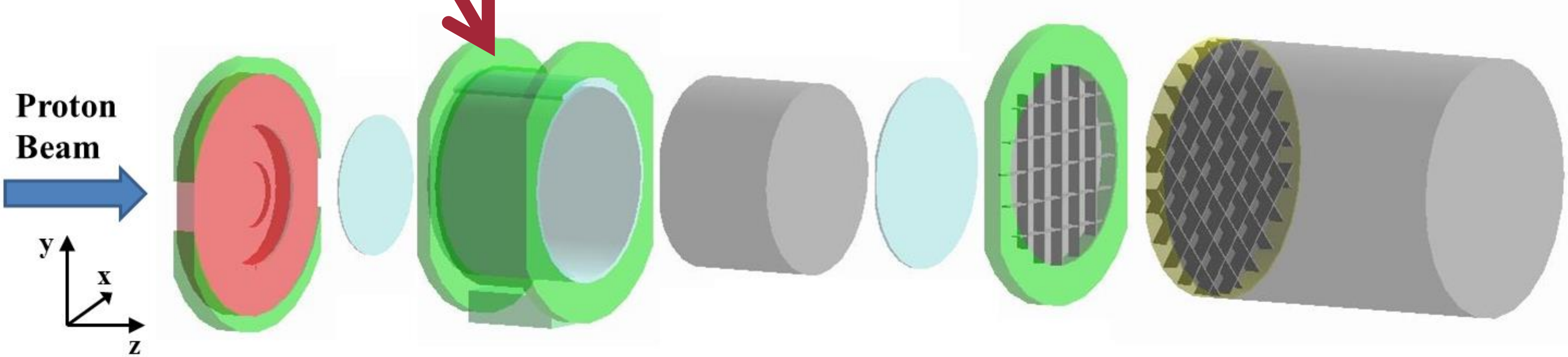
Lead Target with surrounding vessel and structural support (Al-alloys)

Proton Beam



Inner components target assembly:

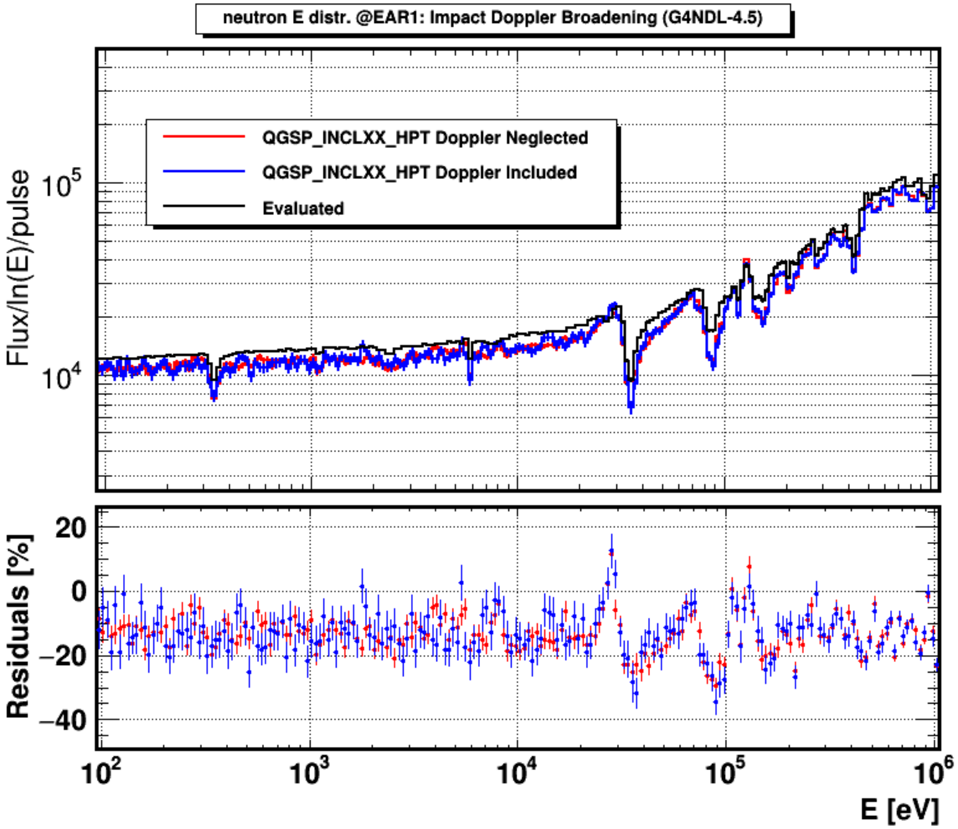
Proton entrance window + vessel+
Lead Core + Moderator/absorber +
neutron exit window + beam line entrance(grid turned 45º)

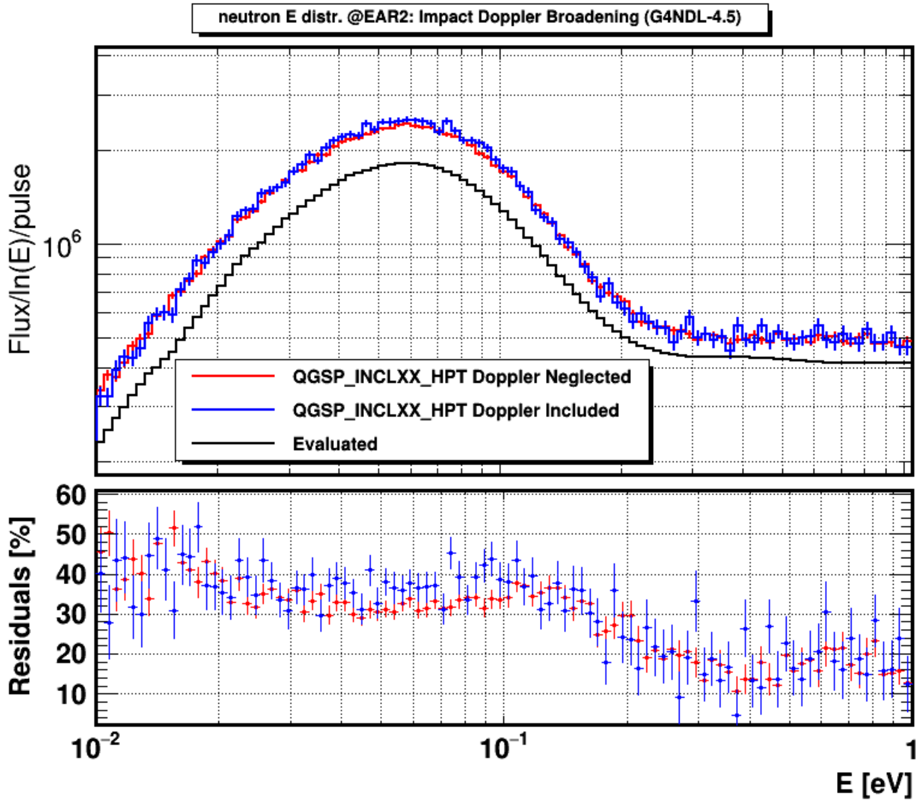


nTOF Geant 4

Impact of the Doppler broadening: QGSP_INCLXX_HPT

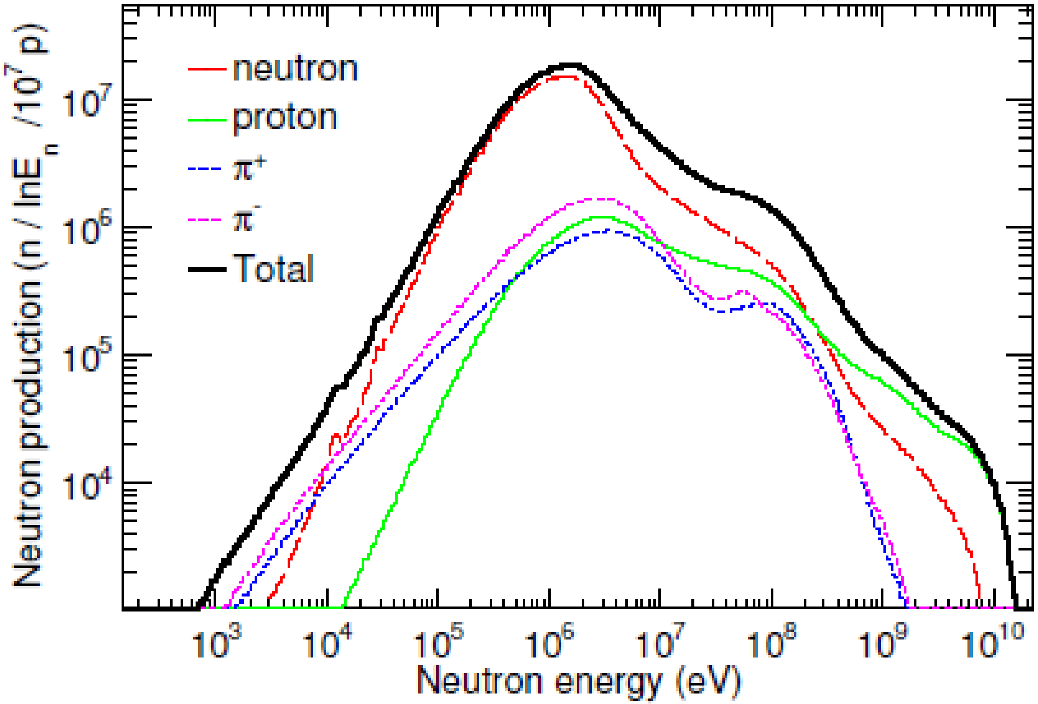
Dips EAR1





Thermal Peak EAR2

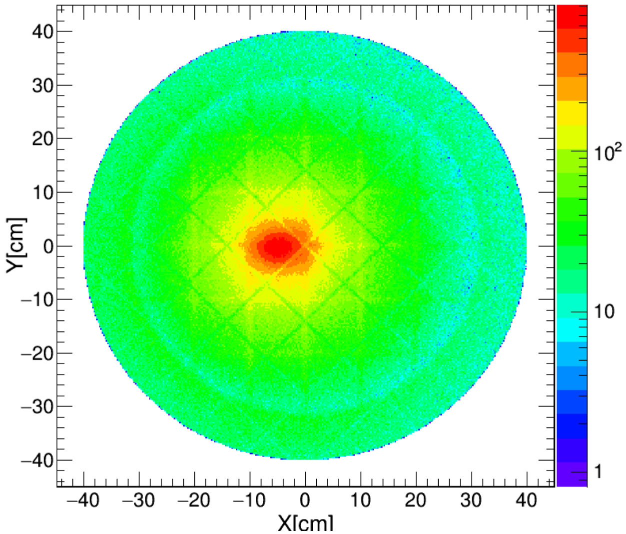
Study of the neutron production

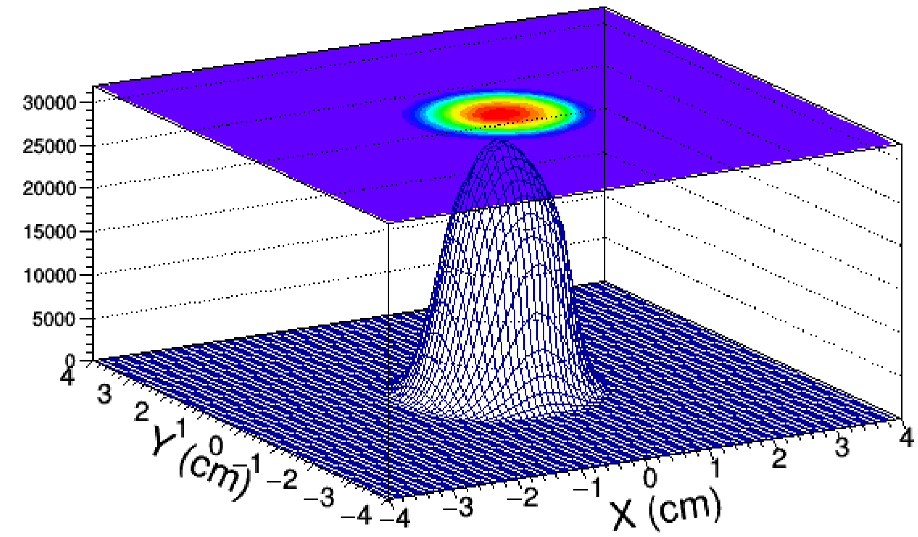


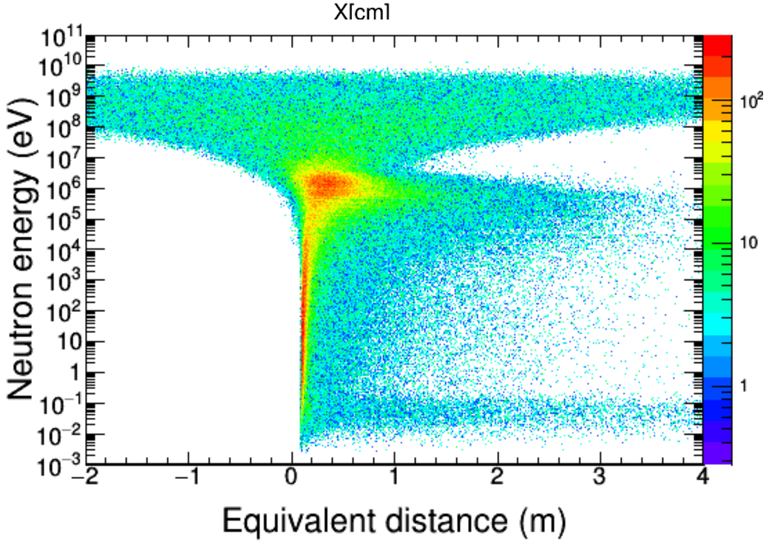
Non-moderated spectrum of neutrons produced in Pb target

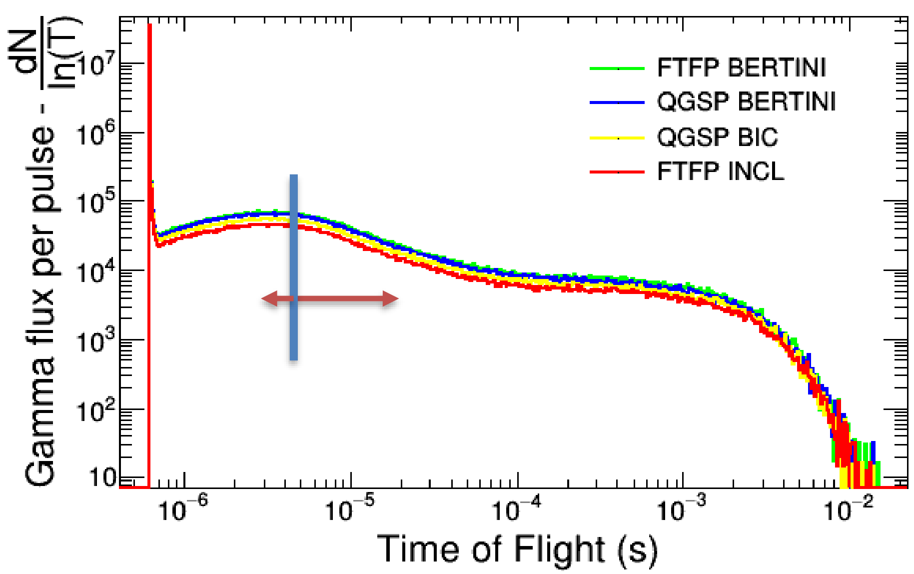
nTOF Geant 4

Additional characteristics of the beam

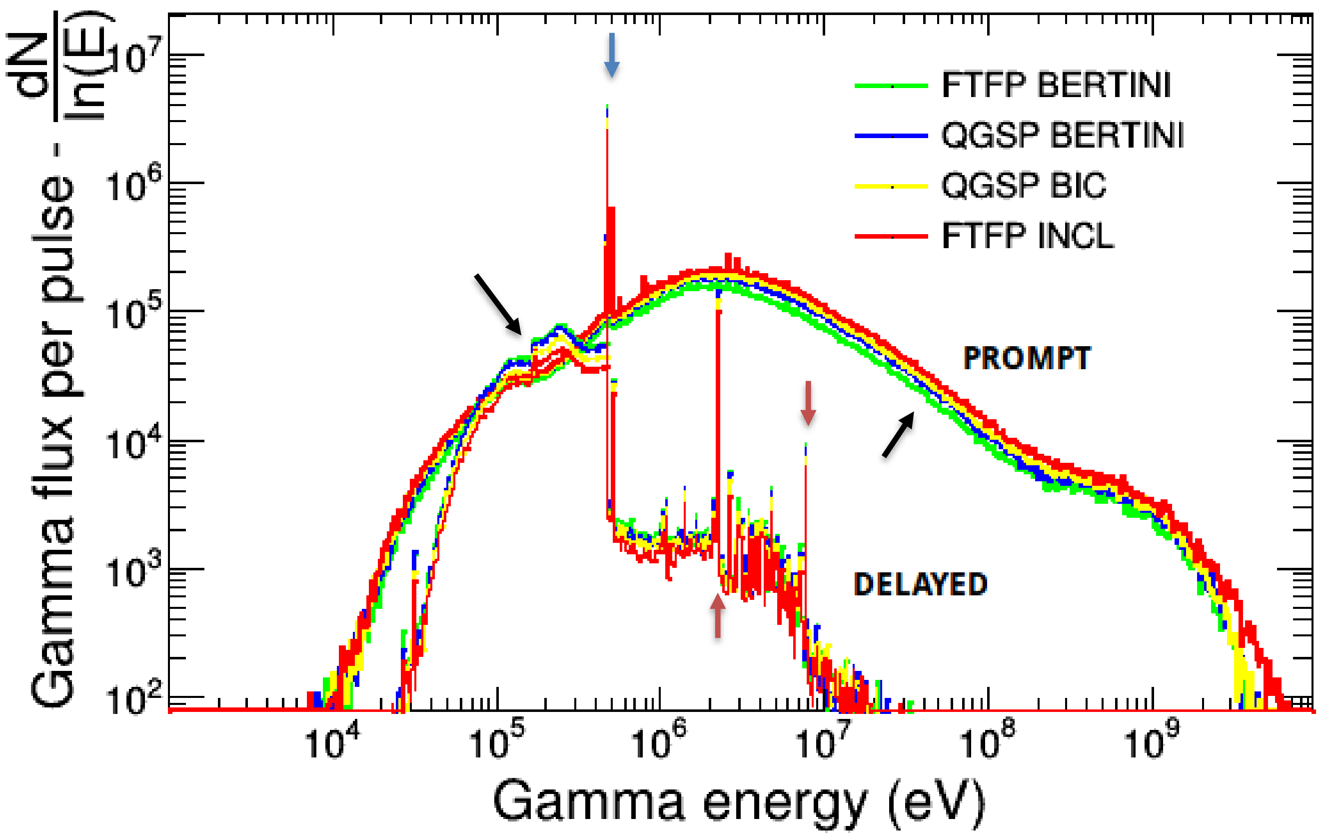








Gamma Energy Distribution @ EAR1



- **Prompt gammas:** Mainly decay of pi_0(and succesive EM cascade→**511keV**).
  - **Anticorrelation gamma-neutron** production for all PL's
- **Delayed:** Moderated neutron capture:**B10 (478keV), H(2.2MeV), Al-27(7.4MeV)**
  - Production of **delayed gammas** follows the **neutron yield** for all PL's

nTOF Geant 4

EAR1 Scorer

Neutron Energy Distribution

(FTFP_INCLXX_HPT,v10.0.3 vs 10.1.1)