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

J. Lerendegui-Marco, Miguel A. Cortés-Giraldo, J. M. Quesada, C. Guerrero

Universidad de Sevilla (Seville, Spain)

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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 ($\Delta E/E @1\text{keV} : \approx 3 \cdot 10^{-4}$)
  - EAR2 (20m): High flux (~$7.5 \cdot 10^6 \text{n/cm}^2/\text{pulse}$)

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

- Diagram: EAR2: 40x higher neutron flux, EAR1: better energy resolution
Pb Spallation Target – Technical Details

- **EAR1**: 1cm Water + 4cm Borated Water (1.28% of H$_3$BO$_3$) before beam pipe.

- **EAR2**: “triangular” shape entrance to beam line. NO Boron, just water.
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

- **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
- 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)

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

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

- 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/
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. Elastic Thermal Scattering (\(E_n < 4 \text{ eV}\)) 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)

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

Upcoming results: PLs will omit the _HPT: (Neutron HP below 20MeV + Thermal Scattering below 4eV)
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)
- **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**
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

- Normalization factors increase:
  - **FTFP_BERT**: 0.664 → 0.749
  - **QGSP_INCLXX**: 0.715 → 0.777

- Shape above 1 MeV presents changes:
  - **FTFP_BERT**: Improves agreement in evaporation peak
  - **QGSP_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
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

<table>
<thead>
<tr>
<th>Physics List</th>
<th>V10.1.1</th>
<th>V10.2.2</th>
<th>V10.5.0</th>
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<tr>
<td>QBBC</td>
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<td>FTFP_BERT_HPT</td>
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<tr>
<td>FTFP_INCLXX_HPT</td>
<td>233</td>
<td>465</td>
<td>208</td>
</tr>
</tbody>
</table>

- 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 FTFP_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

CPU time (min) 5000 protons
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 all 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

Neutrons (meV to GeV)

PS Protons (20 GeV/c)

BEAM LINE EAR1

Better Energy Resolution

Higher Neutron Flux

Neutrons (meV to ~100 MeV)

1+3 cm cooling & moderator (water)

1 cm cooling (water)

4 cm moderator (borated water)
Exit toward EAR2 and Moderator layer with aluminum Support grid

Target support structures, concrete container, cooling circuits,
Geometry Model – Details

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

Inner components target assembly:
- Proton entrance window + vessel +
- Lead Core + Moderator/absorber +
- Neutron exit window + beam line entrance (grid turned 45°)
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
Additional characteristics of the beam
- **Prompt gammas:** Mainly decay of $\pi_0$ (and successive EM cascade $\rightarrow 511$keV).
  - Anticorrelation gamma-neutron production for all PL’s
- **Delayed:** Moderated neutron capture: $\text{B10 (478keV), H(2.2MeV), Al-27(7.4MeV)}$
  - Production of delayed gammas follows the neutron yield for all PL’s
EAR1 Scorer

Neutron Energy Distribution
(FTFP_INCLXX_HPT,v10.0.3 vs 10.1.1)
EAR1SD neutron Kinetic Energy

Counts

\[ \begin{align*}
\text{v10.0.3} \\
\text{v10.1.1}
\end{align*} \]

\[ \begin{align*}
10^3 & \quad 10^4 \\
10^2 & \quad 10^3 \\
10^{-1} & \quad 10^0 \\
10^{-2} & \quad 10^{-1} \\
E [\text{eV}] & \quad 10^0 \\
\end{align*} \]