

New Thermal Scattering Libraries in Geant4

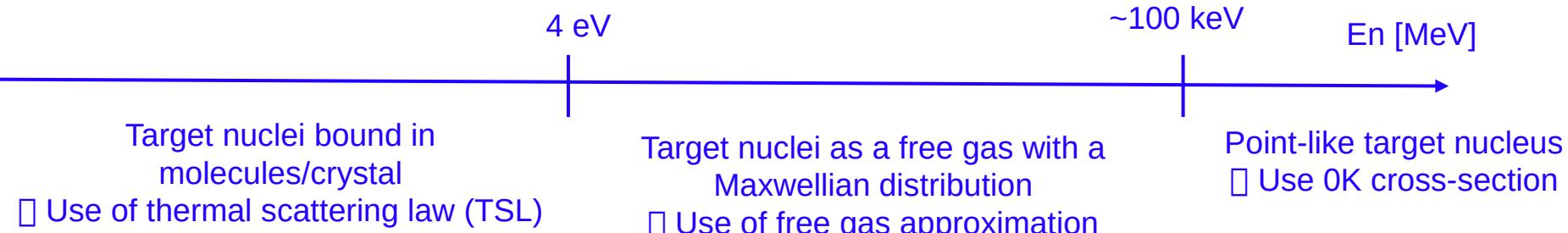
Low Precision and High Precision modes

L. Thulliez, E. Dumonteil
(CEA-Saclay/Irfu/DPhN)

(29/09/2022)

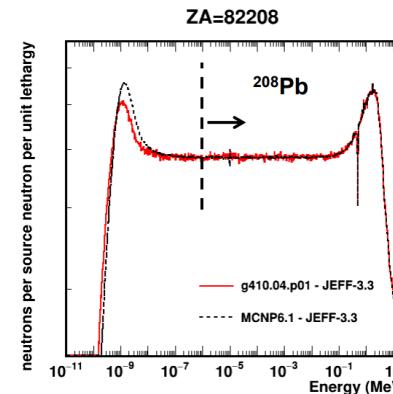
Neutron-HP package used to transport low energy neutrons $E_n < 20$ MeV

- What are the different «models» used to describe the neutron/target interaction?



TSL not updated since ENDF-BVII.1

- How to study moderators and cold moderators with updated and new materials from ENDF-BVIII.0 and JEFF-3.3?



Talk from E. Mendoza Geant4 Hadronic meeting Feb. 2020

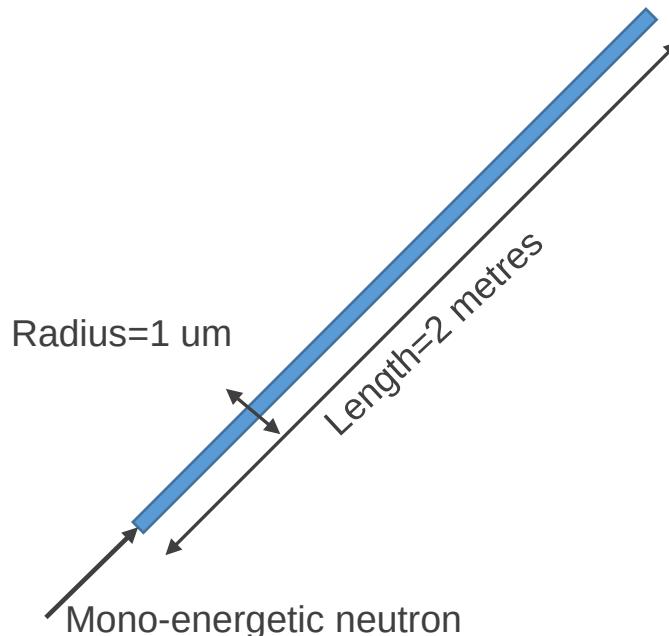
- New TSL processing code ?
- Discrepancies between ref. codes of ~20%

- Free gas approximation implemented in Geant4 has trouble to reproduce MCNP (ref. code) below 1 eV
- Problem in the algorithm?

Two benchmarks are used to compare Geant4 and Tripoli4 results

Microscopic benchmark

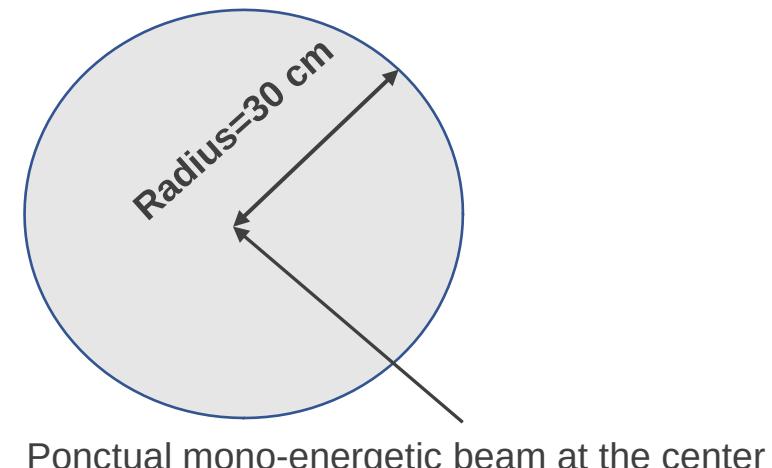
Goal: assessing collision kinematic
One collision geometry



Observables:
Outgoing neutron energy and angle

Macroscopic benchmark

Goal: probing slowing-down and thermalization process



Observables:
Cell flux in the sphere 3

How to compute Doppler broaden cross-section and outgoing particle properties?

→ Threshold, capture reactions : no need to know the target velocity

□ Elastic scattering : need to compute the reaction kinematics, the target velocity

* In Geant4 velocity sampling in Maxwellian distribution NOT preserving the thermal-averaged cross-section – from our understanding?

□ Sampling of the Velocity of the Target (SVT) method

Equation preserving the thermal averaged XS:

$$v_n \bar{\sigma}(v_n, T) = \int d\vec{v}_T \sigma(v_r) \mathcal{M}(\vec{v}_T)$$

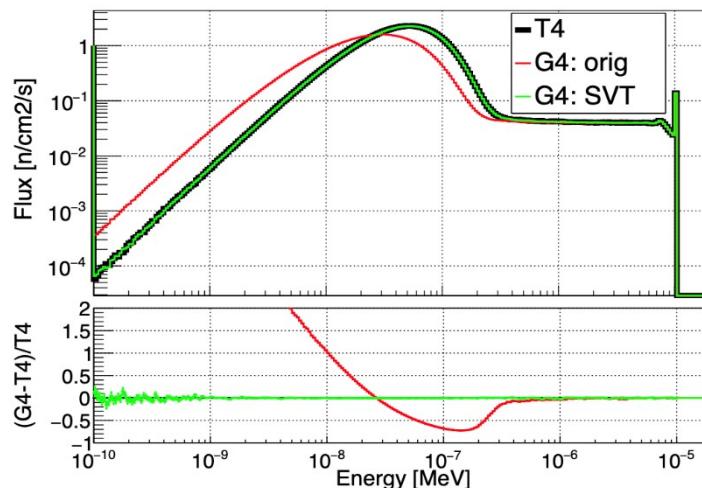
Neutron velocity Thermal averaged cross-section at T Target velocity Neutron/target relative velocity
 Maxwellian distribution OK cross-section

Joint probability distribution:

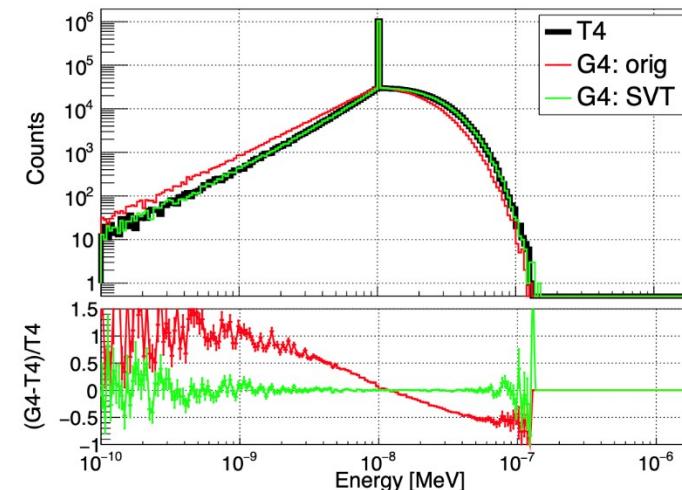
Joint probability distribution:

- 1/ Sampling v_T in (B)
- 2/ Sampling $\mu (= \cos(\theta))$ uniformly
- 3/ Accept the pair (v_T, μ) according to (A)
 □ If not accepted go to step 1/

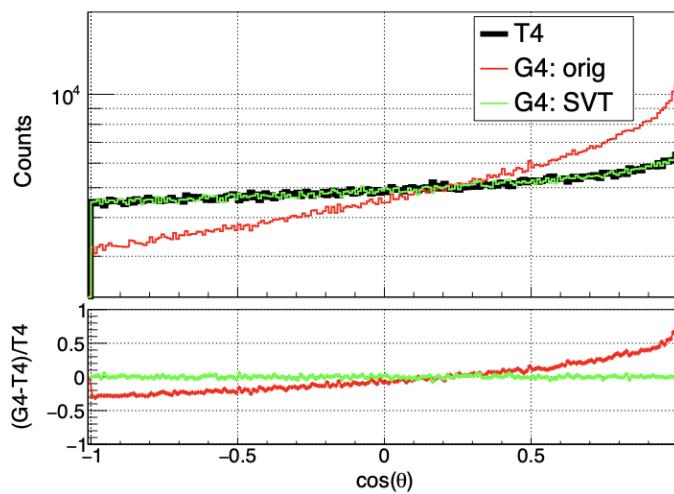
$$p(v_T, \mu) \propto \underbrace{\frac{\sqrt{v_n^2 + v_T^2 - 2v_n v_T \mu}}{v_n + v_T}}_{(A)} \underbrace{(v_n + v_T) \beta^3 v_T^2 e^{-\beta^2 v_T^2}}_{(B)}$$

*Sphere benchmark*

12C – free gas approximation – ENDF-BVII.1

*Thin cylinder benchmark / energy*

12C – free gas approximation – ENDF-BVII.1

*Thin cylinder benchmark / $\cos(\theta)$*

12C – free gas approximation – ENDF-BVII.1

- The SVT method has been implemented in `G4Nucleus::GetBiasedThermalNucleus` (hyp: constant cross-section at these energy)
- Now discrepancies between Tripoli4 and Geant4 less than 1%
- In the futur: need to implement the DBRC algorithm to take into account low energy resonance for heavy nuclei

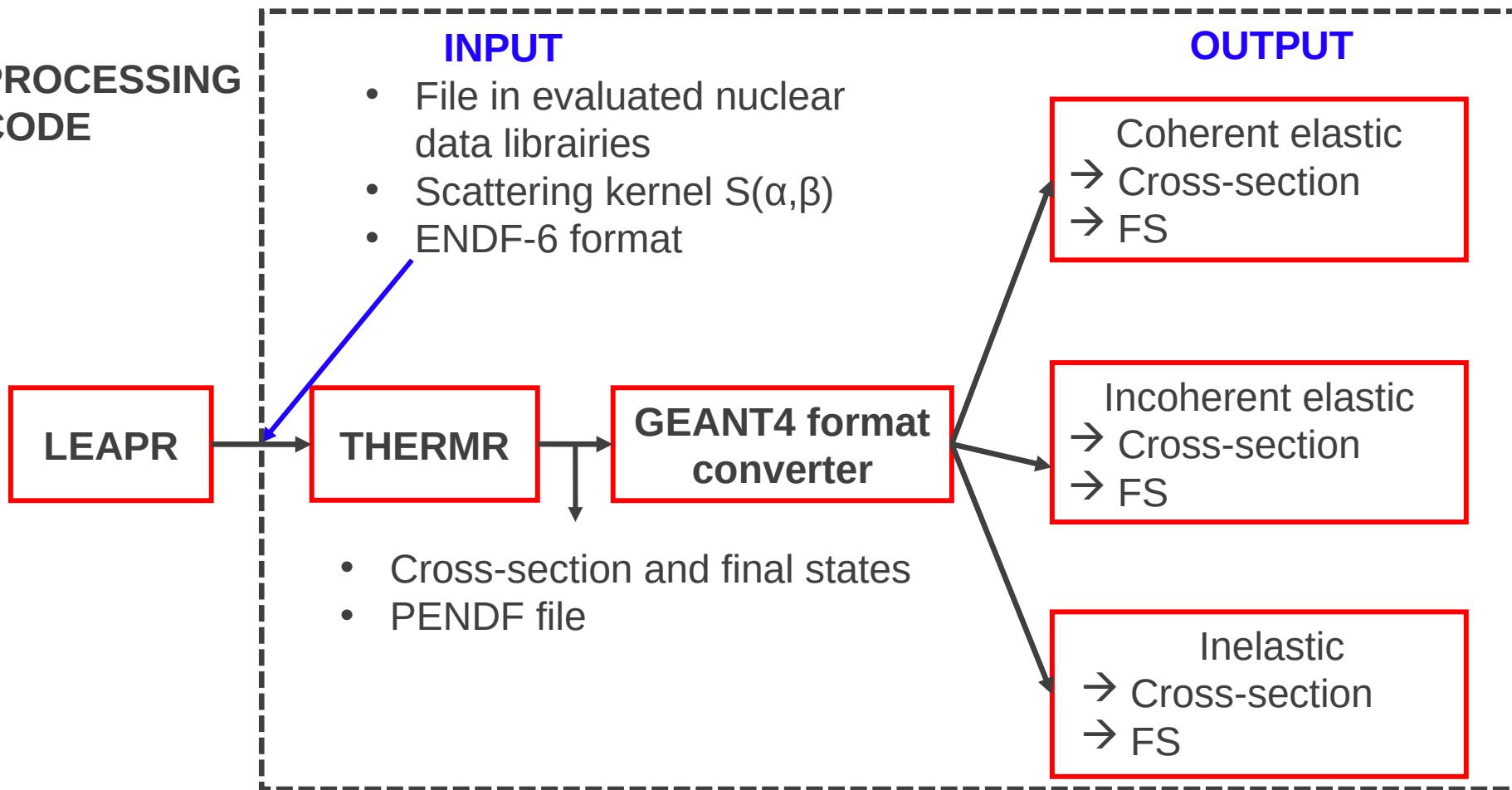
Objectives:

- 1/ Add new TSL from ENDF-BVIII.0 and JEFF-3.3 in Geant4 to study updated and new materials compared to ENDF-BVII.1 (2011)
- 2/ Take into account Hartling et al. recommendations regarding the TSL data processing

(Hartling et al. The effects of nuclear data library processing on Geant4 and MCNP simulations of the thermal neutron scattering law NIMA 891:25-31,5, 2018)

→ Need a new processing code

- 3/ Correct some discrepancies between Geant4 and reference codes.
 Modify the Geant4 regarding TSL data treatment

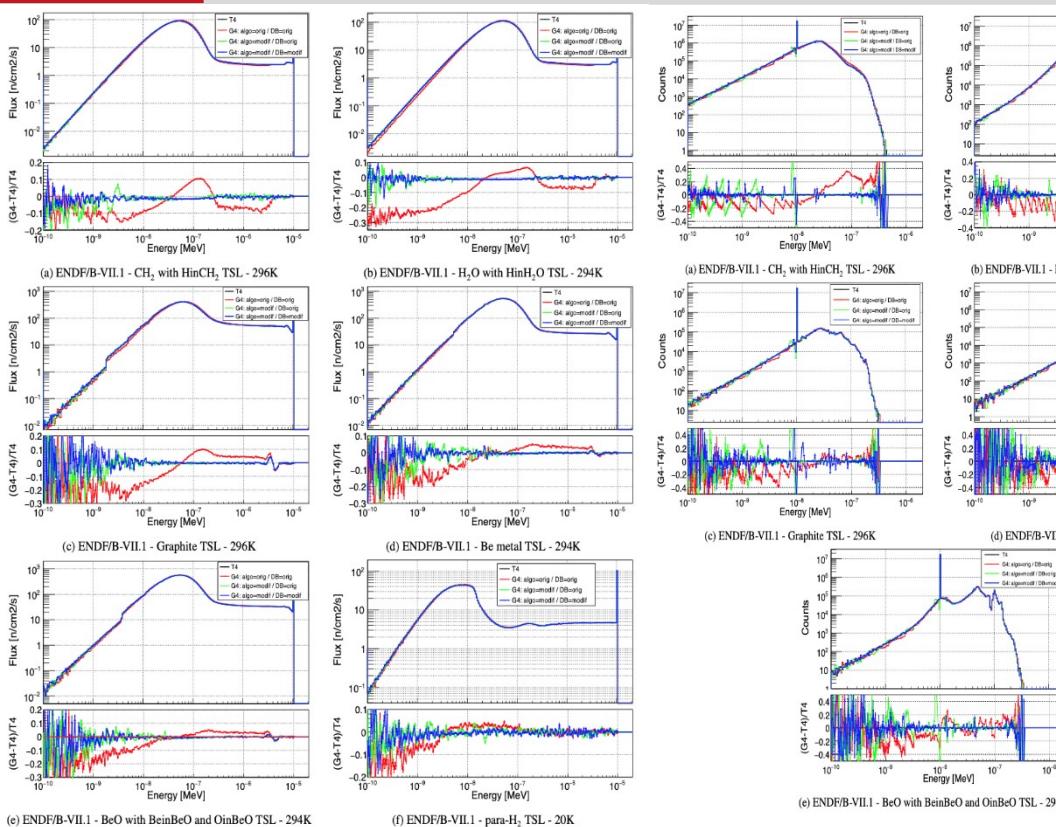
PROCESSING
CODE

THERMR parameters [Hartling et al.]:

- * Tolerance parameters (tol) : tol=0.02 □ 0.001 (energy reconstruction tolerance)
- * Number of equiprobable scattering angle ($N\mu$) : $N\mu=8$ □ 32

(Hartling et al. The effects of nuclear data library processing on Geant4 and MCNP simulations of the thermal neutron scattering law NIMA 891:25-31,5, 2018)

GEANT4 TSL - NEW PROCESSING CODE - VALIDATION

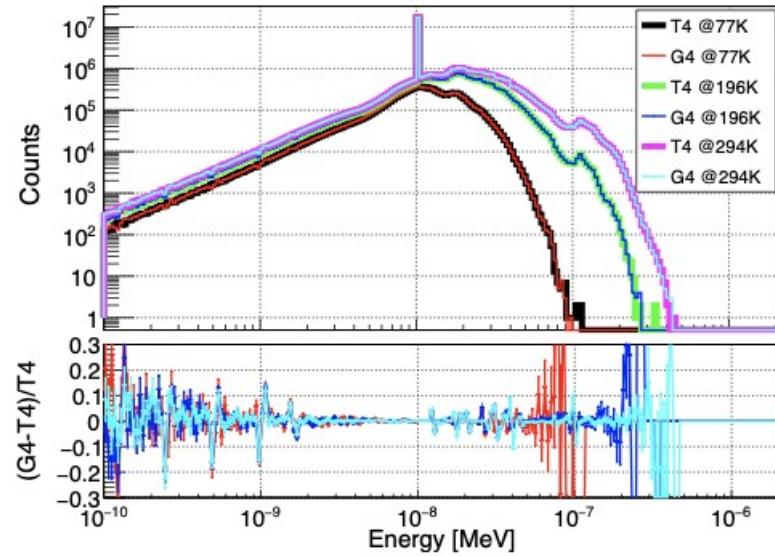
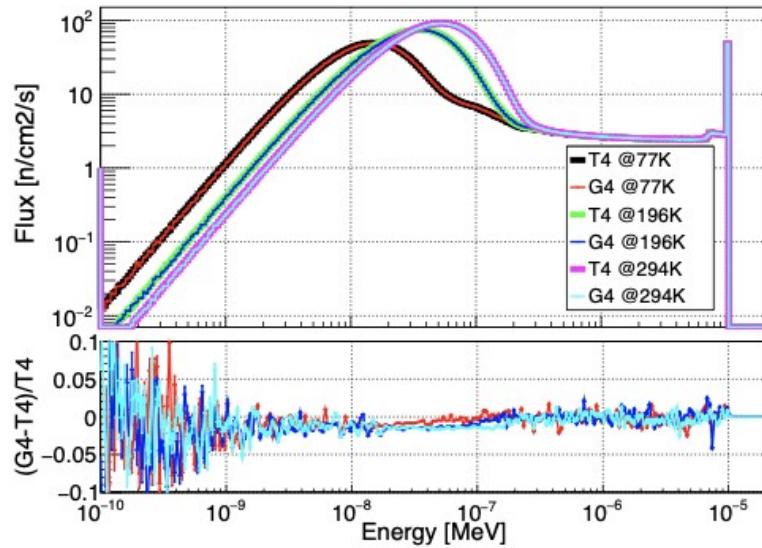


ENDF-BVII.1 – Various moderator materials - Macroscopic benchmark

ENDF-BVII.1 – Various moderator materials - Microscopic benchmark

- Validation of the new processing tool: reprocessed data ~ old data
- New THERMR parameters + Modification of Geant4 code
- => increase Geant4 accuracy, i.e. reduce discrepancies compare to Tripoli4

GEANT4 TSL - NEW PROCESSING CODE - RESULTS



ENDF-BVIII.0 – Polyethylene at various temperature – Macroscopic benchmark (left) and microscopic benchmark (right)

Processing of new libraries: ENDF-BVIII.0 and JEFF-3.3

- New materials
- New temperatures
- Updated evaluations

WHAT ARE THE NEW LIBRARIES?

Thermal scattering data from different libraries couples to JEFF-3.3 nuclear cross-sections, i.e. with G4NDL4.6

ENDF/BVII-1:

ThermalScattering_XS_JEFF33_TSL-ENDFB71_HighPrecision
ThermalScattering_XS_JEFF33_TSL-ENDFB71_LowPrecision

ENDF/BVIII-0:

ThermalScattering_XS_JEFF33_TSL-ENDFB80_HighPrecision
ThermalScattering_XS_JEFF33_TSL-ENDFB80_LowPrecision

JEFF-3.3:

ThermalScattering_XS_JEFF33_TSL_JEFF33_HighPrecision
ThermalScattering_XS_JEFF33_TSL_JEFF33_LowPrecision

Mix JEFF-3.3 and ENDF/BVIII-0, take all TSL data from JEFF-3.3 and add the ENDF/BVIII-0 materials not in JEFF-3.3 :

ThermalScattering_XS_JEFF33_TSL_mix_JEFF33-ENDFB80_HighPrecision
ThermalScattering_XS_JEFF33_TSL_mix_JEFF33-ENDFB80_LowPrecision

Nuclear Inst. and Methods in Physics Research, A 1027 (2022) 166187



Improvement of Geant4 Neutron-HP package: From methodology to evaluated nuclear data library

L. Thulliez^{a,*¹}, C. Jouanne^{b,1}, E. Dumonteil^{a,1}^a IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France^b Université Paris-Saclay, CEA, Service d'études des réacteurs et de mathématiques appliquées, 91191 Gif-sur-Yvette, France

ARTICLE INFO

Keywords:
 Thermal neutrons
 Thermal scattering law
 Geant4
 SVT method
 TRIPOLI-4[®]
 NJOY processing

ABSTRACT

An accurate description of interactions between thermal neutrons (below 4 eV) and materials is key to simulate the transport of neutrons in a wide range of applications such as criticality-safety, reactor physics, compact accelerator-driven neutron sources, radiological shielding or nuclear instrumentation, just to name a few. While the Monte Carlo transport code Geant4 was initially developed to simulate particle physics experiments, its use has spread to neutronics applications, requiring evaluated cross-sections for neutrons and gammas between 0 and 20 MeV (the so-called neutron High Precision – HP – package), as well as a proper offline or on-the-flight treatment of these cross-sections. In this paper we will point out limitations affecting the Geant4 (version 10.07.p01) thermal neutron treatment and associated nuclear data libraries, by using comparisons with the reference Monte Carlo neutron transport code TRIPOLI-4[®], version 11, and we will present the results of various modifications of the Geant4 Neutron-HP package, required to overcome these limitations. Also, in order to broaden the support of nuclear data libraries compatible with Geant4, a nuclear processing tool has been developed (the code is available on a GitLab repository) and validated allowing the use of the code together with ENDF/B-VIII.0 and JEFF-3.3 libraries for example. These changes will be taken into account in an upcoming Geant4 release.

- improvements in the TSL algorithms used in Geant4
 - new TSL processing tool produced to generate new TSL libraries for Geant4 users
- Open source code available online:
https://gitlab.com/lthullie/geant4_tsl_processing

- needed to produce and benchmark new TSL librairies which will be available for Geant4 users

- Free gas approximation algorithm has been rewritten
 - * The results agree well with Tripoli4 with discrepancies around 1%
 - * Long standing issue regarding this part has been solved
- Developement of new TSL processing tool
 - * The results agree well with Tripoli4 with discrepancies less than < 2% (thermal moderators) and <5% (cold moderators) for different benchmarks
 - * New librairies (ENDF-B-VIII.0, JEFF-3.3) have been processed
 - more materials at more temperature available in Geant4
 - TSL data treatment in Geant4 has been modified
 - * Gain in computing time : faster by a factor 2 (temeprature stochastic interpolation)

Geant4 starts to become onpar with reference code such as MCNP and Tripoli4 for low energy neutron (<20 MeV)

THANKS FOR YOUR ATTENTION

Updated class G4ParticleHPTermalScatteringNames.cc ↔ TSL names

→ great attention paid on the coherence of the TSL naming to ease users
comparaison tests between the different librairies

```
names.insert ( std::pair < G4String , G4String > ( "TS_H_of_Para_Hydrogen", "h_para_h2" ) );    ///ENDF/BVIII.0 and JEFFF.3.3 and ENDF/BVII.1
names.insert ( std::pair < G4String , G4String > ( "TS_D_of_Para_Deuterium", "d_para_d2" ) );  ///ENDF/BVIII.0 and JEFFF.3.3 and ENDF/BVII.1
names.insert ( std::pair < G4String , G4String > ( "TS_H_of_Ortho_Hydrogen", "h_ortho_h2" ) ); //ENDF/BVIII.0 and JEFFF.3.3 and ENDF/BVII.1
names.insert ( std::pair < G4String , G4String > ( "TS_D_of_Ortho_Deuterium", "d_ortho_d2" ) );///ENDF/BVIII.0 and JEFFF.3.3 and ENDF/BVII.1
names.insert ( std::pair < G4String , G4String > ( "TS_O_of_Uranium_Dioxide", "o_uo2" ) );      //ENDF/BVIII.0 and ENDF/BVII.1
names.insert ( std::pair < G4String , G4String > ( "TS_O_of_Ice", "o_ice" ) );                  ///ENDF/BVIII.0
names.insert ( std::pair < G4String , G4String > ( "TS_O_of_Heavy_Water", "o_heavy_water" ) ); //ENDF/BVIII.0 and JEFFF.3.3
names.insert ( std::pair < G4String , G4String > ( "TS_O_of_Beryllium_Oxide", "o_beo" ) );     //ENDF/BVIII.0 and ENDF/BVII.1
names.insert ( std::pair < G4String , G4String > ( "TS_N_of_Uranium_Nitride", "n_un" ) );       ///ENDF/BVIII.0
names.insert ( std::pair < G4String , G4String > ( "TS_H_of_Liquid_Methane", "h_l_ch4" ) );     ///ENDF/BVIII.0 and ENDF/BVII.1
```