Recent improvements in NeutronHP package, validated against reference neutron codes MCNP and Tripoli-4

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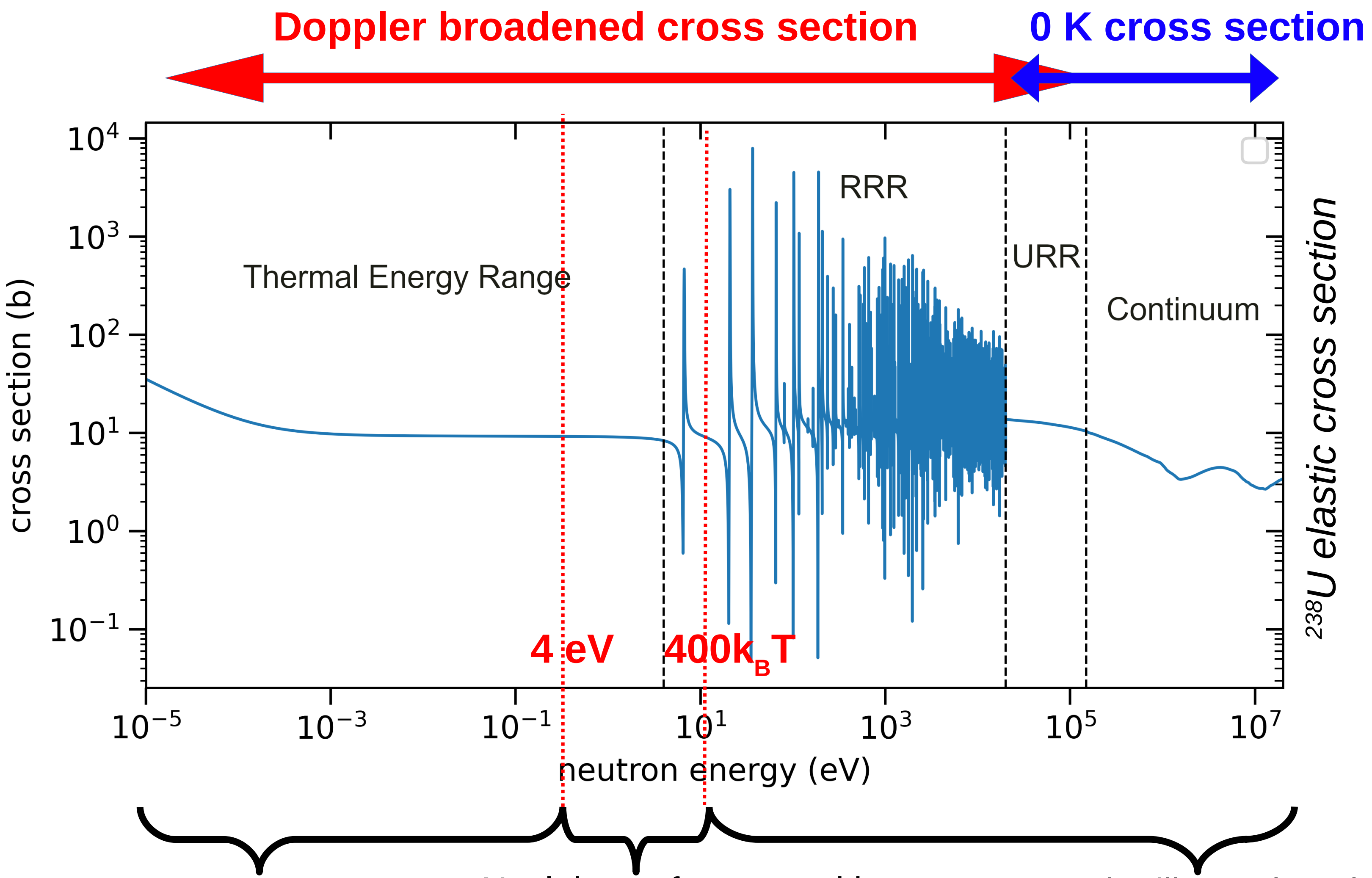
29th Geant4 collaboration meeting – Catania *7 – 11 october 2024*

Simulation of neutron physics for $E_n < 20$ MeV

Based on evaluated nuclear data libraries: ENDF/B, JEFF, JENDL, BROND, CENDL, etc

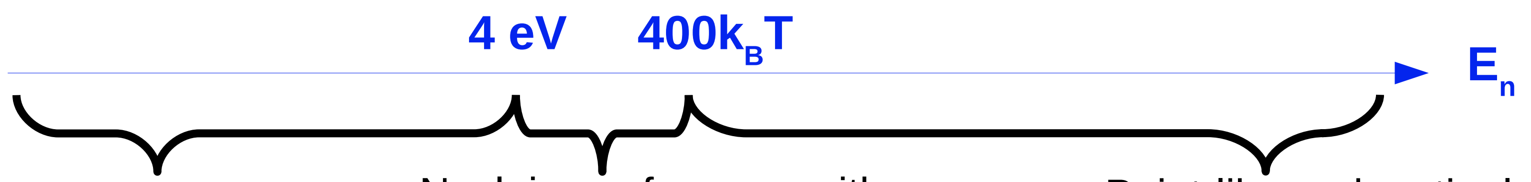


Nuclei bound in molecule/crystal
- Use of thermal scattering data (TSL)

Nuclei as a free gas with Maxwellian distribution

Point-like and motionless nuclei

Status of the Geant4 NeutronHP package (E_n < 20 MeV) in 2021



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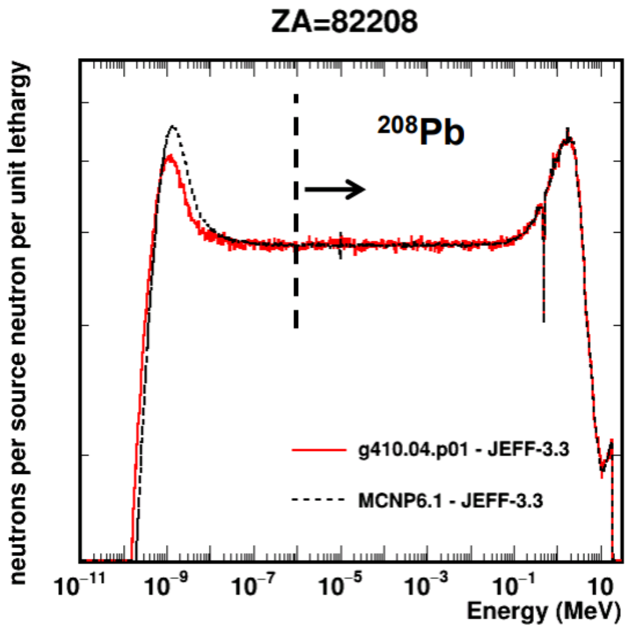
TSL not updated since ENDF/B-VII.1
BUT
ENDF/B-VIII.0 and JEFF3-3 contain ~20 more materials and more temperatures
+
~20% discrepancies with Tripoli-4 and MCNP



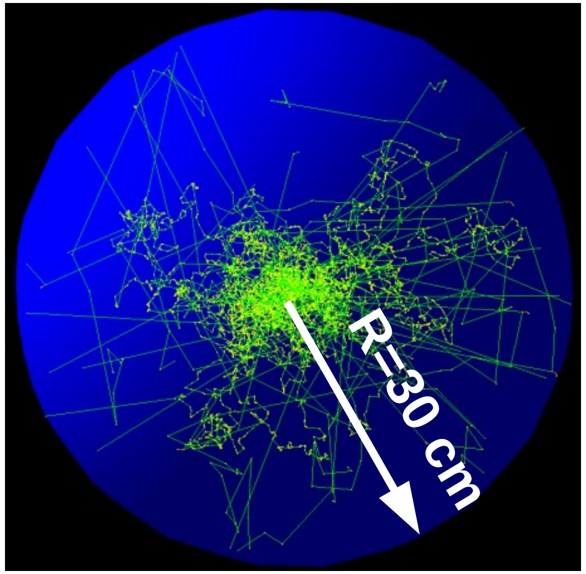
Talk from E. Mendoza, Geant4 Hadronic meeting Feb. 2020

URR NOT described by Probability Table (TP)

Free gas approximation in Geant4 does NOT reproduce Tripoli-4 and MCNP results below few eV

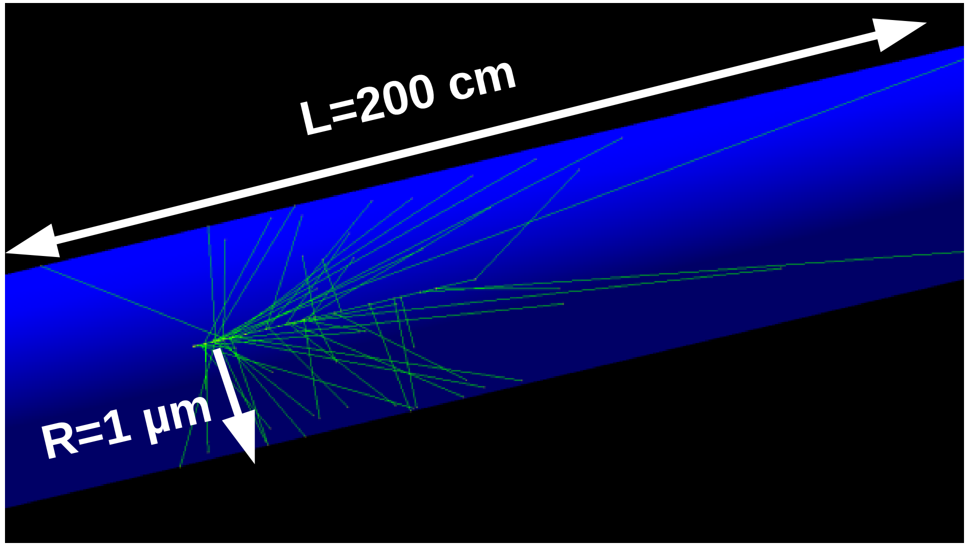
Benchmark methodology

Macroscopic



- **Probe** the neutron slowing down and thermalization
- **Score** the neutron flux in the sphere
- Isotropic neutron source

Microscopic



- **Probe** only one interaction
- **Score** scattered neutron energy and angle
- 0 degree direction neutron beam

Geant4 validated against reference neutron transport codes **Tripoli-4®** [1] and **MCNP6.2** [2]

[1] E. Brun et al., TRIPOLI-4 ® , CEA, EDF and AREVA reference Monte Carlo code. Ann. Nucl. Energy 82, 2015, 151–160. http://dx.doi.org/10.1016/j.anucene.2014.07.053.
[2] C.J. Werner et al., MCNP Version 6.2, Technical Report, LANL, 2018, http://dx.doi.org/10.2172/1419730.

Status of the Geant4 NeutronHP package (E_n < 20 MeV) in 2021

4 eV — $400k_BT$ — E_n

Nuclei bound in molecule/crystal
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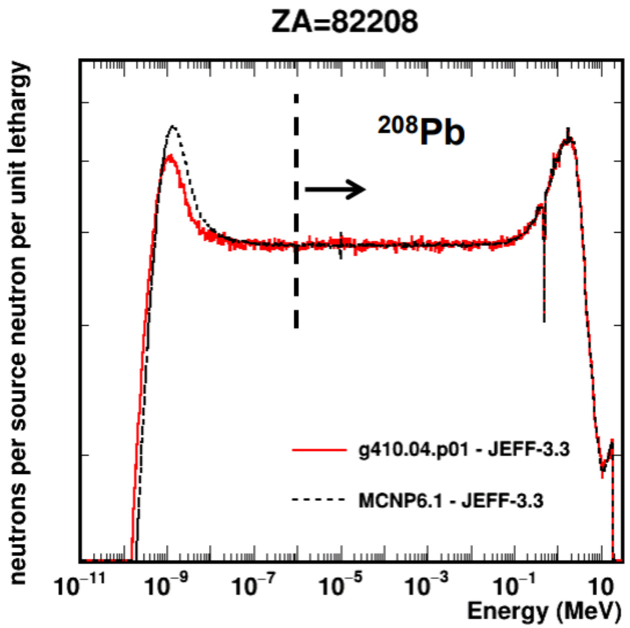

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URR NOT described by Probability Table (TP)

Free gas approximation in Geant4 does NOT reproduce Tripoli-4 and MCNP results below few eV

Effect of thermal motion on cross section

- Need to conserve average thermal reaction rate (Original Geant4 algorithm did not)

$$\sigma_T(v_n) = \frac{1}{v_n} \int v_r \sigma_{T=0\mathrm{K}}(v_r) \mathcal{M}(\mathbf{V}_t, T) d\mathbf{V}_t$$

Thermal average cross section at temperature T

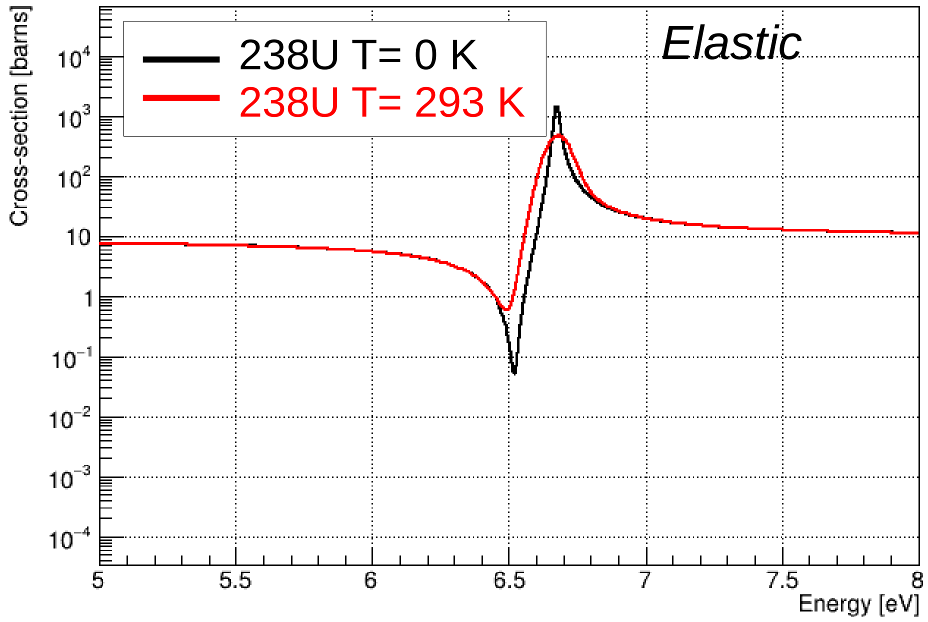
Neutron velocity

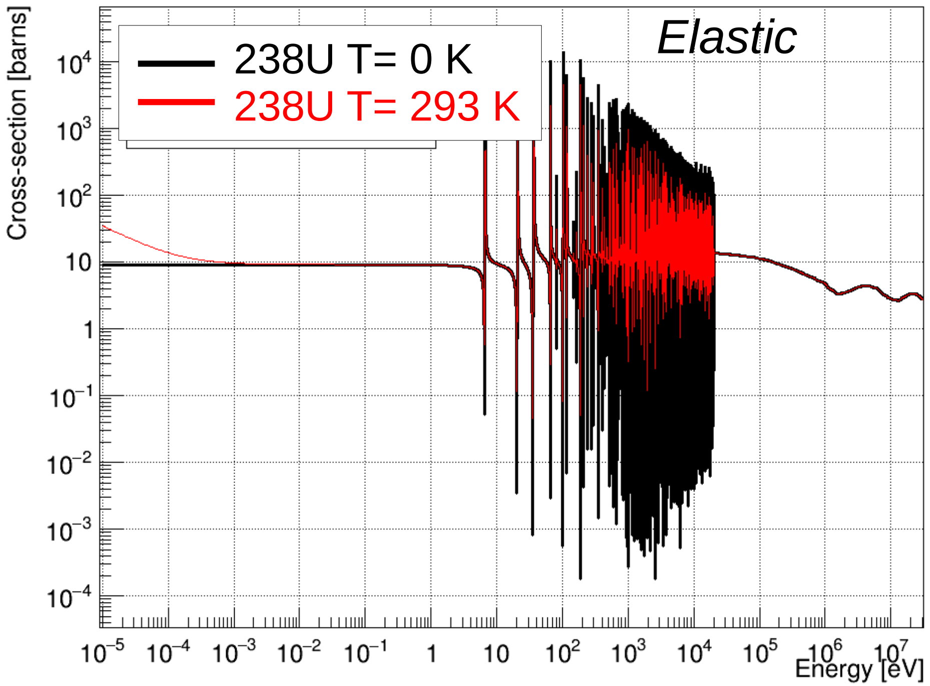
Neutron/Target relative velocity

0 K cross section

Maxwellian distribution

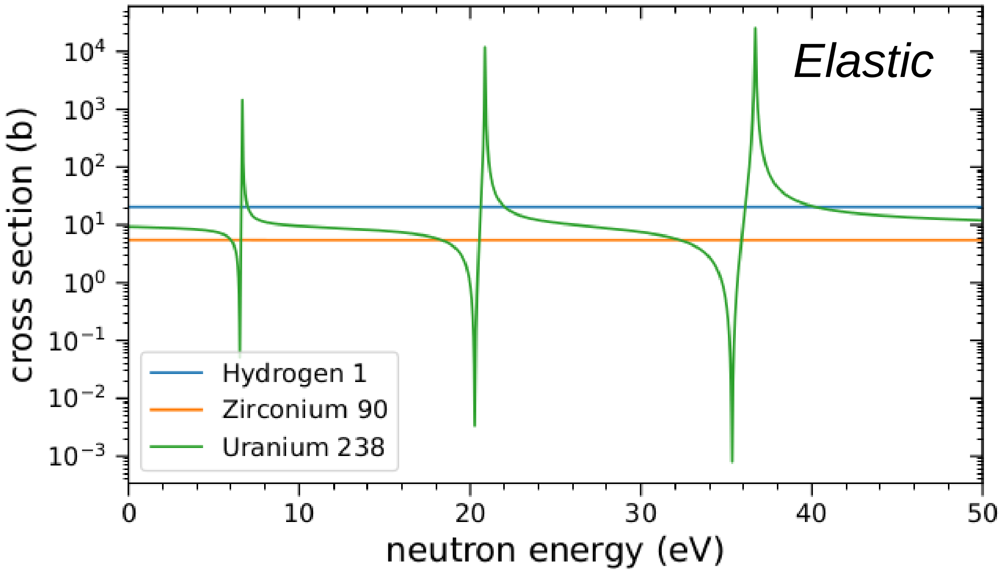
- Final State has to be sampled accordingly!





Doppler Broadening of elastic kernel for light / medium nuclei (1/2) → Sampling of the Velocity of the Target (SVT)

Light / medium nucleus → no resonance at ~10 – 100 eV
→ slowly varying cross section



Thermal average reaction rate conservation

Hyp: $\sigma_{T=0K}$ ~ constant

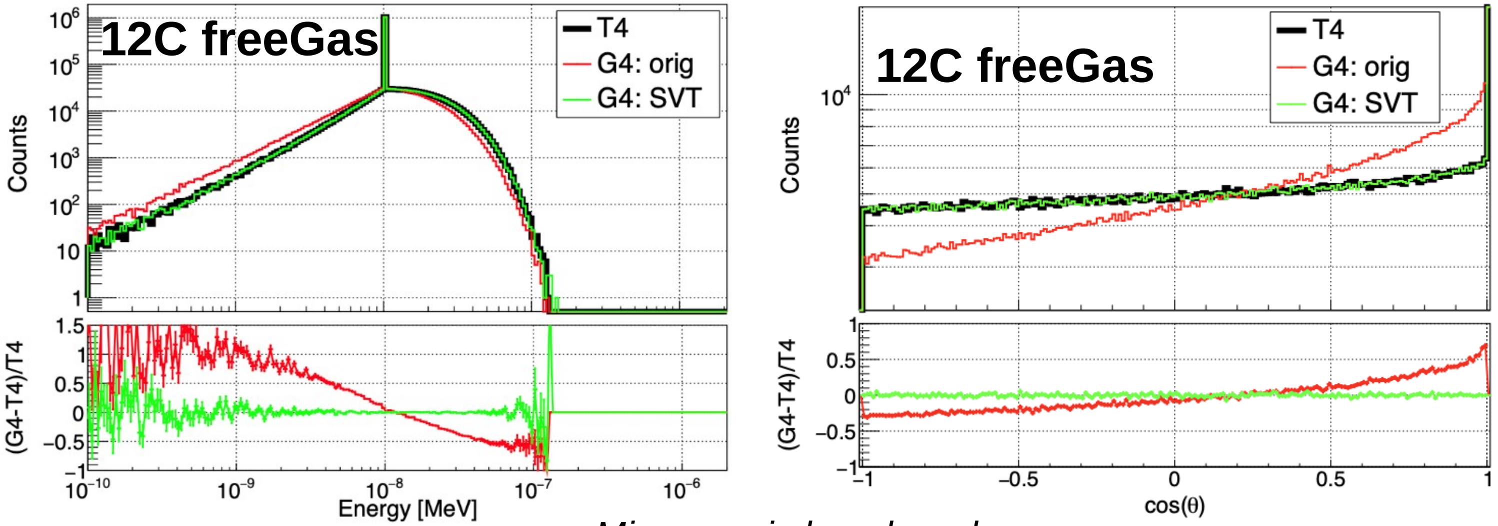
Joint probability distribution

$$p_{SVT}(V_t,\mu)dV_t d\mu = C \underbrace{\frac{d\mu}{2}}_{(A)} \underbrace{(v_n+V_t)\frac{4\beta^3}{\sqrt{\pi}}V_t^2 e^{-\beta^2 V_t^2} dV_t}_{(B)} \underbrace{\left(\frac{v_r}{v_n+V_t}\right)}_{(C)}$$

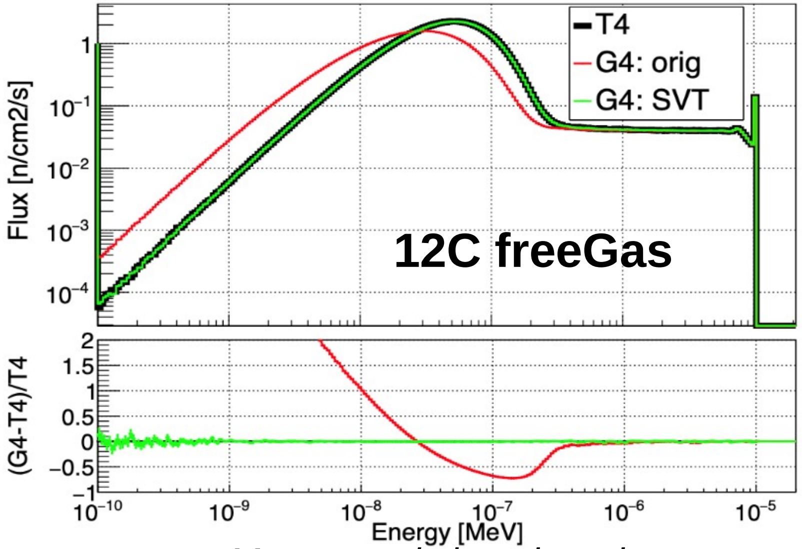
1/ Sample μ in (A)
2/ Sample V_t in (B)
3/ Accept (V_t, μ) with probability (C)
→ if not, go to 1/

L. Thulliez, C. Jouanne, E. Dumonteil, Improvement of Geant4 Neutron-HP package: From methodology to evaluated nuclear data library, Nucl. Instrum. Meth. Phys. Res. Sec. A, Volume 1027, 2022, 166187, ISSN 0168-9002, https://doi.org/10.1016/j.nima.2021.166187 (arXiv:2109.05967)

Doppler Broadening of elastic kernel for light / medium nuclei (2/2)



Microscopic benchmark



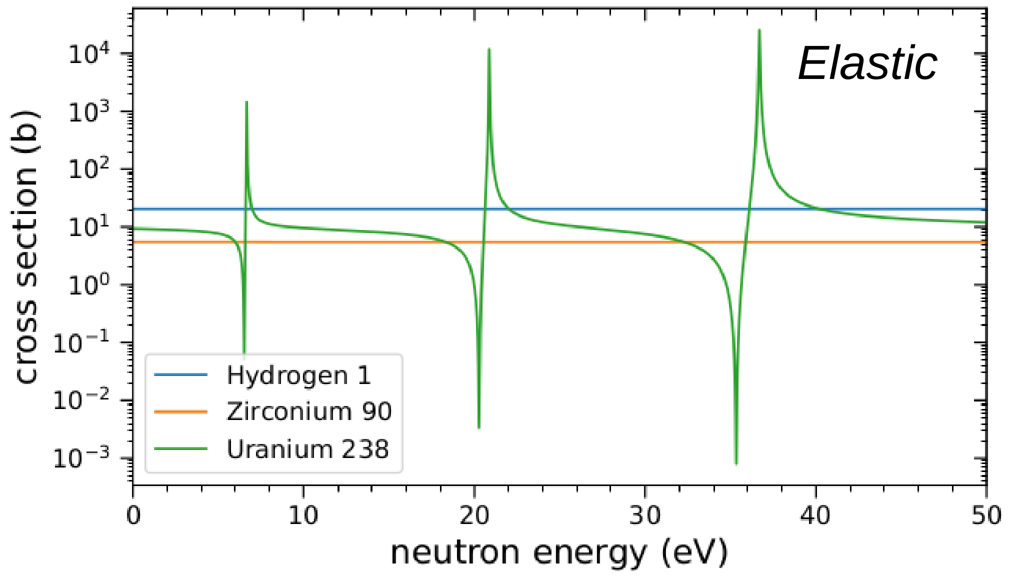
Macroscopic benchmark

- SVT algorithm validated against Tripoli-4 within stat.unc.
- Important for all neutron applications
- In geant4-11.0.0

L. Thulliez, C. Jouanne, E. Dumonteil, Improvement of Geant4 Neutron-HP package: From methodology to evaluated nuclear data library, Nucl. Instrum. Meth. Phys. Res. Sec. A, Volume 1027, 2022, 166187, ISSN 0168-9002, https://doi.org/10.1016/j.nima.2021.166187 (arXiv:2109.05967)

Doppler Broadening of elastic kernel for heavy nuclei (1/2)
→ Doppler Broadening Rejection Correction (DBRC)

Heavy nuclei → resonances at ~10 – 100 eV
→ sharp variation in the cross section



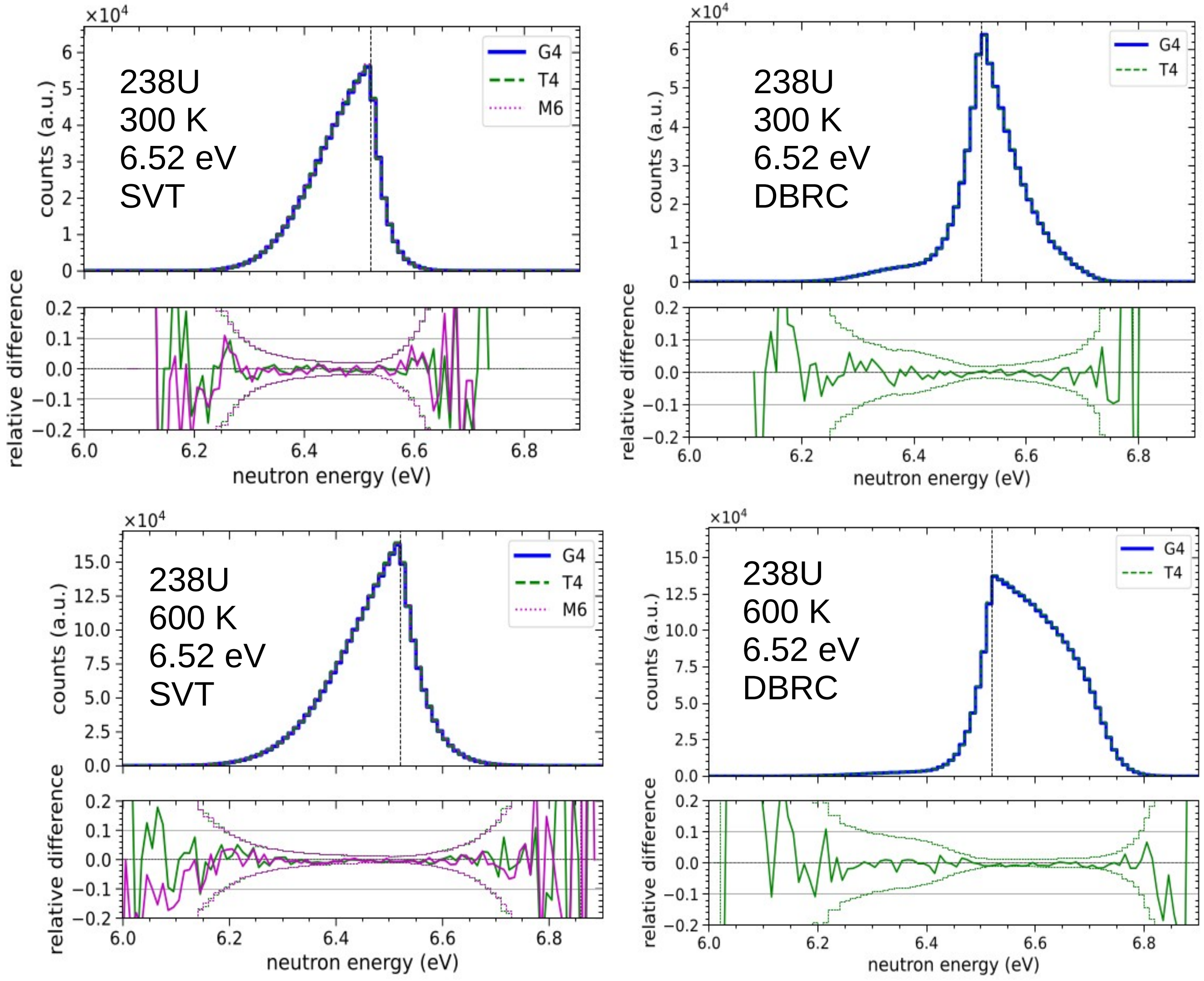
$$p_{\text{DBRC}}(V_t, \mu) = C' p_{\text{SVT}}(V_t, \mu) \underbrace{\left(\frac{\sigma_0(v_r)}{\sigma_0^{\max}(v_\xi)} \right)}_{(D)}$$

1/ Sample μ in (A)
2/ Sample V_t in (B)
3/ Accept (V_t, μ) with probability (C)
→ if not, go to 1/
4/ Accept (V_t, μ) with probability (D)
→ if not, go to 1/

Breaks hyp $\boldsymbol{\sigma_{T=0K}}$ **~ constant** [1]

[1] Becker, B., Dagan, R., Lohnert, G., 2009. Proof and implementation of the stochastic formula for ideal gas, energy dependent scattering kernel. Ann. Nucl. Energy 36, 470–474. http://dx.doi.org/10.1016/j.anucene.2008.12.001.

Doppler Broadening of elastic kernel for heavy nuclei (2/2)



Microscopic benchmark

- SVT algorithm again validated against Tripoli-4 and MCNP6.2, for different temperatures and resonance energies, agreement within stat. unc.
- DBRC algorithm validated against Tripoli-4, within stat. unc.
  (MCNP6.2 does not have this feature!)
- Important for nuclear reactor physics
- Important for nuclear resonance spectroscopy in heavy nuclei (*e.g.* nTOF experiment at CERN)
- In geant4-11.2.0
  with new command lines:
  /process/had/particle_hp/use_DBRC true
  /process/had/particle_hp/DBRC_A_min 200
  /process/had/particle_hp/DBRC_E_min 0.1 eV
  /process/had/particle_hp/DBRC_E_max 210 eV
  /process/had/particle_hp/SVT_E_max 200 eV (default=400kT)

M. Zmeškal, L. Thulliez, E. Dumonteil, Improvement of Geant4 Neutron-HP package: Doppler broadening of the neutron elastic scattering kernel, Annals of Nuclear Energy, Volume 192, 2023, 109949, ISSN 0306-4549, https://doi.org/10.1016/j.anucene.2023.109949 (arXiv:2303.07300)

Status of the Geant4 NeutronHP package (E_n < 20 MeV) in 2021

4 eV $400k_BT$ E_n

Nuclei bound in molecule/crystal
- Use of thermal scattering data (TSL)

Nuclei as a free gas with Maxwellian distribution
- Use free gas approximation

Point-like and motionless nuclei

TSL not updated since ENDF/B-VII.1
BUT
ENDF/B-VIII.0 and JEFF3-3 contain ~20 more materials and more temperatures
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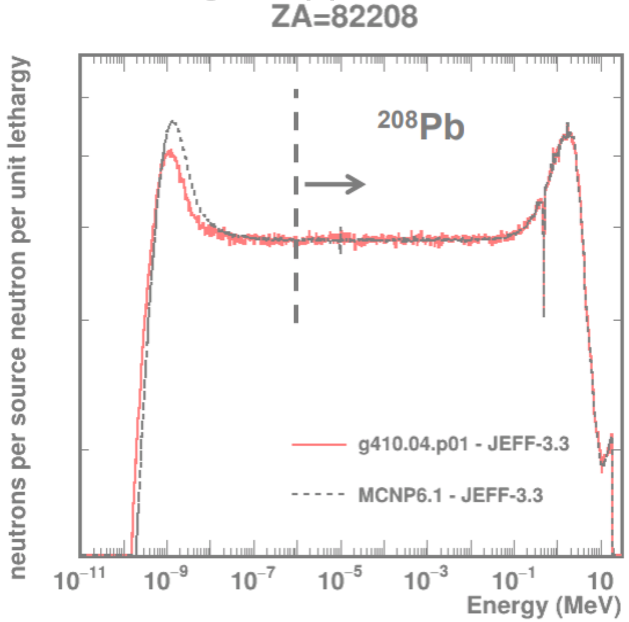


Talk from E. Mendoza, Geant4 Hadronic meeting Feb. 2020

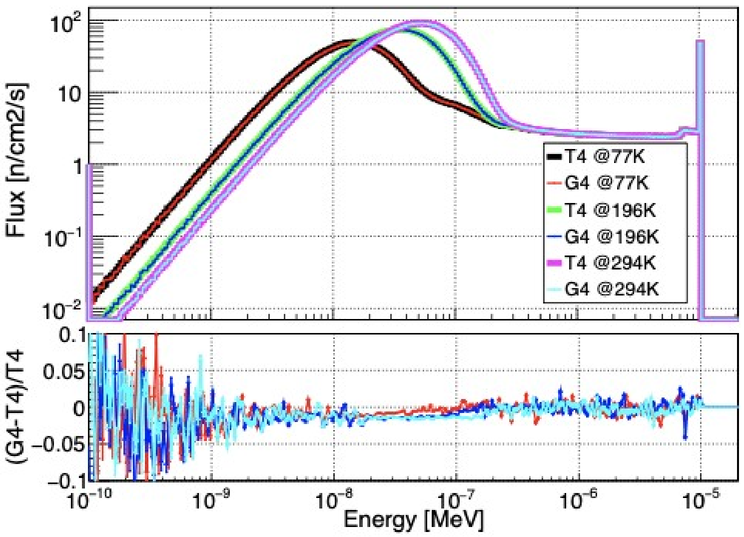
URR NOT described by Probability Table (TP)

Free gas approximation in Geant4 does NOT reproduce Tripoli-4 and MCNP results below few eV

Thermal scattering (TSL) data

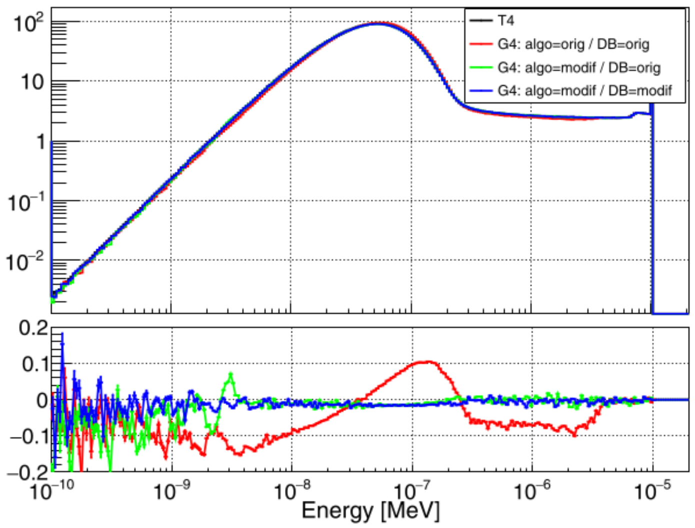
In 2021: → only ENDF/B-VII.1 TSL in Geant4 BUT ENDF/B-VIII.0 and JEFF3-3 available
=> need to develop a new processing tool based on NJOY
→ few corrections in the algorithms needed

New TSL library



Polyethylene – ENDF/B-VIII.0
Macroscopic benchmark

Algorithm corrections

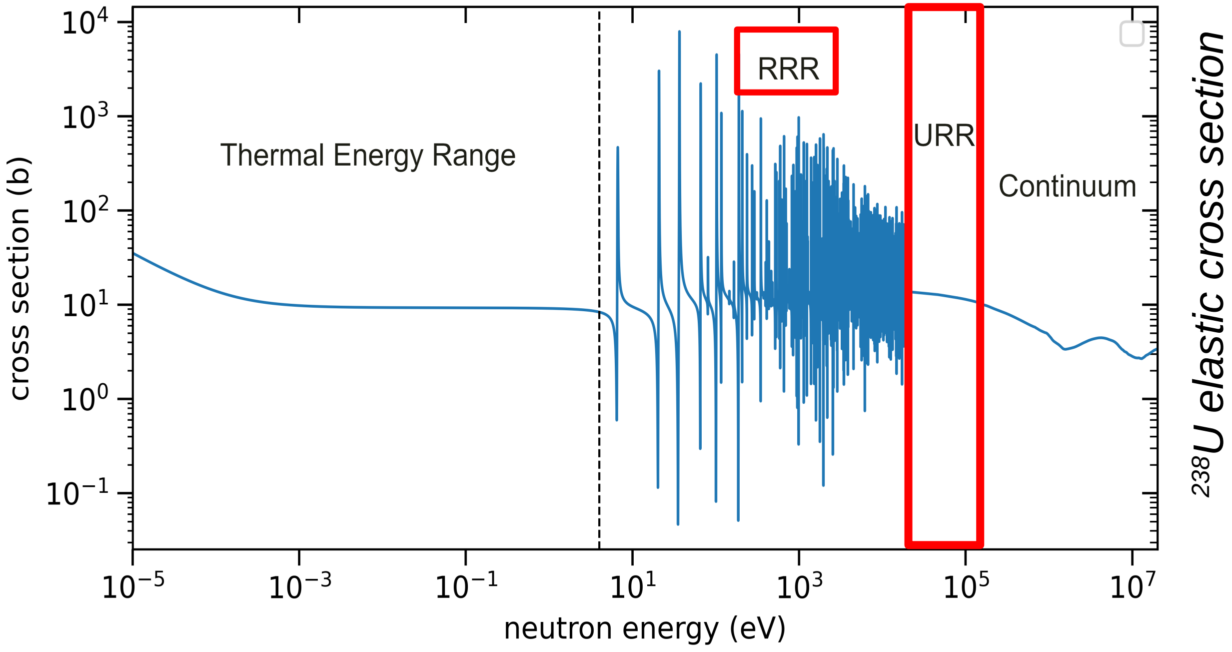


Polyethylene – ENDF/B-VII.1
Macroscopic benchmark

- New TSL processing tool validated against Tripoli-4, agreement better than 2%
- Multiple TSL libraries are available in **LowPrecision** and **HighPrecision**: ENDF/B-VII.1, ENDF/B-VIII.0, JEFF3-3 and mix of JEFF3-3 and ENDF/B-VIII.0
- G4NDL4.7 TSL = mix JEFF3-3 / ENDF/B-VIII.0
  G4NDL4.7.1 taking into account bugzilla 2552 (https://bugzilla-geant4.kek.jp/show_bug.cgi?id=2552)
  → ~20 more materials and temperatures
- Important for all applications with thermal neutrons
- In geant4-11.0.0 / G4NDL4.7

L. Thulliez, C. Jouanne, E. Dumonteil, Improvement of Geant4 Neutron-HP package: From methodology to evaluated nuclear data library, Nucl. Instrum. Meth. Phys. Res. Sec. A, Volume 1027, 2022, 166187, ISSN 0168-9002, https://doi.org/10.1016/j.nima.2021.166187 (arXiv:2109.05967)

Unresolved Resonance Region (URR) description with Probability Table (PT)



Resolved **R**esonance **R**egion (RRR)
- Resonances experimentally observed/resolved
- R-matrix formalism used to extract resonance parameters (energy position, width, spin, parity)

Unresolved **R**esonance **R**egion (URR)
- Resonances NOT experimentally observed/resolved
- BUT where self-shielding is important
- Cross section from adjusted average resonance parameters (average resonance spacing and widths)

Two ways to describe the URR:
- Use smooth cross sections → **Geant4 until now**
- Use Probability Tables (PT) to better take into account self-shielding

URR description with Probability Table (PT)

URR cross section = sampled resonances (spacing from Wigner distribution / width from χ^2 distribution)

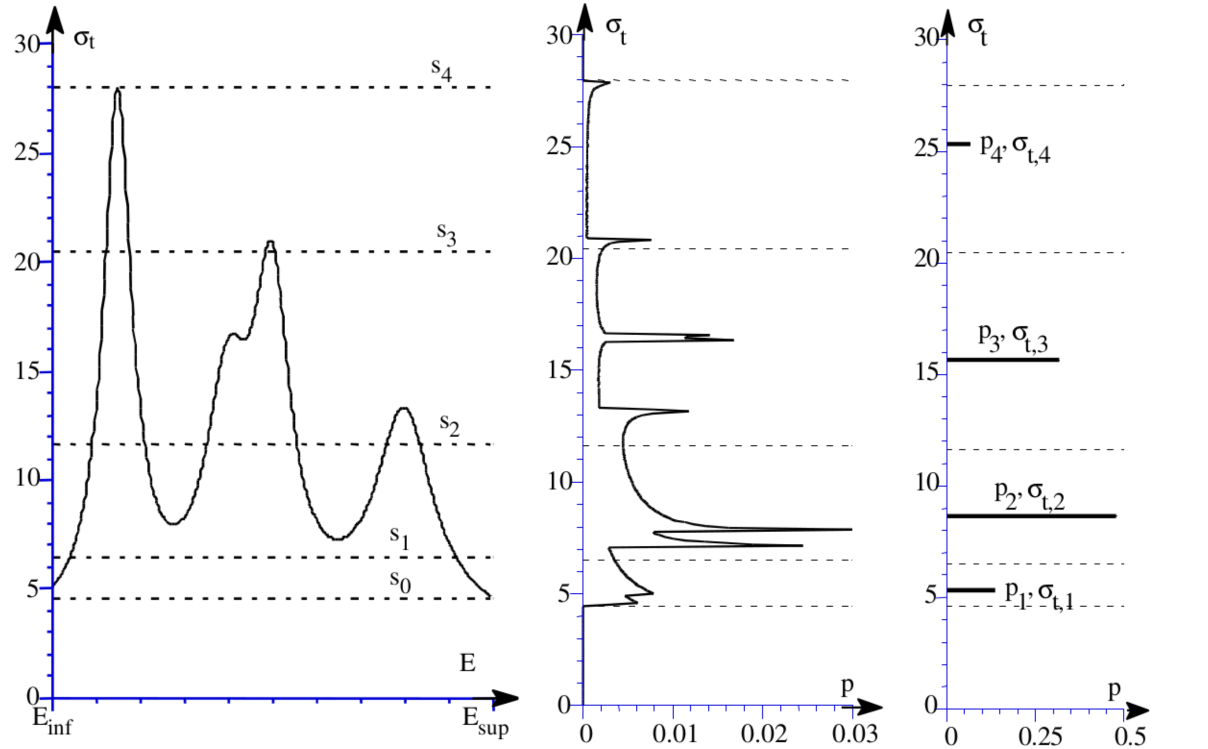


Fig. 1a Cross section versus energy **1b** Exact PT distribution **1c** PT discretisation

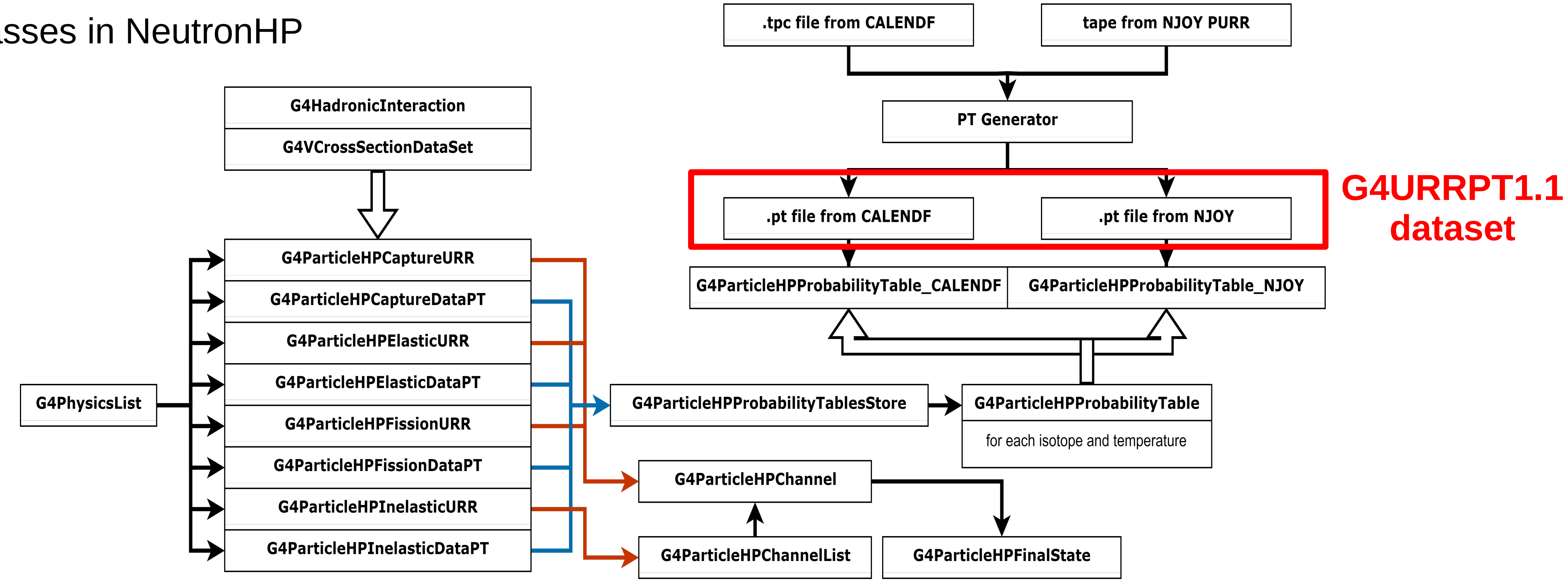
J.C. Sublet, P. Ribon, M. Coste-Delclaux, CALENDF-2010: user manual, Rapport CEA-R-6277, 2011

Processing tools:

- CALENDF: PTs for elastic, capture, fission, inelastic | dense energy grid & few samples
- NJOY: PTs for elastic, capture, fission | few energy points & lot of samples

URR description with PT – Geant4 implementation

12 new classes in NeutronHP

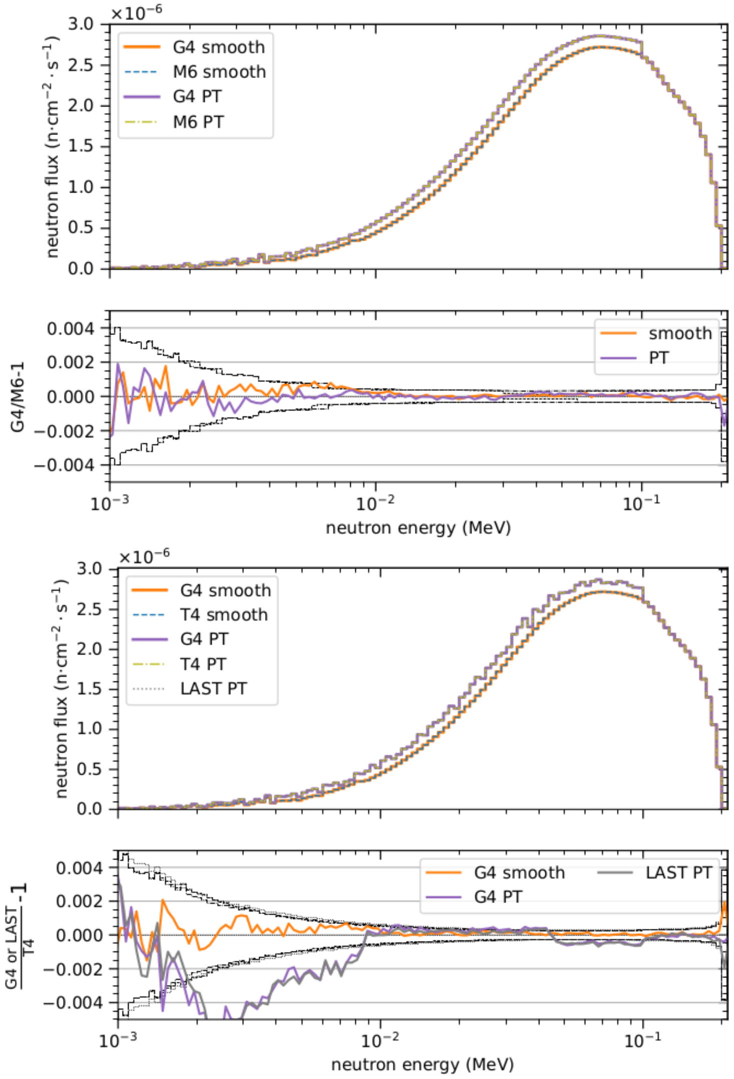


Probability tables from NJOY and CALENDF are:

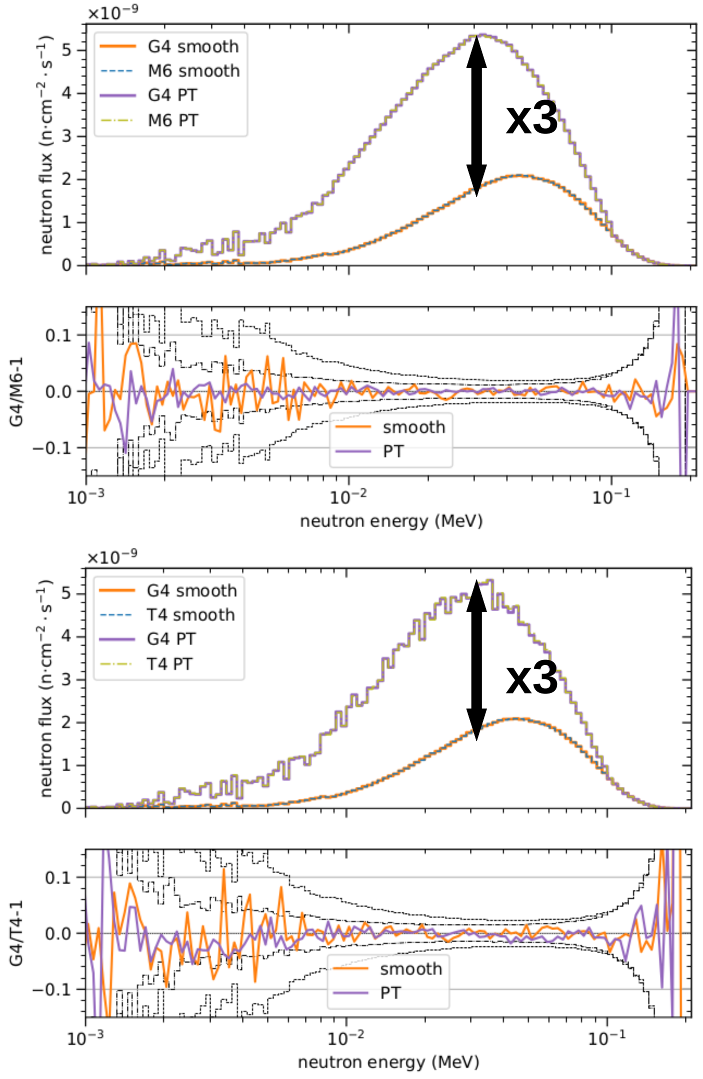
- produced with the geant4_pt_generator available here: https://gitlab.com/lthullie/geant4_pt_generator
- will be in **geant4-11.3.0** in the new dataset **G4URRPT1.1**
- can be choose in setting in main.cc: - G4HadronicParameters::Instance()->SetTypeTablePT("njoy");
  - G4HadronicParameters::Instance()->SetTypeTablePT("calendf");

M. Zmeškal, L. Thulliez, P. Tamagno, E. Dumonteil, Improvement of Geant4 Neutron-HP package: Unresolved resonance region description with probability tables, Annals of Nuclear Energy, Volume 211, 2025, 110914, ISSN 0306-4549, https://doi.org/10.1016/j.anucene.2024.110914 (arXiv:2404.16389)

URR description with PT – Geant4 validation with Tripoli-4 and MCNP6.2



Flux inside the sphere of ^{nat}W



Flux going out of the sphere of ^{nat}W

- Geant4 validated, within stat. unc., against Tripoli-4 (PT from CALENDF) and MCNP6.2 (PT from NJOY)
- Benchmark performed for all W isotopes, 238U, W element, at different temperatures
- To our knowledge first code to handle PTs from both CALENDF and NJOY
  → can compare the impact of the choices made in each code to produce PT
- Important for shielding calculations
- Self-shielding has huge effect
  → factor 3 behind ^{nat}W shield
- In geant4-11.3.0
- Environment variable G4URRPTDATA pointing to G4URRPT1.1
  setting in main.cc:
  G4HadronicParameter:Instance()→SetTypeTablePT(“njoy”)
  G4HadronicParameter:Instance()→SetTypeTablePT(“calendf”)

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Conclusions

In terms of neutron physics Geant4 is now on-par with MCNP6.2 and Tripoli-4®

- Doppler broaden elastic scattering kernel for light/medium nuclei – Sampling of the Velocity of the Target (SVT)

  L. Thulliez, C. Jouanne, E. Dumonteil, Improvement of Geant4 Neutron-HP package: From methodology to evaluated nuclear data library, Nucl. Instrum. Meth. Phys. Res. Sec. A, Volume 1027, 2022, 166187, ISSN 0168-9002, https://doi.org/10.1016/j.nima.2021.166187 (arXiv:2109.05967)

- Doppler broaden elastic scattering kernel for heavy nuclei – Doppler Broadening Rejection Correction (DBRC)

  M. Zmeškal, L. Thulliez, E. Dumonteil, Improvement of Geant4 Neutron-HP package: Doppler broadening of the neutron elastic scattering kernel, Annals of Nuclear Energy, Volume 192, 2023, 109949, ISSN 0306-4549, https://doi.org/10.1016/j.anucene.2023.109949 (arXiv:2303.07300)

- Up-to-date thermal scattering (TSL) data + bug corrections
  → G4NDL4.7=mix of JEFF3-3 and ENDF/B-VIII.0

  L. Thulliez, C. Jouanne, E. Dumonteil, Improvement of Geant4 Neutron-HP package: From methodology to evaluated nuclear data library, Nucl. Instrum. Meth. Phys. Res. Sec. A, Volume 1027, 2022, 166187, ISSN 0168-9002, https://doi.org/10.1016/j.nima.2021.166187 (arXiv:2109.05967)

- Description of Unresolved Resonance Region (URR) with Probability Tables (PT)
  → G4URRPT1.1 dataset with NJOY and CALENDF PTs

  M. Zmeškal, L. Thulliez, P. Tamagno, E. Dumonteil, Improvement of Geant4 Neutron-HP package: Unresolved resonance region description with probability tables, Annals of Nuclear Energy, Volume 211, 2025, 110914, ISSN 0306-4549, https://doi.org/10.1016/j.anucene.2024.110914 (arXiv:2404.16389)

- Agreement between Geant4 NeutronHP package and Tripoli-4 and MCNP6.2 to better than 2%

- Creation of NeutronHP benchmarks in geant-val to ensure its reliability on a long term

How to ensure the validity of the NeutronHP physics on a long term?

Geant-val !

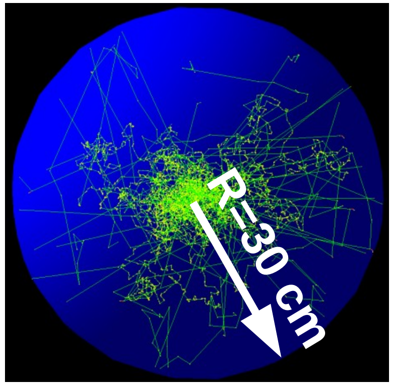
(cf. Dmitri talk on Monday "geant-val: Status and challenges")

Very important steps to ensure the reliability of Geant4 on a **long term** and help disentangle things when someone has a problem

Implementation of the two tests in https://github.com/geant-val (**will be finalized soon !**)

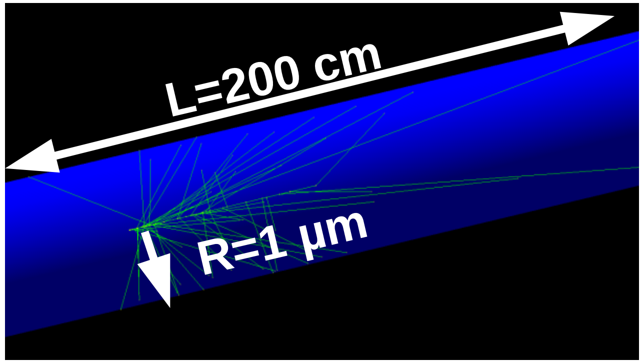
- along with reference database from Tripoli-4 and MCNP6.2
- for the different physics cases presented in this talk (SVT, DBRC, TSL, URR_PT)

Macroscopic



- Probe the neutron slowing down and thermalization
  - ✔ Check TSL data
  - ✔ Check URR description with PT

Microscopic



- Probe only one interaction / Final State:
  - ✔ Check TSL data
  - ✔ Check SVT
  - ✔ Check DBRC

What is next ?

- **Speed-up the code**
  - Create libraries of pre-Doppler broadened cross-sections at given temperatures
    → will speed-up the simulation by a factor from 2 to 10
    Steps: 1) Use available tools *e.g.* NJOY or PREPRO (end 2024 / begin 2025)
    2) Develop a code to Doppler broaden the XS at the initialization steps in Geant4
  - Perform a code review to:
    → spot bottlenecks of computational speed
    → clarify the handling of cross-sections: isotope vs element cross-sections

Soon, Geant4 on-par with MCNP6.2 and Tripoli-4®
for neutron physics and computational performances?!

- **Stay up-to-date**
  - In 2025 (?) new evaluated nuclear data libraries ENDF/B-VIII.1 and JEFF-4.0
    → include them in Geant4
    → Warning: ENDF/B-VIII.1 might be the last ENDF/B release in ENDF format, after it would be GNDS BUT let see…

Thank you for your attention

This works have been supported in part by :

- **IAEA fellowship** of Marek Zmeskal in the framework of national project CZR0011 (5 months)
- **Emilie du Chatelet** grant for Marek Zmeskal (2 months)
  This work was supported by the French government under the France 2030 program (P2I - Graduate School Physics) under reference ANR-11-IDEX-0003