Low energy (E≤20MeV) neutron treatment

Introduction

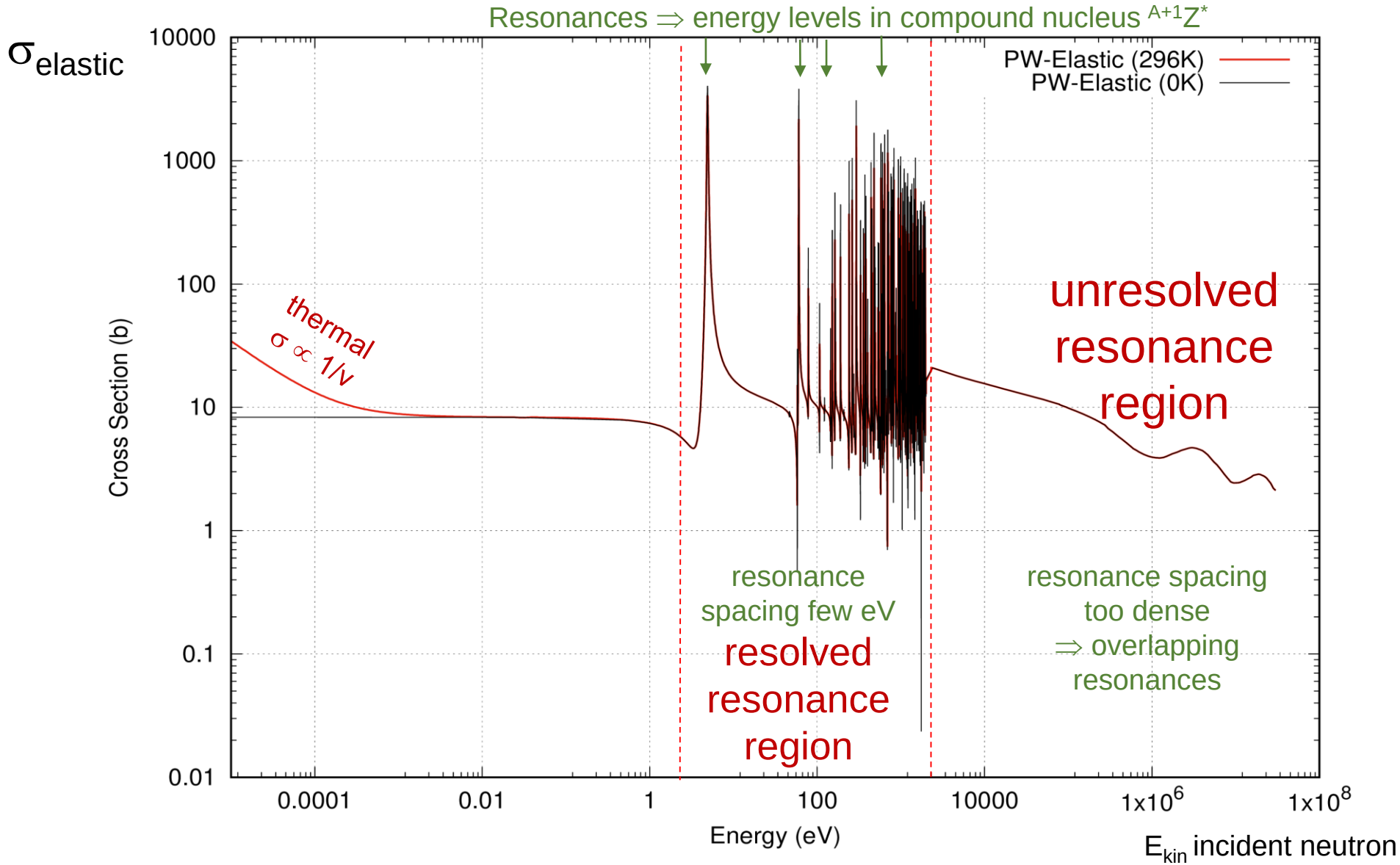
- In FLUKA, neutrons below 20 MeV are called low energy neutrons
- Neutron interactions at higher energy are handled by FLUKA nuclear models
- Transport and interactions of neutrons with energies below E≤20 MeV are handled by a dedicated neutron library
- Why are low Energy Neutrons special?
  - The neutron has no charge

    → can interact with nuclei at low energies, e.g. meV
  - Neutron cross sections (σ) are complicated, depending on the isotope and/or solid state effects on crystalline structures at low neutron energies

    → cannot be calculated by models

    → we rely on data files

Typical neutron cross-section



Evaluated Nuclear Data Files (ENDF)

The neutron data are provided in the Evaluated Nuclear Data Files (ENDF)

Major libraries: ENDF, JEFF, JENDL, TENDL, CENDL, BROND, …

- Organized per isotope
  - per interaction channel (elastic, capture, inelastic, fission, ….)
    - Cross section (resonance parameters + continuum)
    - Final states (uncorrelated) described in a plethora of “laws”
- Most libraries share the same data
- Channels without measurements are completed with “models”
- Old databases contained natural elements

Thermal Scattering Law Data are provided in additional datafiles for a few selected materials/isotopes

Specialized programs NJOY, PREPRO,… are used to preprocess for use in MC

Monte Carlo approaches

Groupwise

- histogram like/group information, was widely used in neutron transport codes
- Advantages
  - fast
  - small memory footprint
  - gives good results for some applications
- Drawbacks:
  - self-shielding not accurately reproduced
  - discrete angular distributions (e.g. 3 angles in FLUKA)
  - no recoils, and other particle emissions

Pointwise

- “continuous” scatter plot of pairs of (Energy, cross section)
- Advantages
  - follows cross section precisely
  - no issues with self-shielding (in the resolved resonance region)
  - accurate reproduction of angular distributions and all final states
- Drawbacks
  - time and memory consuming

FLUKA supports both approaches (since v4.3)

Groupwise

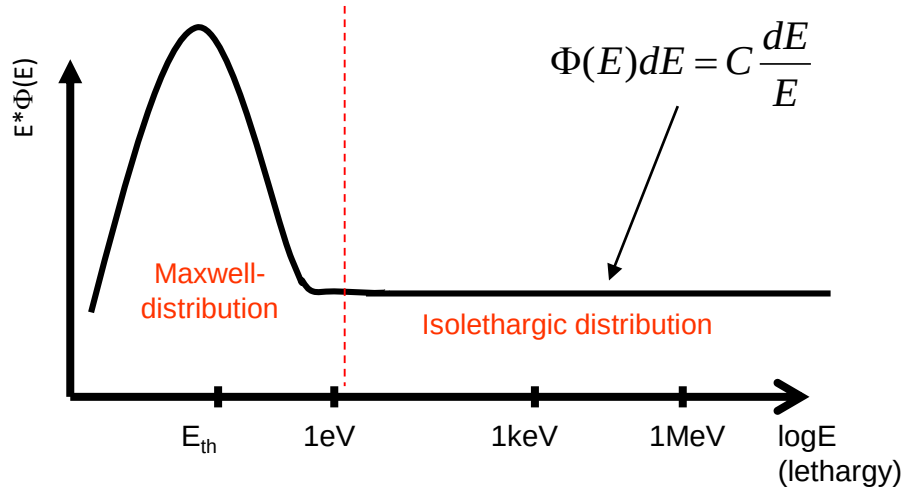
Energy groups:

- 1 – highest energy 20..19.64MeV
  …
  260 – lowest energy 200..10μeV
- Elastic & Inelastic reactions are simulated group-to-group transfer probabilities (down-scattering matrix)
  - Lose energy: down scattering
  - Stay in the same group: in-scattering
  - Thermal energies: could gain energy up-scattering
- Neutron has NO PRECISE ENERGY, except the first time it enters in the low energy domain

- Average cross section in a group is given as:

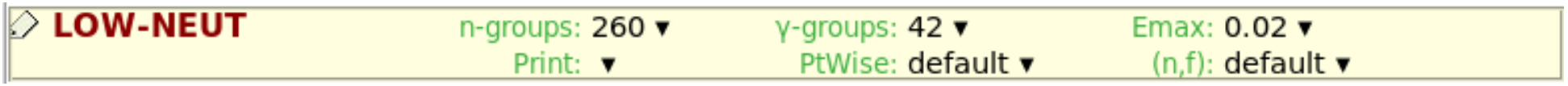
$$< \sigma_i >= \frac{\int_{E_{i,low}}^{E_{i,high}} \sigma(E)\Phi(E)\,dE}{\int_{E_{i,low}}^{E_{i,high}} \Phi(E)\,dE}$$

- Assuming a Φ(E)



Groupwise: cards

- **LOW-NEUT**: to activate, print



and optionally select some old point-wise treatment for a few selected isotopes/channels
NOTE: Group-wise is presently the default model for all FLUKA DEFAULTS

- **LOW-BIAS**: to set a GW neutron cut-off on a region basis

Groupwise: materials

MATERIAL	Name: SODIU_87	#	ρ: 0.97
Z: 11	Am: 22.99	A:	dE/dx: ▼
LOW-MAT	Mat: SODIU_87 ▼	LowMat: 23Na. Sodium 23, 87K ▼	

LOW-MAT sets the correspondence between FLUKA material and the GW low energy neutron cross sections

If material name = library name, there is no need of a LOW-MAT card.
The first match will be used.

It is a **mandatory** card if the names you give do not match the ones in the table

Chapter 10

Material			Temp.	Origin	RN	Name	Identifiers			Gam
9Be		Beryllium 9	296K	ENDF/B-VIIR0	Y	BERYLLIU	4	9	296	Y
9Be		Beryllium 9	87K	ENDF/B-VIIR0	Y	BERYLLIU	4	9	87	Y
B		Natural Boron	296K	ENDF/B-VIIR0	Y	BORON	5	-2	296	Y
B		Natural Boron	87K	ENDF/B-VIIR0	Y	BORON	5	-2	87	Y
10B		Boron 10	296K	ENDF/B-VIIR0	Y	BORON-10	5	10	296	Y
10B		Boron 10	87K	ENDF/B-VIIR0	Y	BORON-10	5	10	87	Y
11B		Boron 11	296K	ENDF/B-VIIR0	Y	BORON-11	5	11	296	Y
11B		Boron 11	87K	ENDF/B-VIIR0	Y	BORON-11	5	11	87	Y
C		Free gas natural Carbon	296K	ENDF/B-VIIR0	Y	CARBON	6	-2	296	Y
C		Graphite bound nat. Carbon	296K	ENDF/B-VIIR0	Y	CARBON	6	-3	296	Y
C		Free gas natural Carbon	87K	ENDF/B-VIIR0	Y	CARBON	6	-2	87	Y
N		Natural Nitrogen	296K	ENDF/B-VIIR0	Y	NITROGEN	7	-2	296	Y
N		Natural Nitrogen	87K	ENDF/B-VIIR0	Y	NITROGEN	7	-2	87	Y
14N		Nitrogen 14	296K	ENDF/B-VIIR0	Y	NITRO-14	7	14	296	Y
14N		Nitrogen 14	87K	ENDF/B-VIIR0	Y	NITRO-14	7	14	87	Y
16O		Oxygen 16	296K	ENDF/B-VIR8	Y	OXYGEN	8	16	296	Y
16O		Oxygen 16	87K	ENDF/B-VIR8	Y	OXYGEN	8	16	87	Y
19F		Fluorine 19	296K	ENDF/B-VIR8	Y	FLUORINE	9	19	296	Y
19F		Fluorine 19	87K	ENDF/B-VIR8	Y	FLUORINE	9	19	87	Y
23Na		Sodium 23	296K	JENDL-3.3	Y	SODIUM	11	23	296	Y
23Na		Sodium 23	87K	JENDL-3.3	Y	SODIUM	11	23	87	Y
Mg		Natural Magnesium	296K	JENDL-3.3	Y	MAGNESIU	12	-2	296	Y
Mg		Natural Magnesium	87K	JENDL-3.3	Y	MAGNESIU	12	-2	87	Y
27Al		Aluminium 27	296K	ENDF/B-VIIR0	Y	ALUMINUM	13	27	296	Y
27Al		Aluminium 27 SelfShielded	296K	ENDF/B-VIIR0	Y	ALUMINUM	13	1027	296	Y

Pointwise: key features

- Modern C++ implementation → keeping in mind the future evolution of FLUKA
- Heavily optimized:
  - Caching a lot of necessary information (pre-tabulation of cumulative distributions)
  - Using adaptive algorithms to improve performance
  - Improved sampling of secondary distributions (using tight envelopes in case of rejection)
  - An innovative idea: a fast indexing of cross-sections using a cheap CPU $\log_2$ approximation
  - Hierarchical sampling of channels
- Thermal Scattering Law (TSL) S(α,β,T) for several materials
- Doppler broadening at any temperature on loading
- Preform “fully” correlated emission of reaction products by treating an N-body final state as consecutive 2-body emissions (kinematics gradually constraining database distributions)

Pointwise: data sets

- Due to huge size, the neutron data are provided as separated packages to download. One per major dataset (newest evaluation).
- The “default” of FLUKA v4.3 is the JEFF-3.3 library

  {FlukaDir}/data/neutron/{library}
- Old evaluations are provided as well for comparison purposes

Structure:

- JEFF-3.3
  - Elastic
    - CrossSection
    - FS
  - Capture
    - CrossSection
    - FS
    - FSMF6
  - Inelastic
    - …
  - Fission
    - …
  - ThermalScattering
    - Coherent
    - Incoherent
    - Inelastic

One file per isotope, per channel, XS & FS

Cross-sections

- Preprocessed at 0K [except TSL]

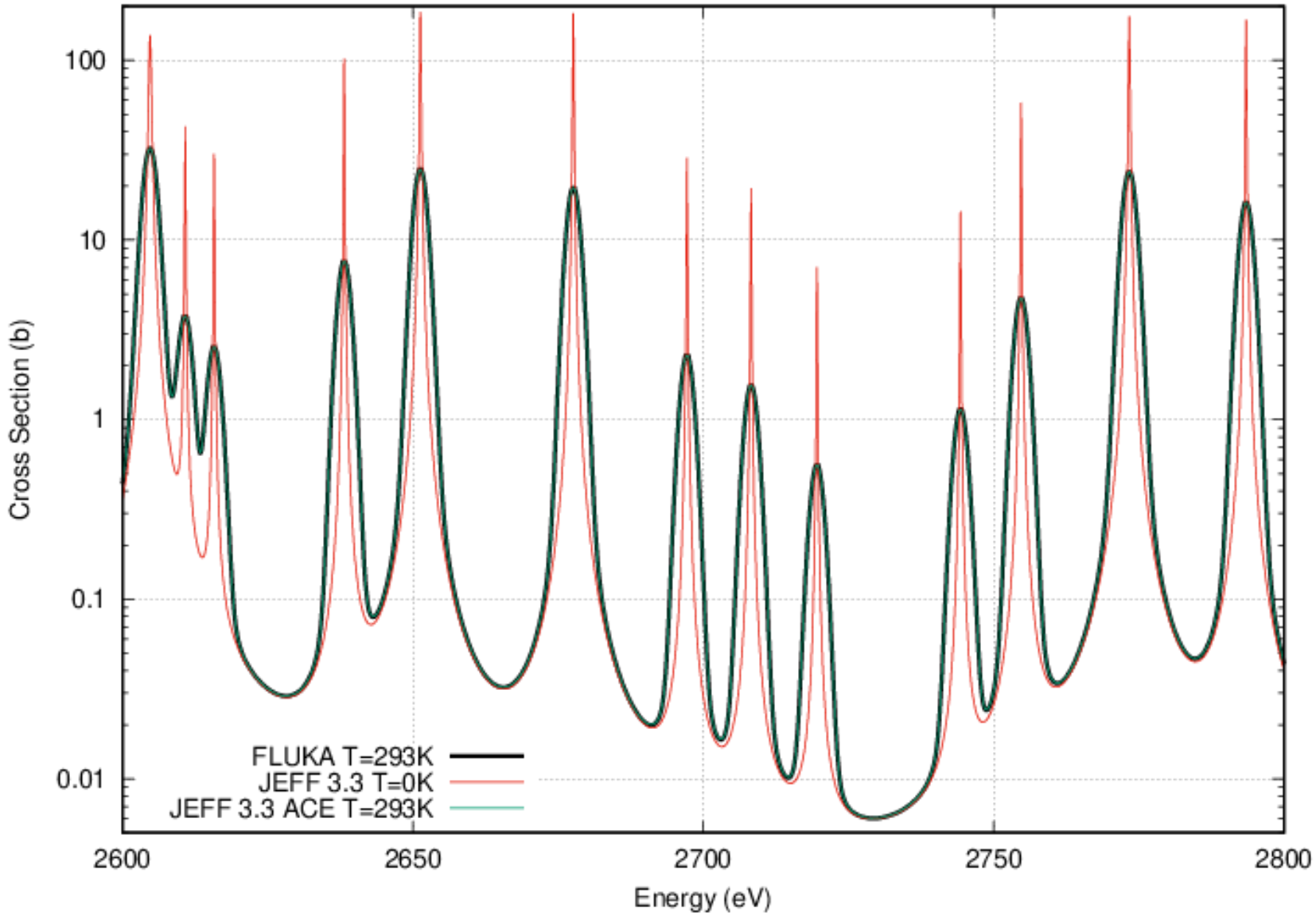
- Tabulation of (Ei,σi) with accuracy < 0.1%
  Energy grid is not uniform among channels to ensure the best representation of the resonances

- During Initialization:
  - Doppler broadened to the T required using a fast adaptive numerical integration

$$\sqrt{E}\sigma(E,T_2) = C\int_0^{\infty}\sigma(x,T_1)\sqrt{x}\left[e^{-\alpha\left(\sqrt{E}-\sqrt{x}\right)^2} - e^{-\alpha\left(\sqrt{E}+\sqrt{x}\right)^2}\right]dx$$

  - Always ensuring precision better than 0.1% (as provided in the initial data)

Doppler broadening



Online Doppler Broadening example of ^{113}Cd vs JEFF processed with NJOY

Interactions

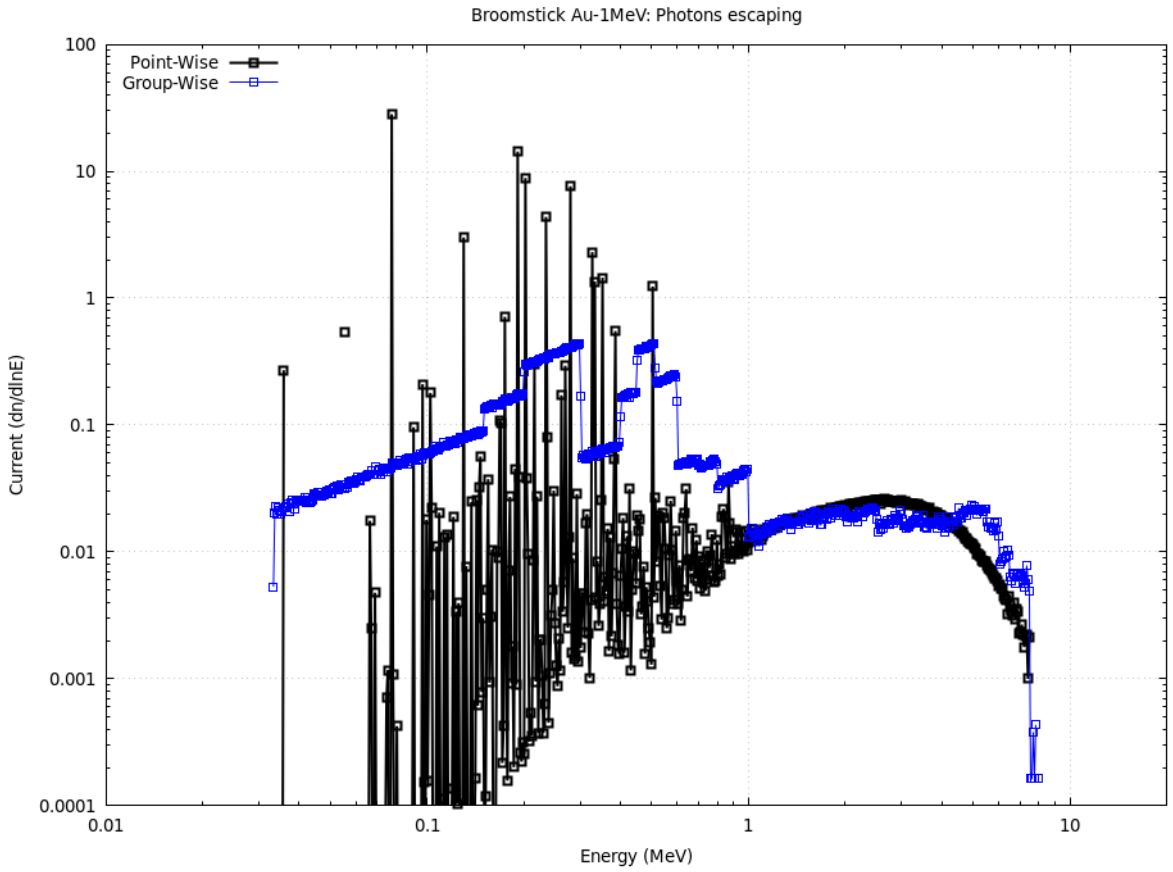
- Divided into 4 main categories
  - Elastic
  - Capture
  - Inelastic
    - Further subdivided into 36 channels
    - (n,n'), (n,p), (n,d), (n,3He), (n,α) have special treatment
  - Fission
    - Fission fragments (database or Wahl systematics)
- All isotopes have elastic, capture and some inelastic channels (typically open at high energies, with a few exceptions)
  Few isotopes have fission channel

Elastic

- Above ~5eV the target nucleus is considered at rest
- Below ~5eV the target nucleus motion is sampled from a weighted Maxwell Boltzmann distribution (using the constant cross section model)
  → Can lead to an impossible situation moving in the same direction with higher speed…
- The recoils are explicitly calculated and pushed in the stack
- On user request S(α,β,T) treatment can be enabled for a handful of isotopes / materials

Radiative Capture

- The neutron is absorbed leading to an excited nucleus
  → calling the standard FLUKA de-excitation module
- All known γ lines will be reproduced
- Currently all isotopes will de-excite to the ground state.
  Work is going on to properly use the probability to end in an isomeric state if the information is available in the database
- The recoil is properly generated

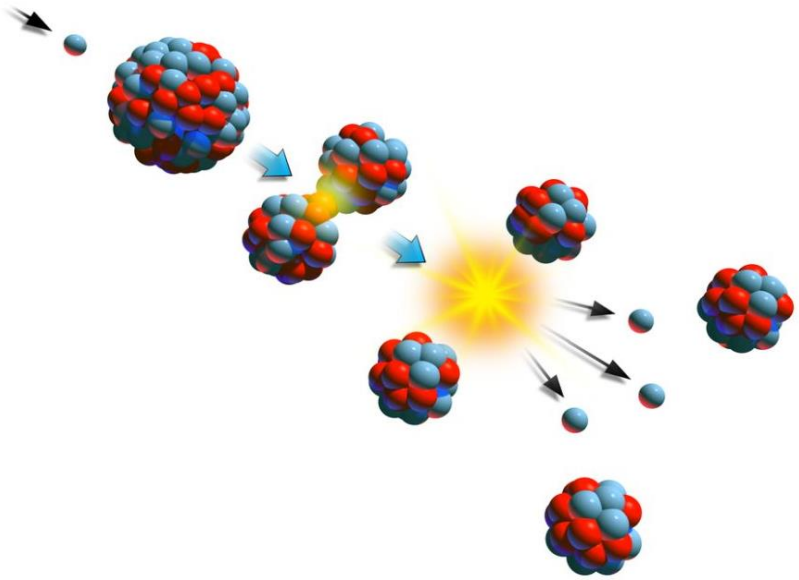


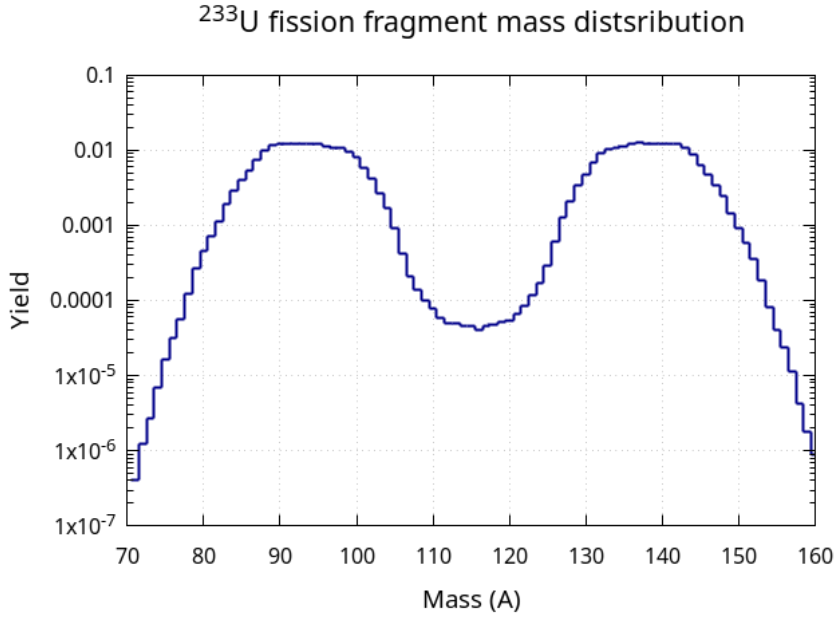
Inelastic

- FLUKA will select a sub-channel based on the XS, request the secondaries, Q-value and residual, and it will try to perform the interaction
- It will sample one-by-one the secondaries (except the photons) from the distributions, getting back the Energy and $cos\theta$ of the ejectile, either in LAB or in CMS.
- Impossible situations can arise → It will reset the interaction and try to perform it again. If after several trials the interaction still fails, it will abort the inelastic scattering and request another channel
- On success it will de-excite the nucleus with the standard FLUKA module.

Fission timeline

- Compound nucleus n+(Z,A)→ (Z,A+1)
- ~10% neutrons emitted pre-scission if kinematically possible
- Scission → Split into two or three fragments
- Excited fragments emit prompt neutrons proportionally to their neutron excess and gammas from the database distribution
- Fragments are sampled either from the database or from Wahl systematics
- Fragments can further emit delayed neutrons not implemented!
- Beta decay of fission fragments via a decay run
- Neutrino emission of fission fragments – not implemented





Thermal Scattering Law S(α,β,T) (1/2)

- For neutrons with thermal energies, generally less than ~4 eV, the kinematics of scattering can be affected by chemical binding and crystalline effects of the target molecule. If these effects are not accounted in a simulation, the reported results may be highly inaccurate.

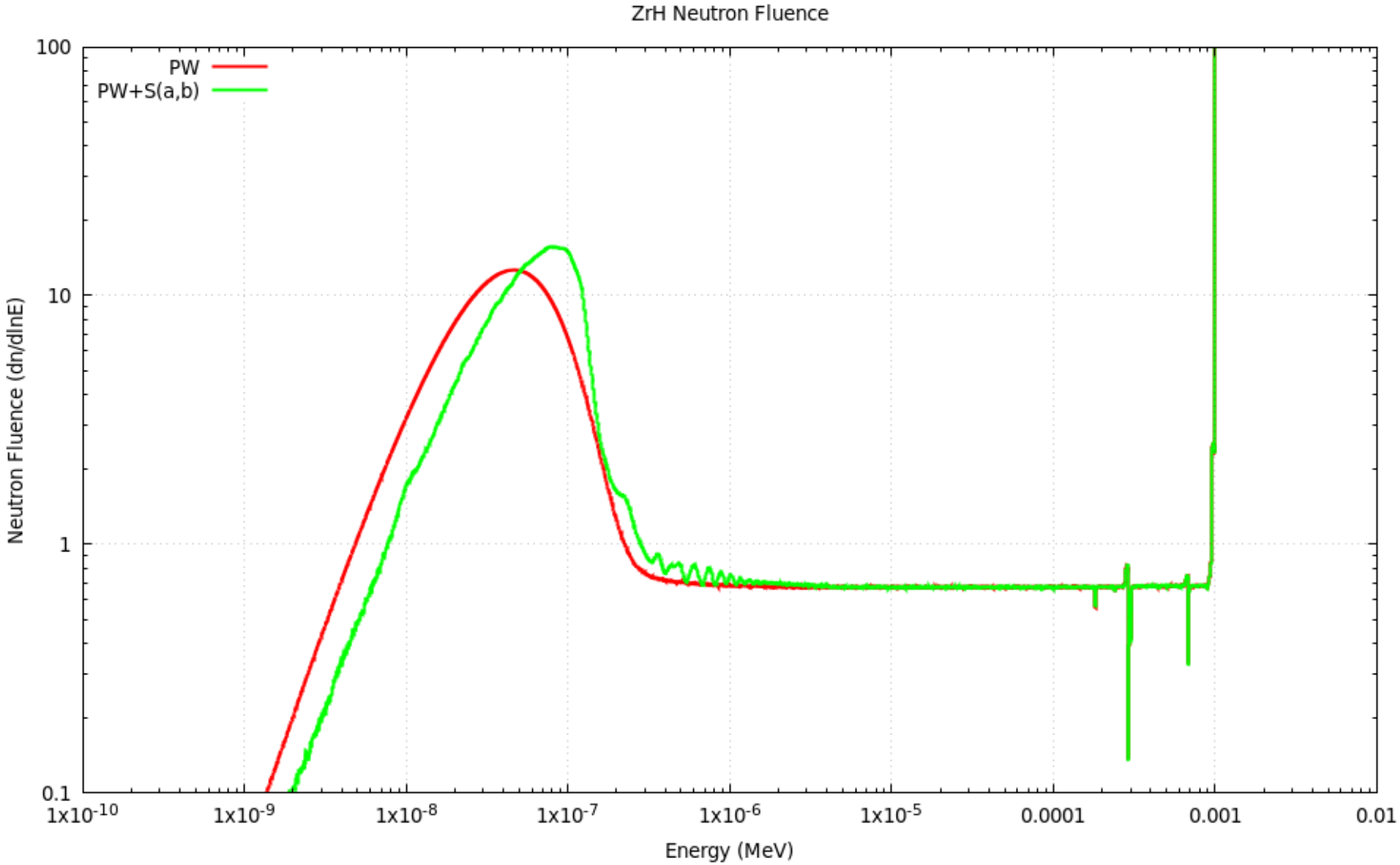
- The theory behind S(α,β,T) is rooted in quantum mechanics and is quite complex.

- Luckily NJOY can preprocess the Thermal Cross section data and prepare 3D tabulations with:
  - [Incoming neutron energy; Outgoing energy; Outgoing angular distribution]
  - [Incoming neutron energy; Bragg Edge; Outgoing angular distribution]

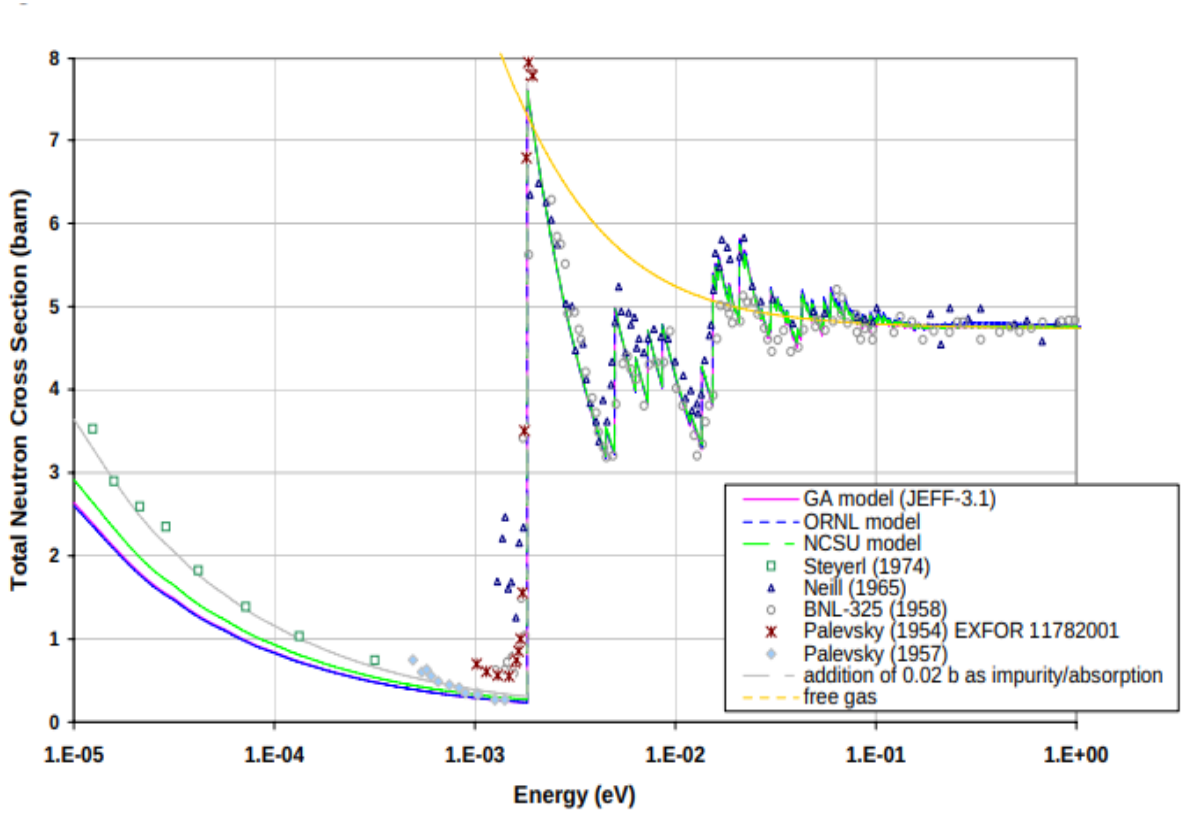
Thermal Scattering Law S(α,β,T) (2/2)

- Channels:
  the names do not refer to the nuclear interaction but at which state they leave the scattering system
  - **Elastic** – the neutron energy remains the same, the angle is changing
    - **Coherent** – discrete angles depending on the crystal direction vs neutron direction and Bragg edge selected, on crystal lattice
    - **Incoherent** – continuous distribution of angles mostly on hydrogenous materials
  - **Inelastic** – the scattering system is left in an excited state
- 58 materials available
  - al_metal, be_beo, be_metal, benzen, d_heavy_water, d_ortho_d2,
  - d_para_d2, fe_metal, graphite, h_l_ch4, h_ortho_h2, h_para_h2,
  - h_polyethylene, h_s_ch4, h_water, h_zrh, o_beo, o_uo2, u_uo2,
  - zr_zrh, …
- At various fixed temperatures per material: 4 .. 800 °K

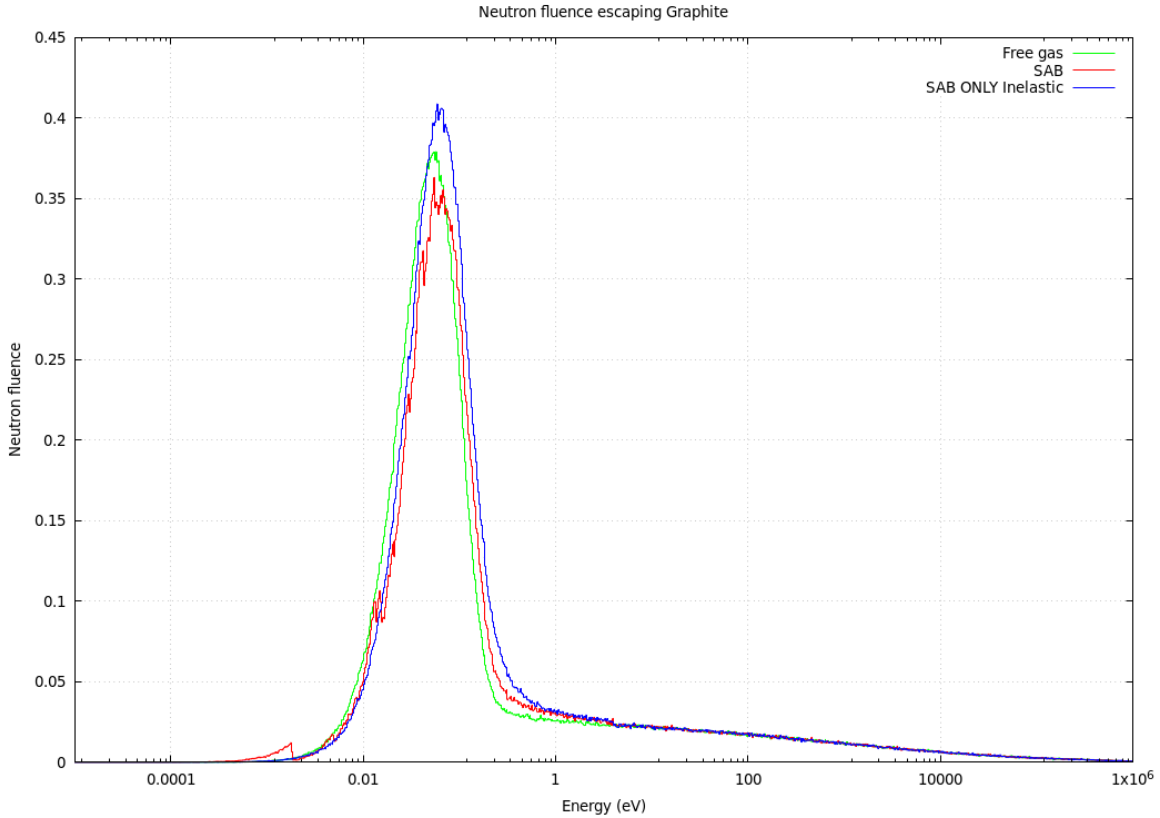
Example S(α,β,T) on ZrH_2



Example S(α,β,T) on Graphite



https://www-nds.iaea.org/publications/indc/indc-nds-0475.pdf



https://fluka-forum.web.cern.ch/t/4528/7

Usage: LOW-PWXS

- **`LOW-PWXS`** card controls the new pointwise treatment in FLUKA
- WHAT(1):
  - **empty/0** = use PW treatment for this isotope (default)
  - **>0** Isotope code **Z*10000 + A*10 + iso**
  - **-1** = switch to OLD behavior, use GW/Old PW treatment for this isotope
- WHAT(2):
  - **S(α,β,T)** database to associate with this isotope
- WHAT(3):
  - **Temperature in °K** to Doppler broaden XS (default 296 °K)
- WHAT(4,5,6):
  - **FLUKA material** range
- SDUM:
  - Select **database** to be used. Empty = **default** (For the present v4.3 default = JEFF-3.3)

LOW-PWXS: examples

- Without any argument to enable PW treatment for all isotopes

```
LOW-PWXS          Mat: ▼      to Mat: ▼      Step:
          db: ▼   IAZ:        S(α,β): ▼      T:
```

- With WHAT(1) = -1 to use OLD way GW+PW for some isotopes

```
LOW-PWXS          Mat: ▼      to Mat: ▼      Step:
          db: ▼   IAZ: -1     S(α,β): ▼      T:
```

- Enable PW for HYDROGEN (natural 1H + 2H)
  Load from **endf** database
  Doppler broaden to **350 °K**
  Select the **h_water** S(α,β,T) **ONLY** for **^{1}H**

```
LOW-PWXS          Mat: HYDROGEN ▼   to Mat: ▼      Step:
          db: endf ▼  IAZ: 10010      S(α,β): h_water ▼   T: 350
```

- *At present the full pointwise treatment is not enabled by default in FLUKA.*
  It will be the default in the coming releases.

Scoring: USR{BDX, TRACK, YIELD, COLL}

Groupwise:

- When low-energy neutrons are requested to be scored, FLUKA will use the FIXED energy group structure of 260 groups, independent on what is supplied on the card

Pointwise:

- FLUKA will honor the user histogram settings:
  ONLY IF the materials of the regions involved have ALL constituents declared as point wise.
- Special attention on VACUUM which can be declared as point or groupwise with the `LOW-PWXS` card

FLUKA output

- Search for the section:
  Low energy neutron Point Wise materials

- For each FLUKA material that contains PW isotopes it will dump the natural composition, temperature, abundance, dataset used, and time for the Doppler broadening

- When something goes wrong verify that what was asked was what you got

```
*** Low energy neutron Point Wise materials
  ###  Material   Z   A m     T(K)    Dataset
    3  HYDROGEN   1   1 0    296.0    default
         S(a,b)   1   1 0             h_water
    6  CARBON     6   0 0    296.0    default
                  12 0    0.9893
                  13 0    0.0107
    7  NITROGEN   7   0 0    296.0    default
                  14 0    0.9963
                  15 0    0.0037
    8  OXYGEN     8   0 0    296.0    default
                  16 0    0.9976
                  18 0    0.0020
                  17 0    0.0004
Doppler broadening Z= 1 A=  1 to T=296K time=0.018041s
Doppler broadening Z= 6 A= 12 to T=296K time=0.002211s
Doppler broadening Z= 6 A= 13 to T=296K time=0.002787s
Doppler broadening Z= 7 A= 14 to T=296K time=0.00405s
Doppler broadening Z= 7 A= 15 to T=296K time=0.001994s
Doppler broadening Z= 8 A= 16 to T=296K time=0.002313s
Doppler broadening Z= 8 A= 18 to T=296K time=0.002716s
Doppler broadening Z= 8 A= 17 to T=296K time=0.003154s
Doppler broadening Z=12 A= 24 to T=296K time=0.006679s
Doppler broadening Z=12 A= 26 to T=296K time=0.005807s
Doppler broadening Z=12 A= 25 to T=296K time=0.008832s
Doppler broadening Z=13 A= 27 to T=296K time=0.011427s
Doppler broadening Z=26 A= 56 to T=296K time=0.080996s
Doppler broadening Z=26 A= 54 to T=296K time=0.037268s
Doppler broadening Z=26 A= 57 to T=296K time=0.066767s
Doppler broadening Z=26 A= 58 to T=296K time=0.149089s
```

Summary

- Low energy neutrons ≤20MeV have special treatment in FLUKA.
- Two methods are available:
  - **Groupwise**: old coarse, but fast treatment. Few isotopes/channels are in point wise.
    It is currently the FLUKA default for compatibility reasons (to be revised)
  - **Pointwise**: superior model, highly optimized, giving access to all latest available neutron data, explicit treatment of interactions in fully correlated way
- What to use:
  - Prefer the use of **pointwise**
    - **unless:** Speed is an issue and you are not interested in the detailed neutron treatment
      Warning: Neutrons can be indirectly responsible for many effects (activation, damage, SEU)
    - When unsure, use pointwise to properly take into account all physical effects
  - Groupwise can work nicely for shielding applications
  - Optionally you can mix point- and groupwise treatment in the same problem


FLUKA