Low energy (≤20MeV) neutron interactions

Outline

- Some neutron physics and neutron interactions below 20 MeV
  (small reminder above 20 MeV in passing)

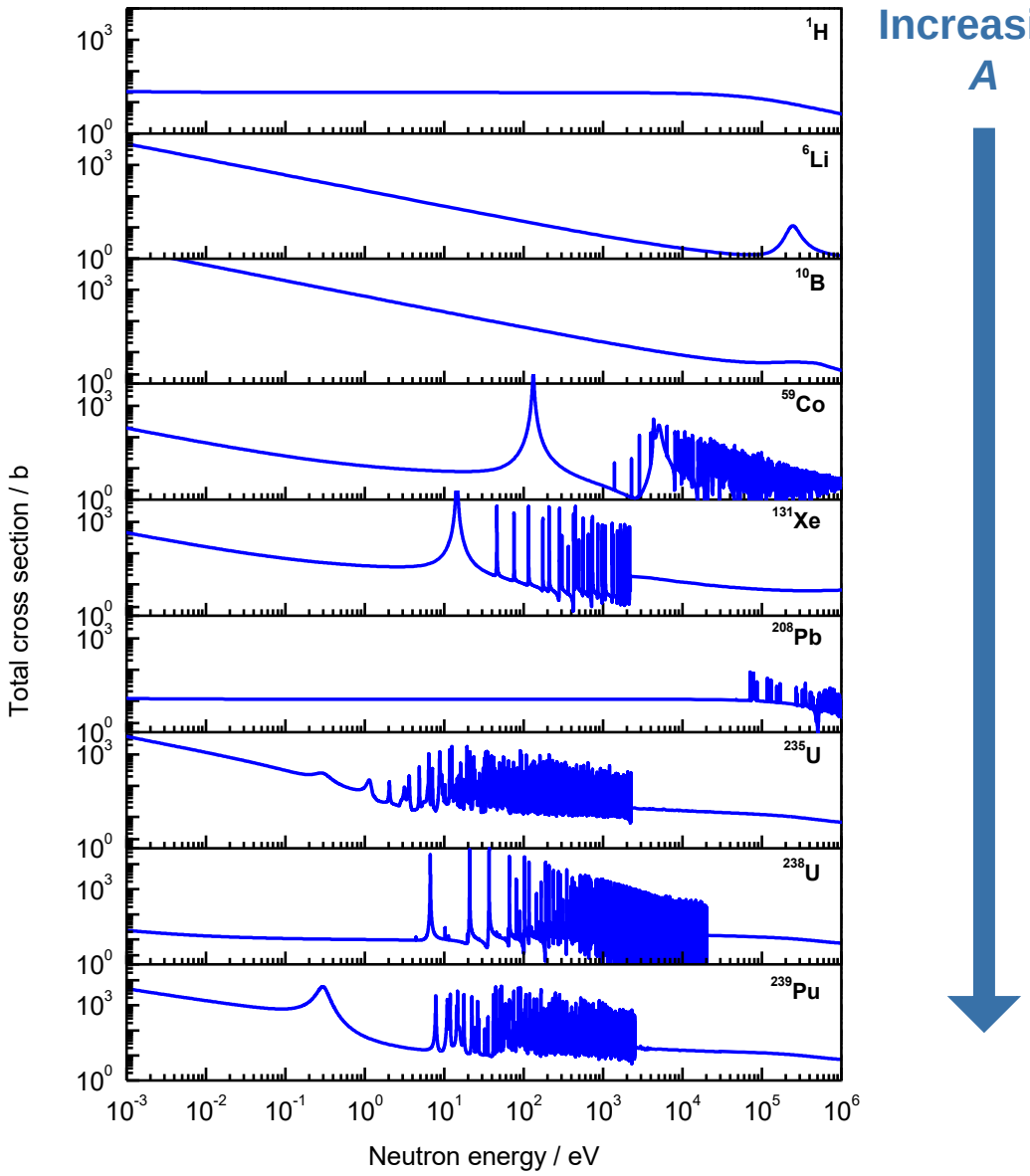
- Group-wise treatment:
  - Legacy treatment

- Point-wise treatment:
  - Introduced in v4-3.0
  - Default from v4-4.0
    for DEFAULTS: NEW-DEFA, PRECISION, DAMAGE

- *Reminder: lethargy units*

Why neutrons?

- Even when not studying a neutronics problem, neutrons can be generated as secondary particles
- They can induce significant backgrounds in detectors, e.g. via neutron capture or recoil generation
- Important for shielding considerations: high penetration (and even multiplication)
- They can activate/damage materials
- Significant even at very low energies (transport down to 10^{-14} GeV in FLUKA): high-energy secondaries can be produced by near zero-energy neutrons
- Interaction probability varies wildly with neutron energy and target nucleus →
  - …and cannot be theoretically predicted
- A special treatment is clearly required



P. Schillebeeckx et al., "Neutron Resonance Spectroscopy for the Characterisation of Materials and Objects", Report EUR 26848 EN (2014) DOI: 10.2787/98278

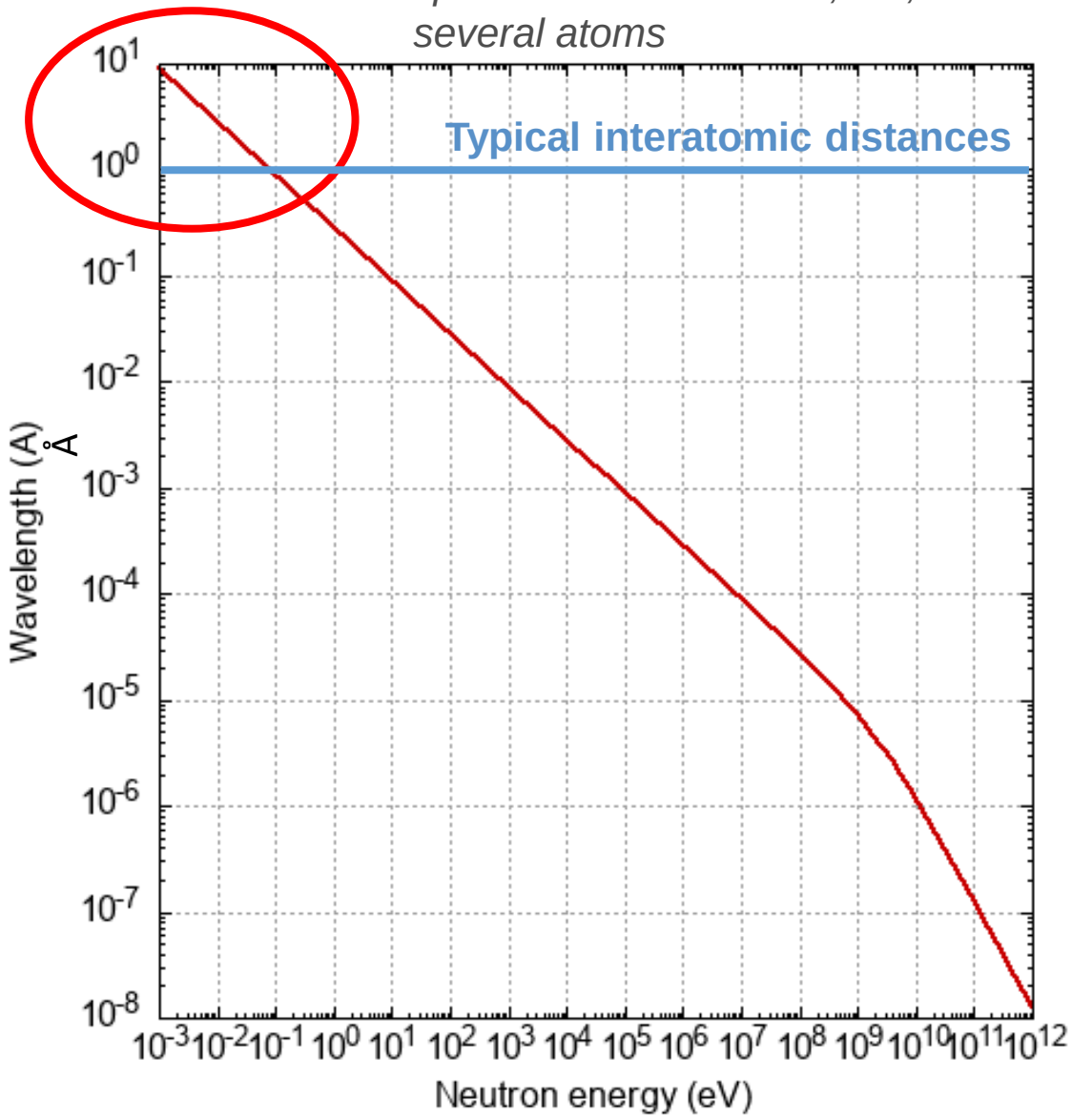
Low-energy neutron interactions

Neutron (n) interaction generalities

- Neutrons **do not feel the Coulomb force**:
  - No Coulomb scattering on atoms
  - No interaction with target electrons (no dE/dx)
  - No Bremsstrahlung
- They **feel the strong force** (nuclear interaction):
  - Elastic scattering: (n,el)
  - Capture: (n,γ)
  - Fission: (n,f)
  - Inelastic channels: (n,n'),(n,p),(n,2n),(n,d),(n,a)…
- Below ~eV energies, they:
  - become sensitive to local atomic arrangement
  - scatter coherently on molecules / crystal lattice
  - thermal scattering laws S(α,β,T)
- Spin-1/2: neutrons probe magnetic/spin densities in matter*

** usually not accounted for in MC codes*

Below O(1) eV, neutron wavelength spreads over several Å, i.e., over several atoms



Neutron interactions in FLUKA - in a nutshell

- Above 20 MeV, neutrons are treated in FLUKA on equal footing with other hadrons:
  - **Nuclear elastic** scattering: based on the Ranft model *(J. Ranft, Part. Acc. 3 129-161, 1972)*
  - **Nuclear inelastic** interactions: FLUKA's hadron-nucleus reaction model (PEANUT)

- Below 20 MeV (**"low energy neutrons"** in FLUKA slang), cross sections exhibit a rich structure of **resonances**:
  - No effective model to capture/describe resonances in a systematic way
  - One must resort to evaluated nuclear data (for both group- and point-wise approaches, see below)

- Neutron **decay** (mean life-time of 879.6 s, *i.e.* about 15 min): $n \rightarrow p + e^- + \bar{\nu}_e$

- **Gravitational** effects* (meV n over 100s of m, e.g. in time-of-flight experiments)

** not modelled in FLUKA*

Neutron moderation

- Neutrons are “moderated” (*i.e.* their kinetic energy is progressively reduced) through successive scattering with the surrounding nuclei in which a fraction of the energy is transferred to the nucleus

- An ideal neutron **moderator** has low atomic mass (to maximise energy transfer per collision), a high neutron scattering cross section (to maximise collisions), a low neutron capture cross section (to reduce depletion of the neutron population) and is resistant to high levels of radiation
  - Typically in reactors: light/heavy water (^{1}H and ^{2}H) (and ^{16}O present), carbon (graphite) ^{12}C

- Eventually, neutrons are “thermalised”

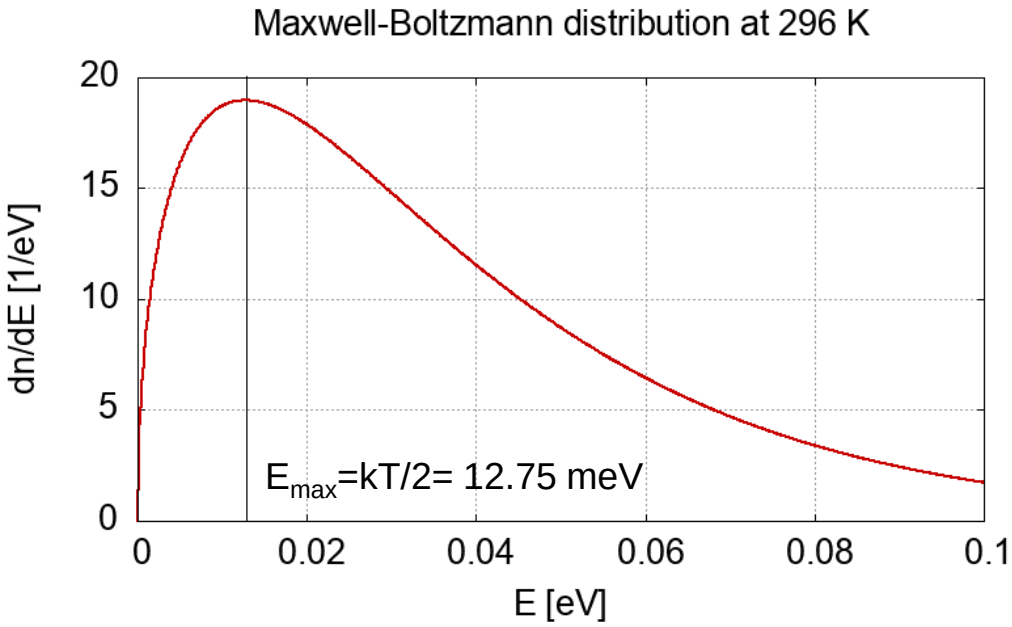
Neutron thermalisation

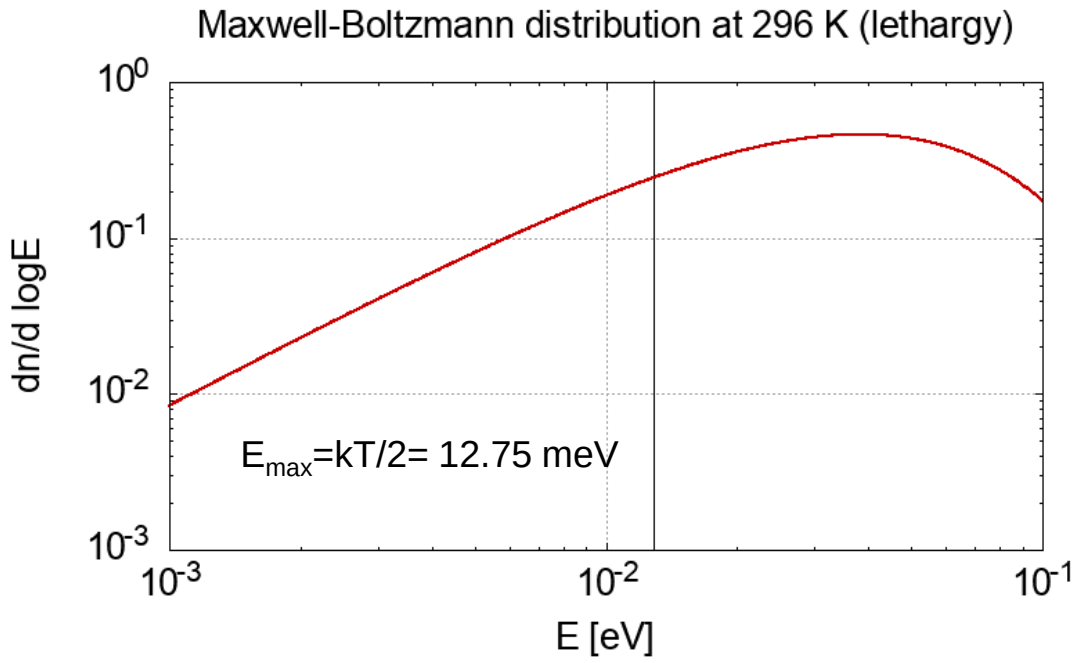
- Thermal motion energy: O(*kT*)
- **At 296 K, *kT*=25.5 meV**
- At/near these energies, neutrons collide elastically (losing or gaining energy) in a “gas” of nuclei, eventually reaching **thermal equibrium**
- The energy distribution of non-relativistic classical particles in thermodynamic equilibrium at temperature *T* is given by the **Maxwell-Boltzmann distribution**:

$$\frac{\mathrm{d}n}{\mathrm{d}E} = 2\sqrt{\frac{E}{\pi}}\left(\frac{1}{kT}\right)^{3/2} \mathrm{e}^{-E/kT} \qquad \mathrm{argmax}(E) = \frac{kT}{2}$$

- In lethargy representation*, maximum shifts to higher energies

** recall the scoring lecture, and see later*





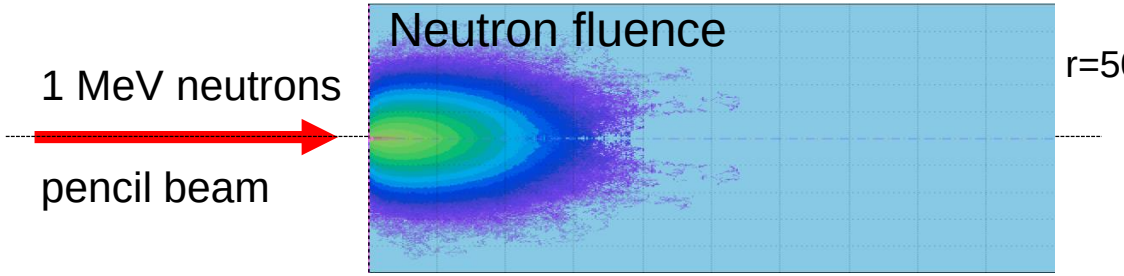
Thermalisation in H_2O

- Example: n pencil beam, E=1 MeV, impinging on a water cylinder (r=50 cm, varying h)
- $\lambda_{(n,el)}$(1 MeV) = 3.5 cm (in water)
- **For h ≪ $\lambda_{(n,el)}$, n barely scatter**
- **For h ~ $\lambda_{(n,el)}$, n start to scatter elastically:**
  - Change direction (possibly staying longer in the cylinder)
  - Lose energy: possibly probing energy ranges where (n,el) cross section drastically increases
- **For h ≫ $\lambda_{(n,el)}$:**
  - Intensive elastic scattering
  - Thermal equilibrium: Maxwell-Boltzmann flux*:

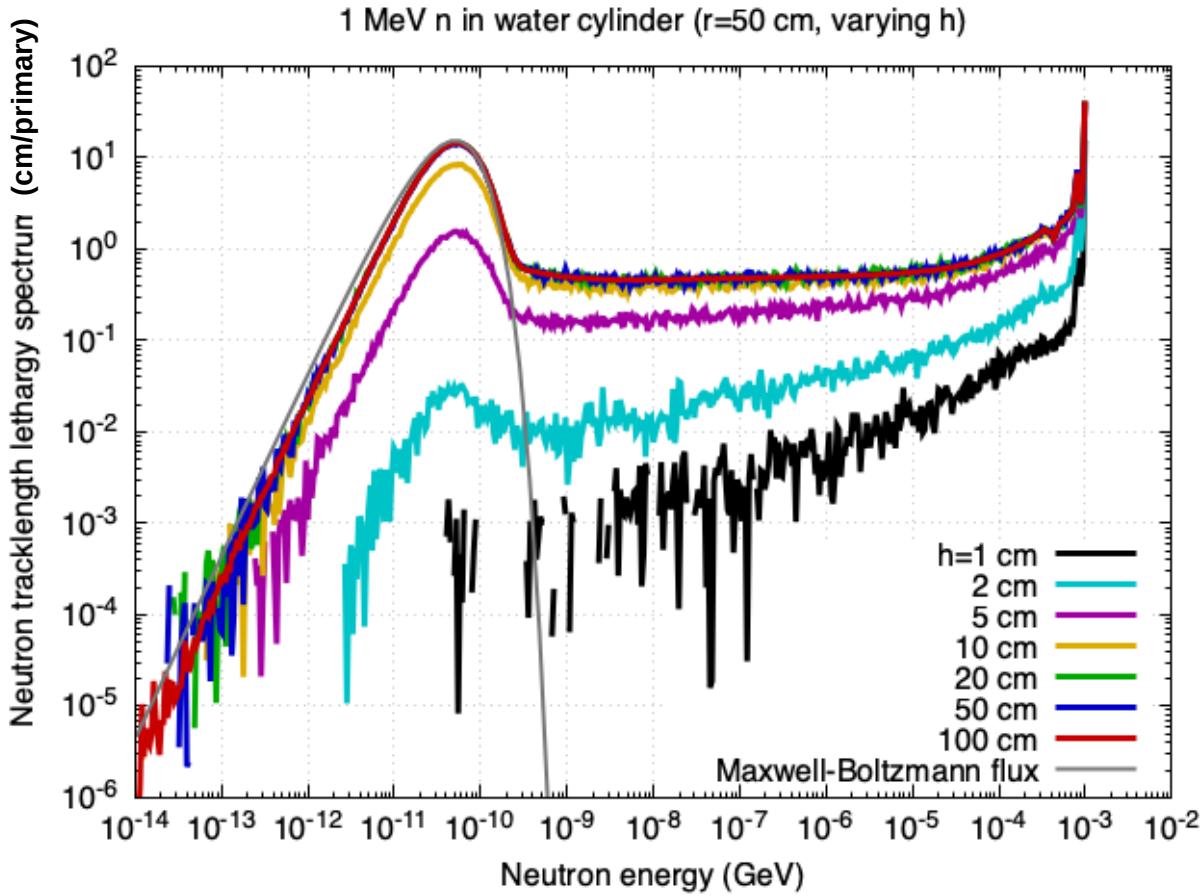
$$\frac{\mathrm{d}\Phi}{\mathrm{d}E} = \frac{\mathrm{d}n}{\mathrm{d}E} v(E) = 2^{3/2} \frac{E}{\sqrt{m\pi}} \left(\frac{1}{kT}\right)^{3/2} \mathrm{e}^{-E/kT}$$

- (n,γ) on either ^{1,2}H or ^{16,17,18}O eventually consumes the neutron flux in favor of MeV photons

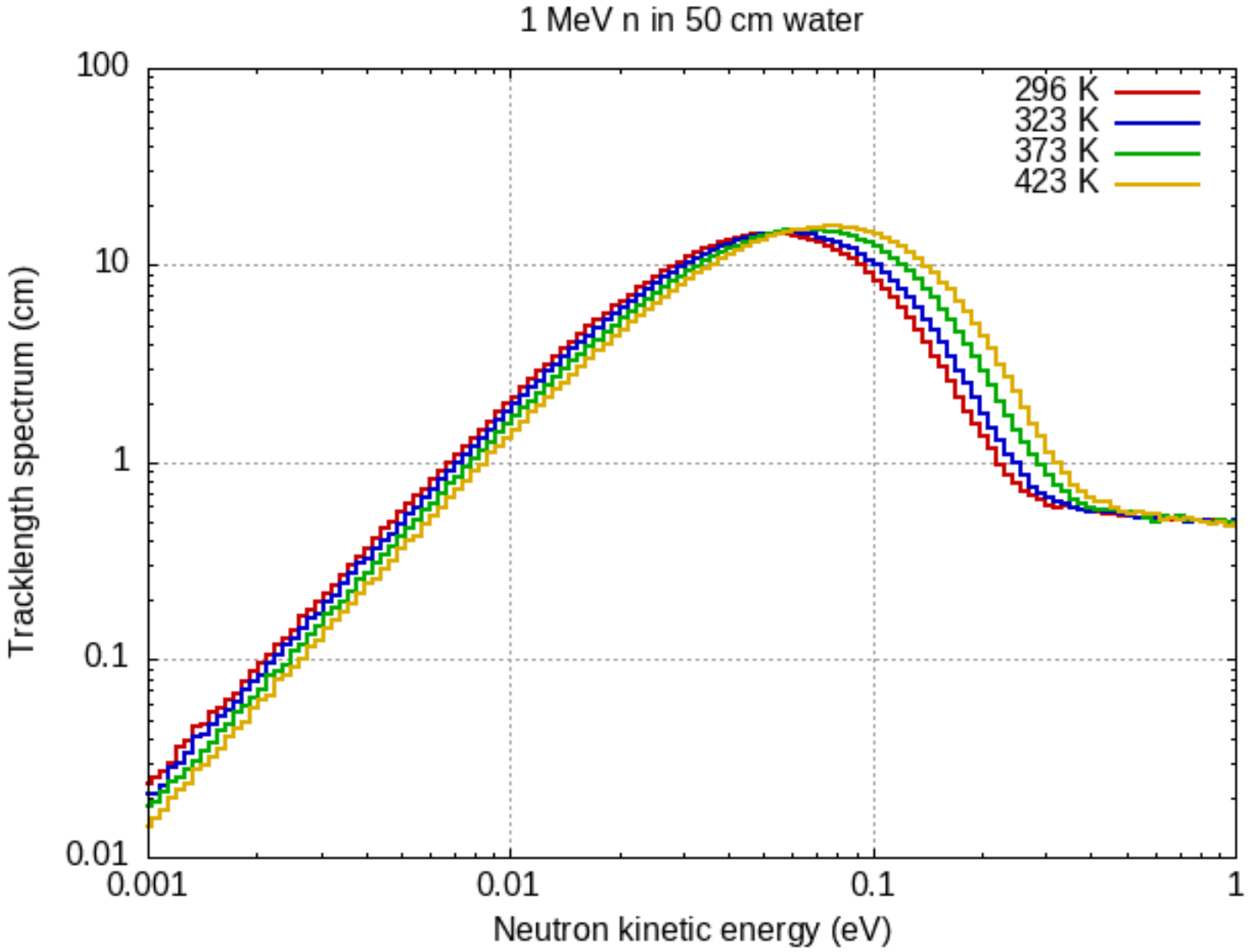
** Small detail discussed later: S(α,β,T)*



Varying h, here e.g. h=100 cm



Thermalisation at different temperatures



- The thermal peak indeed shifts linearly with the temperature
- Energies below about O(1) eV are loosely called **“thermal”**

Neutron reactions of interest

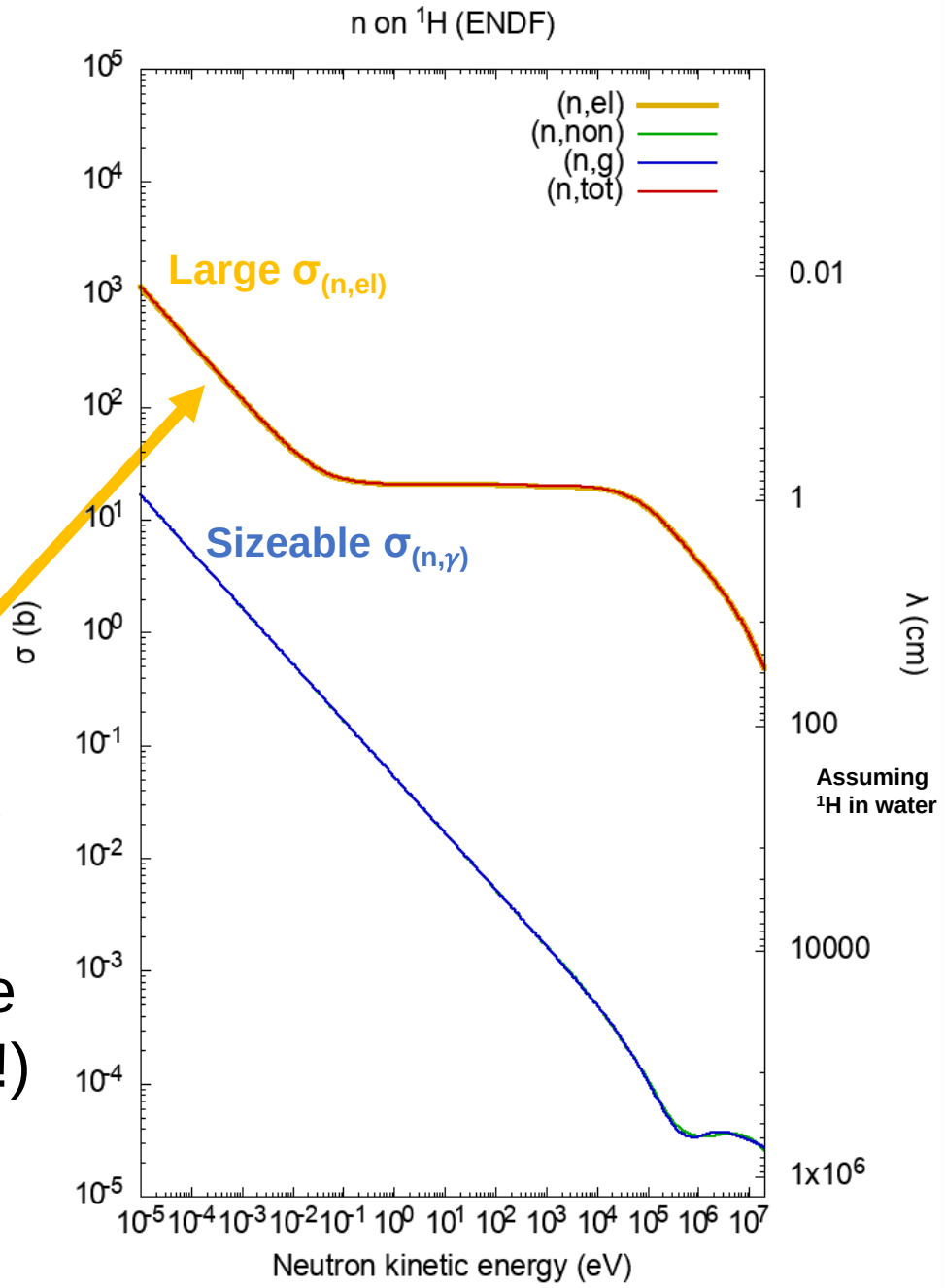
$^{1}H(n,el)$ | $^{2}H(n,el)$ | $^{10}B(n,\alpha)$ | $^{nat}Cd(n,\gamma)$ | $^{235}U(n,f)$

^{1}H(n,el)

- Maximum energy transfer from n to ^{1}H, i.e. a proton (for $E_{kin} \ll m_n$):

$$E_{\mathrm{rec,max}} = \frac{4 m_p m_n E_{\mathrm{kin}}}{(m_p + m_n)^2} \approx E_{\mathrm{kin}}$$

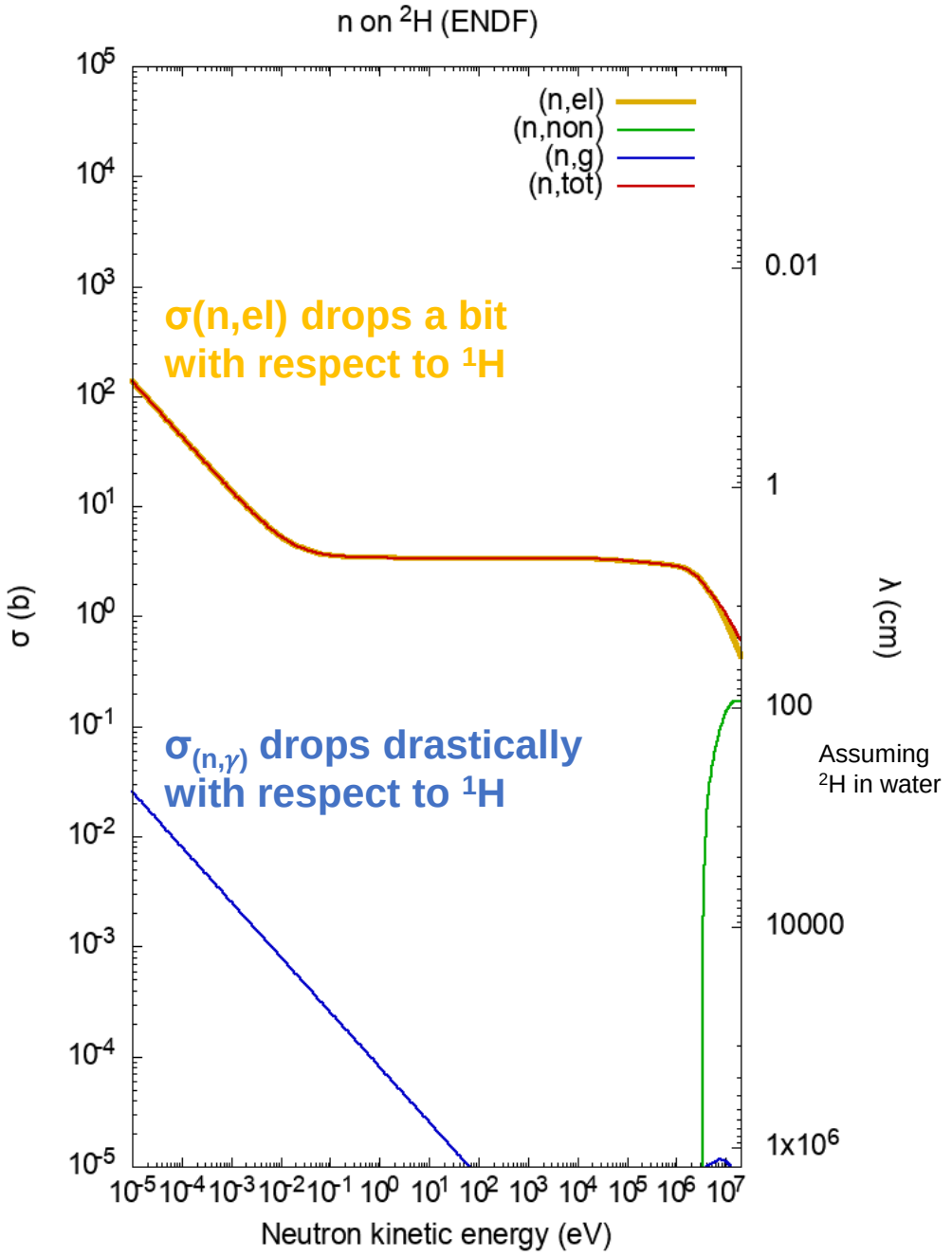
  - (not necessarily the most likely energy transfer!)
- In few collisions, n have the chance to transfer a large fraction of kinetic energy to target ^{1}H
- n energy quickly drops below the eV domain, where $\sigma_{(n,el)}$ increases drastically as $1/v$, i.e. $1/\sqrt{E}$
- At these energies, σ(n,γ) becomes sizeable: capture depletes the neutron flux generating MeV photons (!)
- One must track neutrons down to thermal energies



^{2}H(n,el)

- We already saw: compounds containing ^{1}H are good neutron moderators
- But ^{1}H has a sizeable (n,γ) cross section.
  At thermal energies:
  - $\sigma_{(n,\gamma)}/\sigma_{(n,el)} \sim 10^{-2}$ for ^{1}H
  - $\sigma_{(n,\gamma)}/\sigma_{(n,el)} \sim 10^{-4}$ for ^{2}H
- For applications requiring a high thermal neutron flux, it is advantageous to employ ^{2}H (fewer neutrons captured on the way to thermalisation)
- ^{2}H still has good moderator properties:

$$E_{\mathrm{rec,max}} = \frac{4 m_d m_n E_{\mathrm{kin}}}{(m_d + m_n)^2} \approx \frac{8}{9} E_{\mathrm{kin}}$$



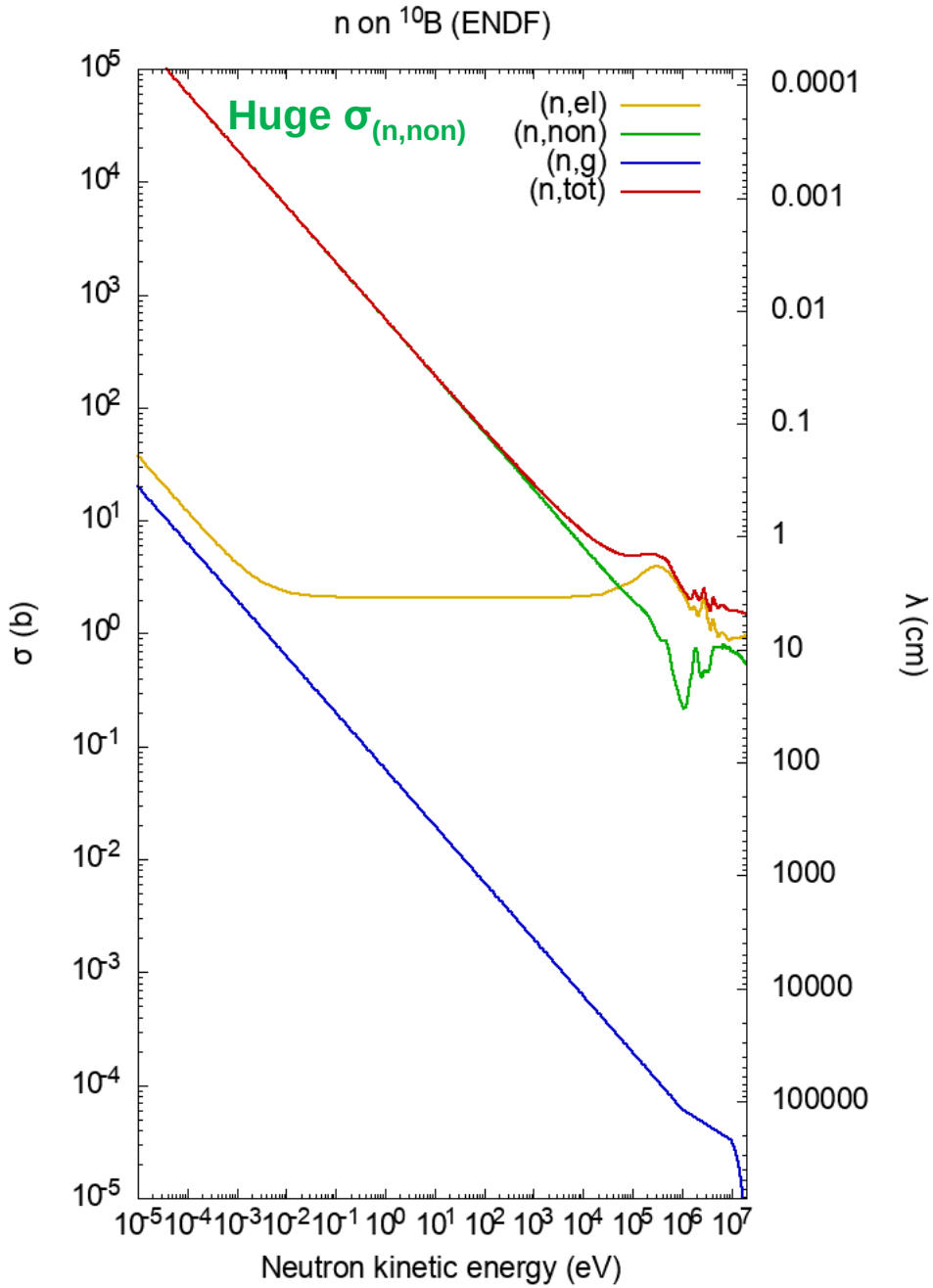
$^{10}B(n,\alpha)$

- $\sigma_{(n,el)}$ is only slightly lower than for $^{1,2}H$
  - But: $E_{rec,max}$(n on ^{10}B) ≪ E_{kin}
  - ^{10}B is not as effective a moderator as $^{1,2}H$
- However, the **$^{10}B(n,\alpha)$** channel has a very large σ:

$$^{10}B + n \rightarrow {}^{7}Li + \alpha + \gamma$$

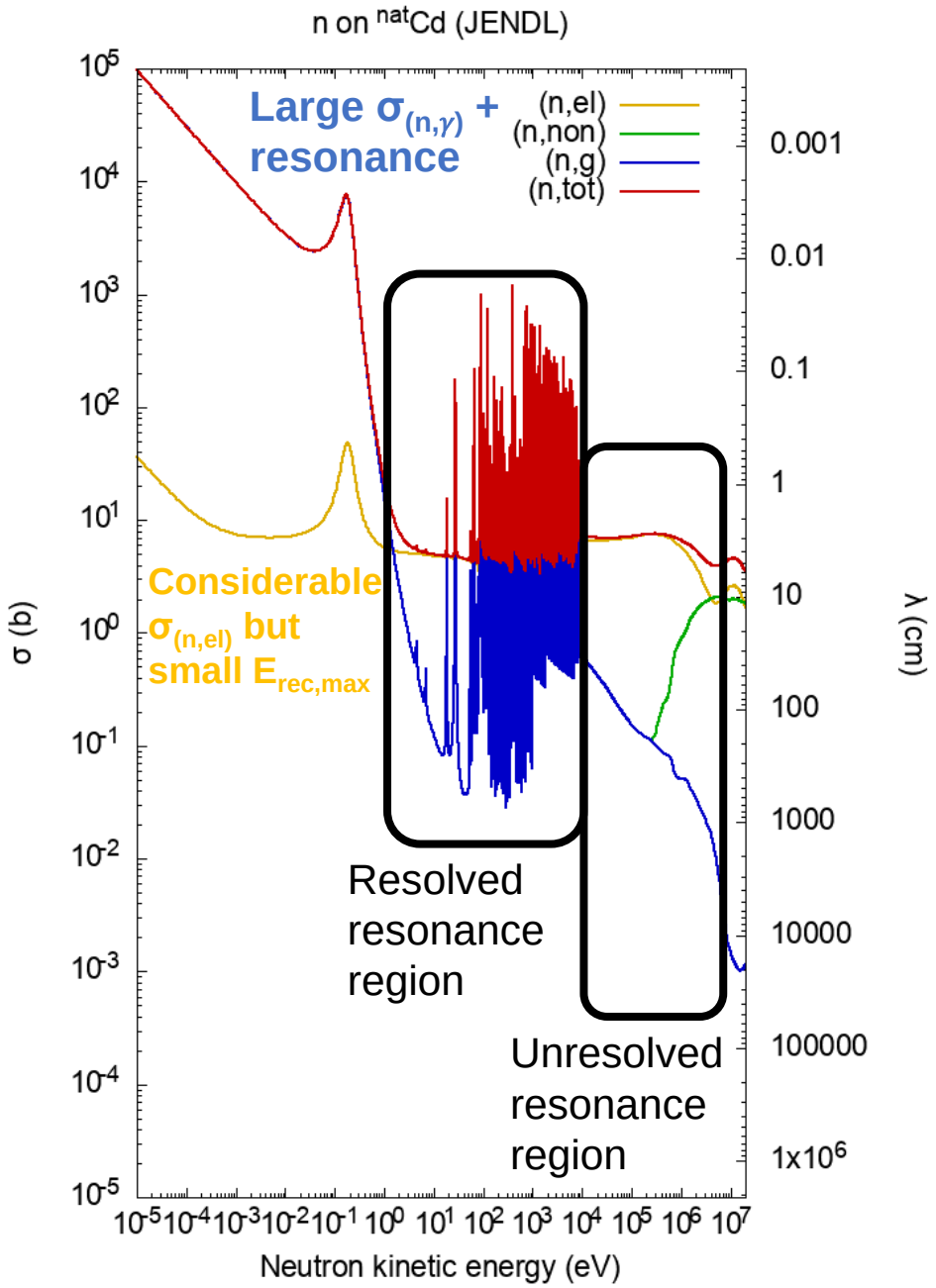
  - σ~10^3-10^5 b, i.e. mean free paths ≪ 100 μm
  - ^{7}Li and α have short range (< 10 μm)
- Basis for various applications:
  - boron neutron capture* therapy (BNCT)
  - boron rods in nuclear power plants to control n flux
  - borated moderators: reduction of neutron fluence and of MeV photon background from neutron capture in ^{1}H

**should rather be "absorption"*



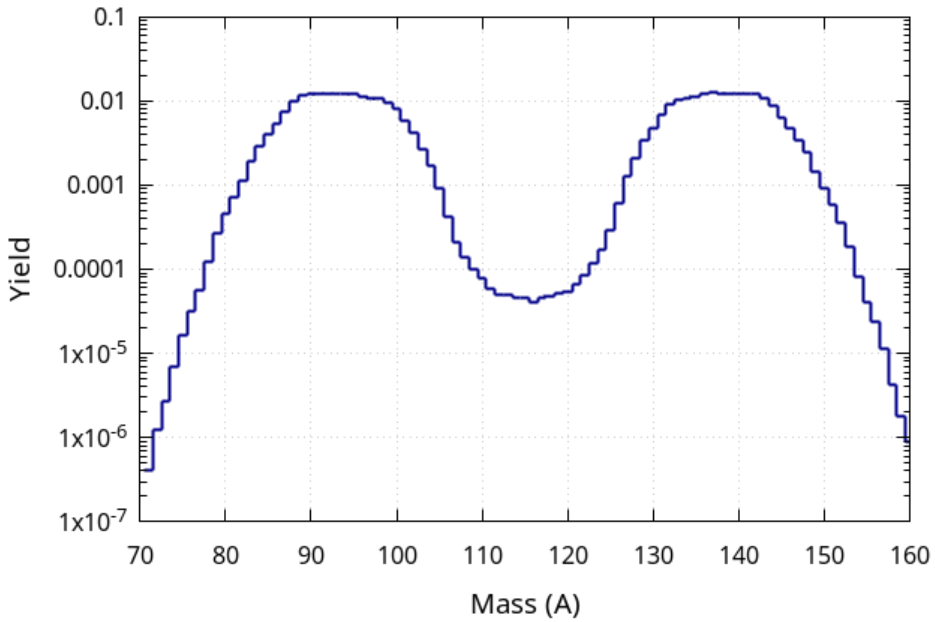
^{nat}Cd(n,γ)

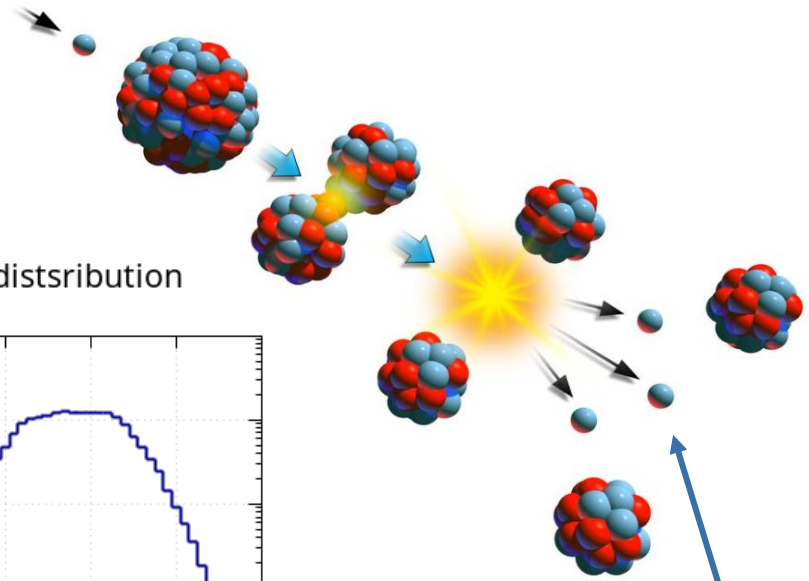
- $\sigma_{(n,el)}$ is slightly lower than for ^{1,2}H, but
  $E_{rec,max}$(n on ^{nat}Cd) ≪ E_{kin}
- ^{nat}Cd is less effective than ^{1,2}H as a moderator
- (n,γ) dominates at energies below 1 eV:
  - Resonance (thousands of barns!) at ~0.2 eV
  - Mean free paths ≪ 100 μm (!)
- neutrons with energies below eV are promptly converted
  into photons of O(100 keV)-O(10 MeV)
- Resonances:
  - Present in neutron cross sections in all but the lightest nuclei
  - Resolved vs unresolved resonance region



^{235}U(n,f)

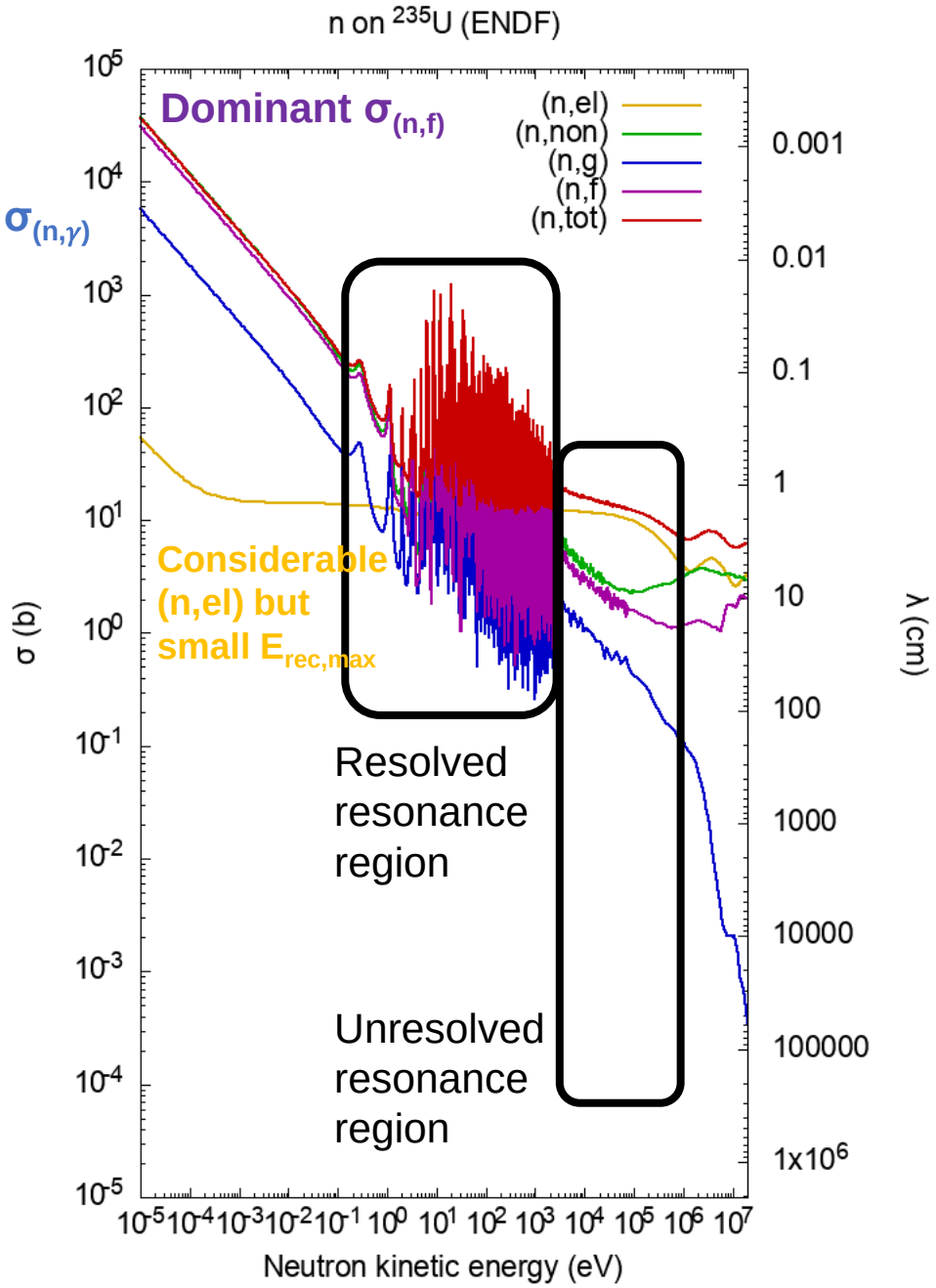
- For heavy targets (n,f) tends to dominate at thermal energies





Fission neutrons with energies O(1) MeV

Considerable $\sigma_{(n,\gamma)}$

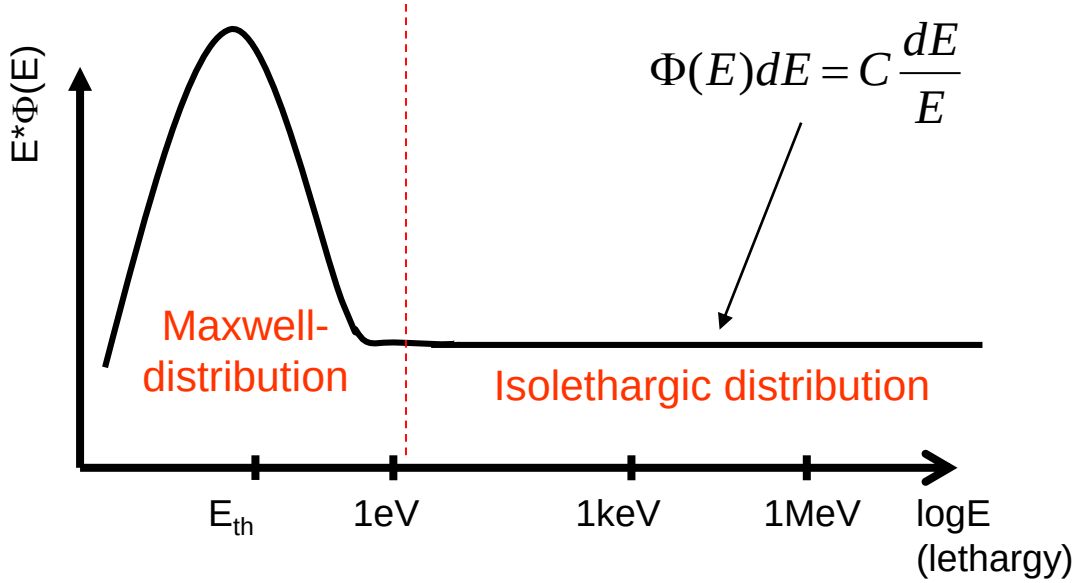


Group-wise treatment of neutron interactions below 20 MeV in FLUKA

The legacy approach

Group-wise approach

- Energy scale is divided into i=1,…,260 fixed bins (**groups**)
- At each group, cross sections from evaluated nuclear databases (ENDF, JEFF, JENDL…) are averaged over a typical neutron fluence:



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

- Energy (**continuous variable**) becomes a group index *g* (**discrete variable**)
- Effect: continuous cross sections become histograms

Low-energy neutron groups in FLUKA

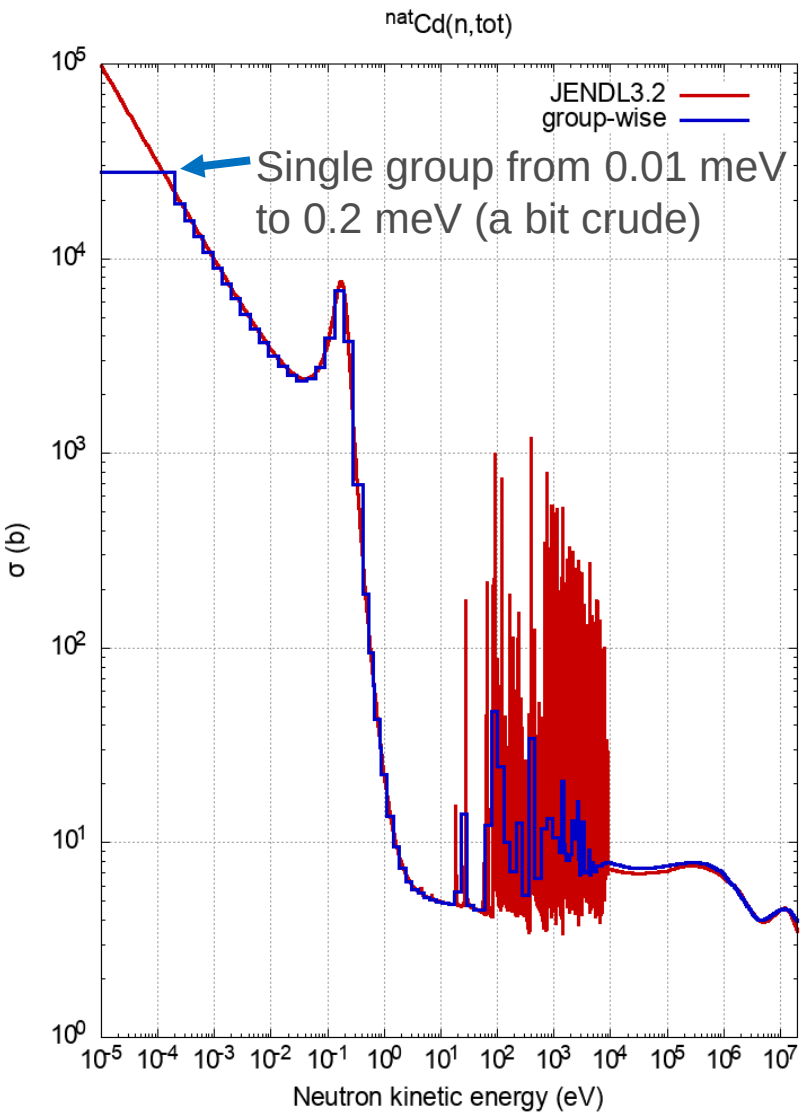
- Highest energy group index: 1
- Lowest energy group index: 260

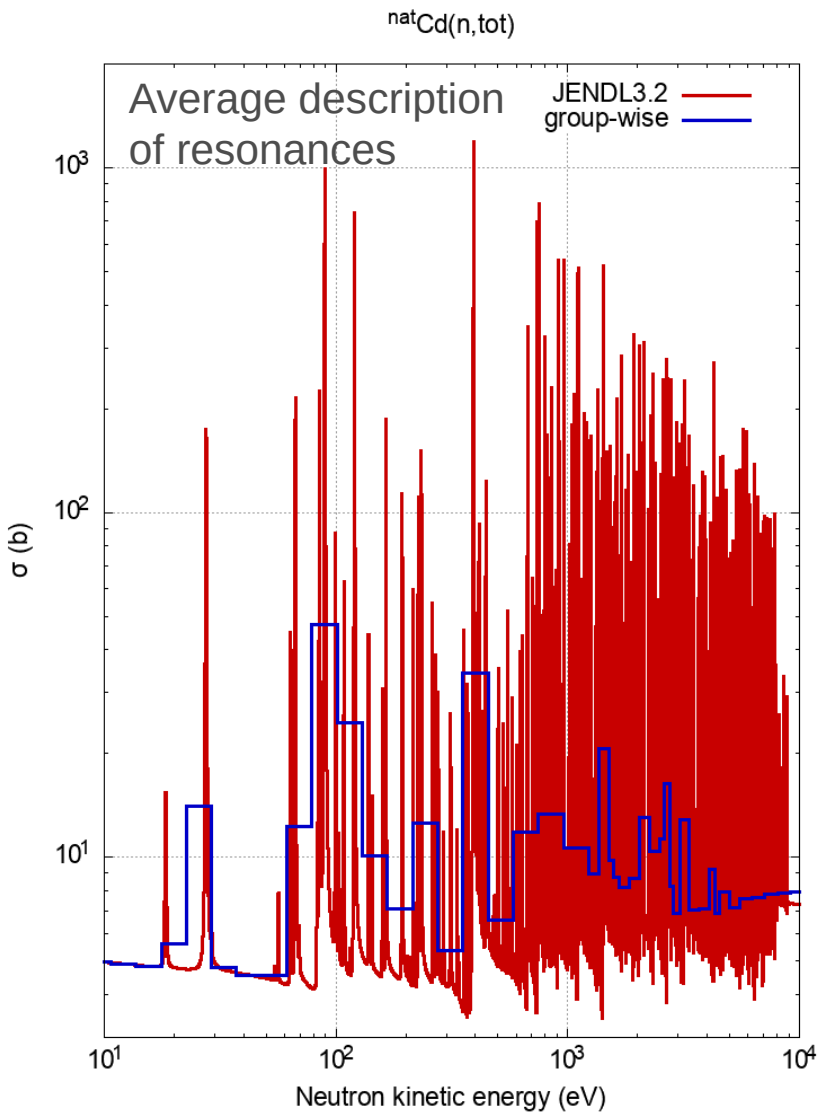
- All energy-resolved quantities involving low-energy neutrons default to this fixed binning

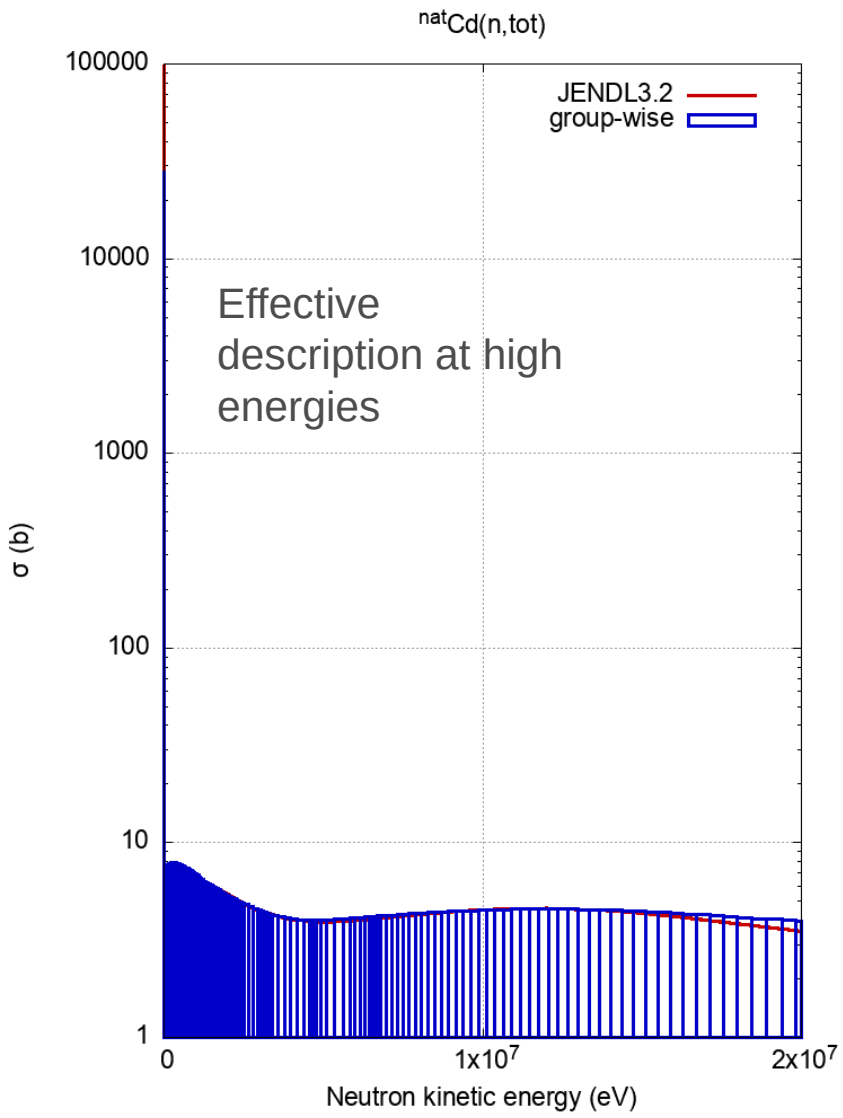
- This affects USRTRACK, USRBDX, USRYIELD, USRCOLL

# Group	Elow (GeV)	Ehigh(GeV)
1	1.9640E-02	2.0000E-02
2	1.9155E-02	1.9640E-02
3	1.8683E-02	1.9155E-02
4	1.8221E-02	1.8683E-02
5	1.7771E-02	1.8221E-02
6	1.7333E-02	1.7771E-02
7	1.6905E-02	1.7333E-02
8	1.6487E-02	1.6905E-02
9	1.6080E-02	1.6487E-02
10	1.5683E-02	1.6080E-02
(...)		
250	6.2118E-12	9.0994E-12
251	4.2405E-12	6.2118E-12
252	2.8948E-12	4.2405E-12
253	1.9761E-12	2.8948E-12
254	1.3490E-12	1.9761E-12
255	9.2092E-13	1.3490E-12
256	6.2867E-13	9.2092E-13
257	4.2917E-13	6.2867E-13
258	2.9297E-13	4.2917E-13
259	2.0000E-13	2.9297E-13
260	1.0000E-14	2.0000E-13

Group-wise cross sections

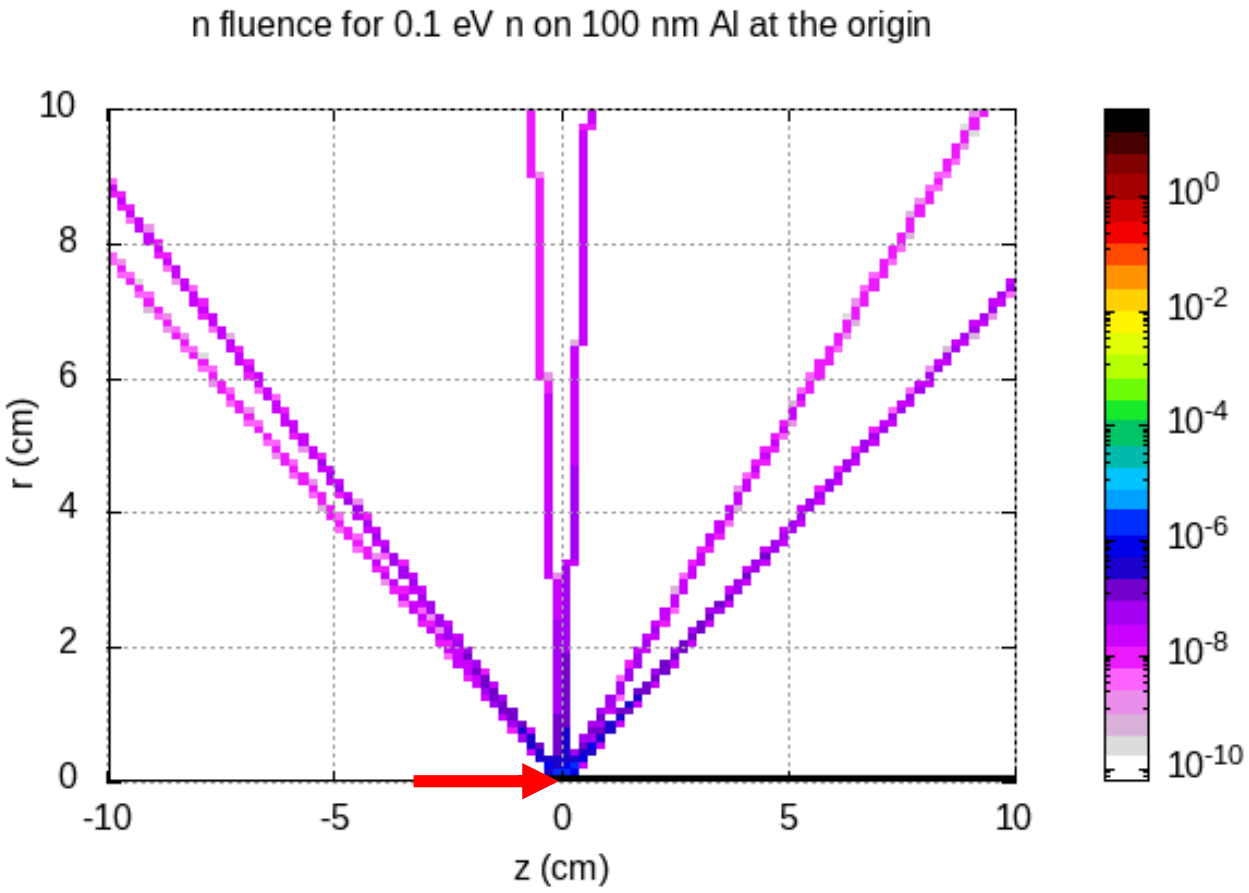






Angular distributions

- (n,el) and reaction channels with secondary neutrons are described in terms of an **up/down-scattering matrix** $M_{gg'}$ providing the likelihood for a neutron to transition from group *g* to group *g'*:
  - $E_{g'} > E_g$: *up-scattering (thermal neutrons!)*
  - *g' = g: in-scattering*
  - $E_{g'} < E_g$: *downscattering*
- Several *g'* may be accessible to a given *g*
- For a given *g→g'* transition, the **continuous distribution of polar scattering angles is discretised into 3 possible directions** (respecting first 6 moments of the original distribution)



Two g→g' transitions happened to be accessible here, hence two groups of 3 outgoing directions

Other aspects of FLUKA's group-wise treatment

- **Charged secondaries** from low-energy neutron interactions **are not produced**
  - Except for **few selected channels**, among which $^{1}H(n,el)$, $^{10}B(n,a)$, $^{14}N(n,p)$
  - Their energy is deposited locally via *kerma factors*
- Gamma generation from (n,γ) and (n,n') accounted for (42 groups,1 keV - 50 MeV), correlated only for a few isotopes. Photon energy sampled uniformly in group, transport is done in EMF module
- **Uncorrelated sampling of residual nucleus** from average distribution
- Cross sections available at a few database temperatures (**no arbitrary material temperature**)

- The group-wise approach **is not applicable** to event-by-event analyses, detector simulations, applications sensitive to details of a particular cross section resonance, a specific temperature not contained in the database, etc.
- But it has its merits:
  - It is **fast** and has **small memory requirements**
  - It is sufficient for some applications, e.g. to score energy deposition in thick materials

Group-wise low-energy neutron interactions in FLUKA

- Group-wise cross sections available for a series of materials:
  https://flukafiles.web.cern.ch/manual/chapters/low_energy_neutrons/multigroup_neutron_transport/neutron_cross_section_library/available_cross_sections.html

Table 8 Available low-energy neutron groupwise cross sections

Material		Temp.	Source	RN	Name	Identifiers			GP
H	H_2O bound natural Hydrogen	296 K	ENDF/B-VIIR0	✓	HYDROGEN	1	-2	296	✓
H	CH_2 bound natural Hydrogen	296 K	ENDF/B-VIIR0	✓	HYDROGEN	1	-3	296	✓
(…)									
Fe	Natural Iron	296 K	ENDF/B-VIR8	✓	IRON	26	-2	296	✓
Fe	Natural Iron	87 K	ENDF/B-VIR8	✓	IRON	26	-2	87	✓
Fe	Natural Iron	4 K	ENDF/B-VIR8	✓	IRON	26	-2	4	✓
Fe	Natural Iron	430 K	ENDF/B-VIR8	✓	IRON	26	-2	430	✓
(…)									
^{241}Am	Americium 241	296 K	ENDF/B-VIIR0	✓	241-AM	95	241	296	✓
^{241}Am	Americium 241	87 K	ENDF/B-VIIR0	✓	241-AM	95	241	87	✓
^{243}Am	Americium 243	296 K	ENDF/B-VIIR0	✓	243-AM	95	243	296	✓
^{243}Am	Americium 243	87 K	ENDF/B-VIIR0	✓	243-AM	95	243	87	✓

- Processed from ENDF, JENDL, JEFF
- Available at 296 K, and at a few fixed temperatures for selected materials

Using FLUKA's group-wise library

- Every FLUKA material (except VACUUM and BLCKHOLE) must be assigned to a group-wise library material

- If 'FLUKA material name' = 'group-wise library material name', the association is automatic
- Otherwise, the **LOW-MAT** card must be used:

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 ▼	

- The first match of FLUKA material name to group-wise library material name present in the input is taken into account

Point-wise treatment of neutron interactions below 20 MeV in FLUKA

General treatment introduced in FLUKA v4-3.0

Default from v4-4.0 for DEFAULTs: NEW-DEFA, PRECISION, DAMAGE

See V. Vlachoudis et al., *Recent developments in the point wise neutron treatment for FLUKA v4*, EPJ WoC 284 (2023) 03021 doi.org/10.1051/epjconf/202328403021

Point-wise interactions in FLUKA

- Nearly direct sampling from evaluated nuclear data libraries:
  - **JEFF** (Joint Evaluated Fission and Fusion library): https://www.oecd-nea.org/dbdata/jeff/
  - **ENDF** (Evaluated Nuclear Data Files): https://www-nds.iaea.org/exfor/endf.htm
  - **JENDL** (Japanese Evaluated Nuclear Data Library): https://wwwndc.jaea.go.jp/jendl/jendl.html
  - **CENDL** (Chinese Evaluated Nuclear Data Library): https://en.cnnc.com.cn/2020-06/17/c_501119.htm
  - **BROND** (Russian evaluated neutron data library): https://vant.ippe.ru/en/brond-3-1

- FLUKA's point-wise code implementation relies on the G4NDL data:

Evaluated neutron cross section libraries for the GEANT4 code (v2.0, 17/05/2018)

Emilio Mendoza and Daniel Cano-Ott, Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT), Spain

FLUKA point-wise data libraries

- Due to large size, the neutron data libraries are provided as separate packages to download*, installed in `${FlukaDir}/data/neutron/` :

BROND-2.2	ENDF-VII0	JEFF31N	JENDL-4.0
BROND-3.1	ENDF-VII.1	JEFF-3.2	JENDL-4.0u
CENDL-31	ENDF-VIII0	JEFF-3.3	JENDL-5.0
ENDF-VI8	JEFF30N	JENDL330	TENDL21

- The **default** point-wise library for FLUKA v4-4.0 is **JEFF-3.3**
- Older evaluations are also provided for comparison purposes
- Thermal Scattering Law S(α,β,T) for several materials

* https://fluka.cern/download/neutron-data-libraries

- **Directory structure:**
  - **Elastic/**
    - CrossSection/
    - FS/
  - **Capture/**
    - CrossSection/
  - **Inelastic/**
    - …
  - **Fission/**
    - …
  - **ThermalScattering/**
    - Coherent/
    - Incoherent/
    - Inelastic/

Containing one file per isotope, per channel, cross section, and final state

Point-wise interaction libraries used by FLUKA

- Interactions are divided into 4 kinds:
  - Elastic: (n,el)
  - Capture: (n,γ)
  - Inelastic
    - Further subdivided into 36 channels, e.g. (n,n'), (n,p), (n,d), (n,^{3}He), (n,α)
  - Fission: (n,f)
    - Fission fragments from database if present, otherwise Wahl [1] systematics
- All isotopes have (n,el) and (n,γ), as well as inelastic channels (typically open at high energies, with a few exceptions)
- A few isotopes have a fission channel

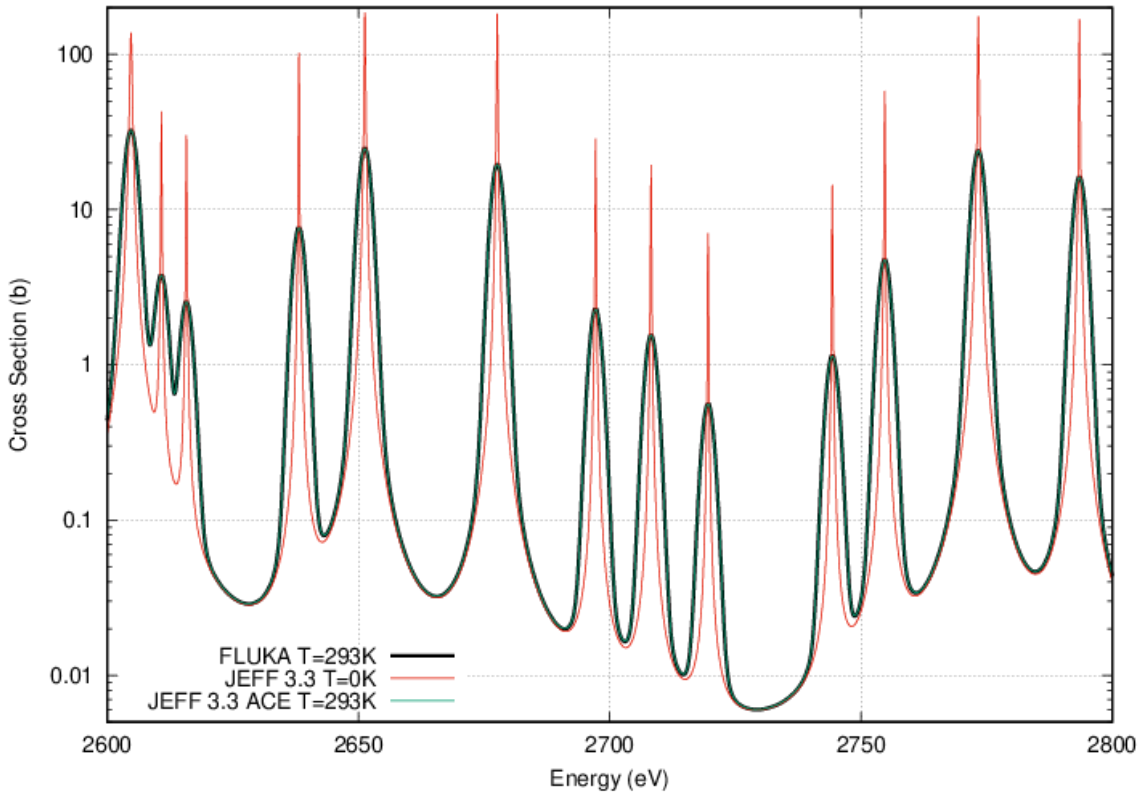
[1] A. Wahl, *Systematics of Fission-Product Yields,* LA-13928 May (2002)
http://cds.cern.ch/record/747754/files/34035670.pdf

Point-wise interactions in FLUKA: key features

- Nearly direct sampling from evaluated nuclear data libraries
- (E_i,σ_i) tables with accuracy < 0.1%
- Modern C++ implementation
- Heavily optimised:
  - 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
- Fast Doppler broadening at arbitrary temperature performed at initialisation
- “Fully” correlated emission of reaction products: N-body final states populated by subsequent 2-body emissions (the kinematics gradually constraining database distributions)

Doppler broadening

- Integrated cross sections are Doppler-broadened to the temperature *T* required using an adaptive numerical integration
- Performed at initialisation
- Fast: CPU time reported in output file (see below)



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

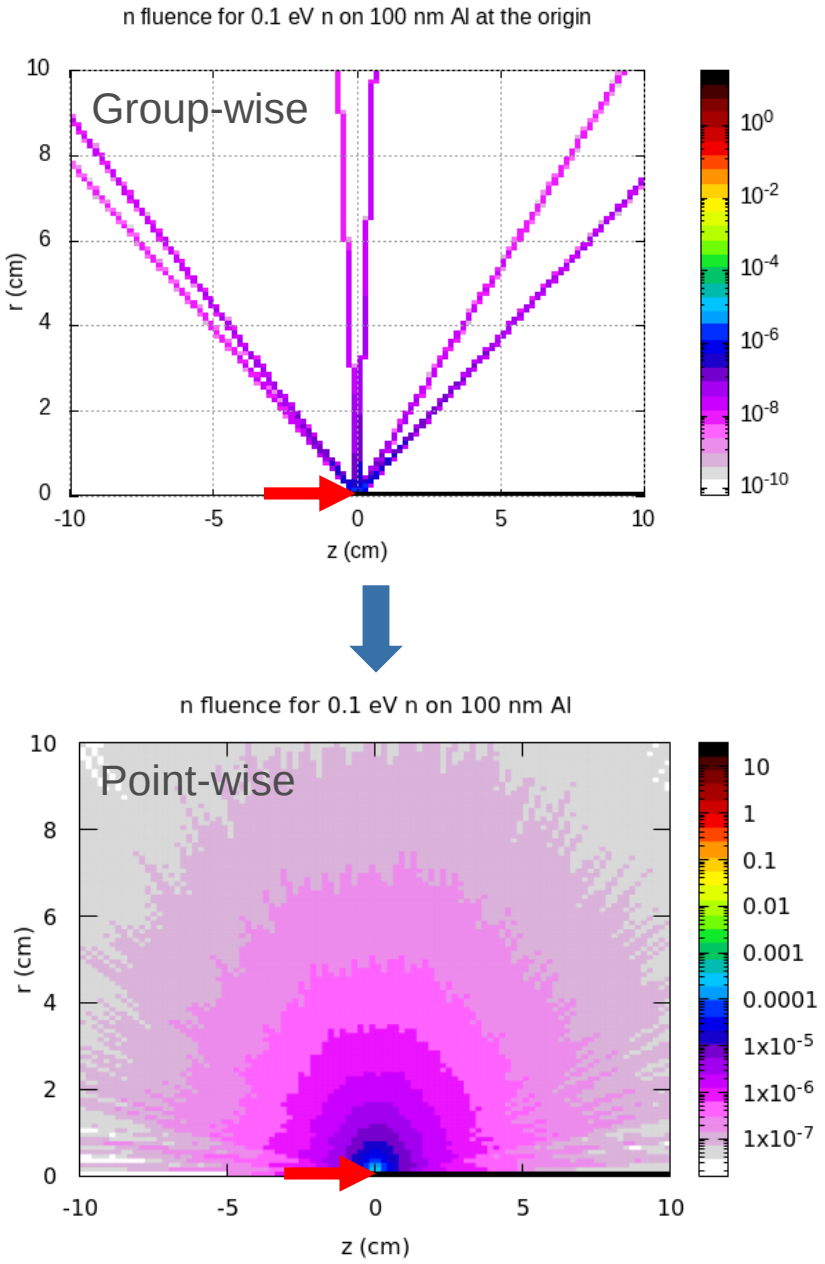
Online Doppler broadening example at 293 K for ^{113}Cd(n,γ):

- FLUKA
- JEFF (T=0 K)
- JEFF processed with NJOY

Point-wise (n,el) in FLUKA

- Continuous distribution of polar scattering angles ↘

- Above ~5 eV the **target nucleus is effectively at rest**
- Below ~5 eV the **target nucleus motion** is sampled from a Maxwell-Boltzmann distribution
- Recoils are explicitly calculated and pushed to the stack
- Below ~eV, neutron wavelength spreads over several atoms. Neutron scattering cross sections are sensitive to the molecular/ crystalline binding of the target nuclide.
  - E.g. H(n,el) will be different depending on whether H is bound in H_2, H_2O, ZrH, etc.
- To account for binding effects, thermal scattering laws S(α,β,T) are available upon user request for a handful of isotopes / materials (more below)

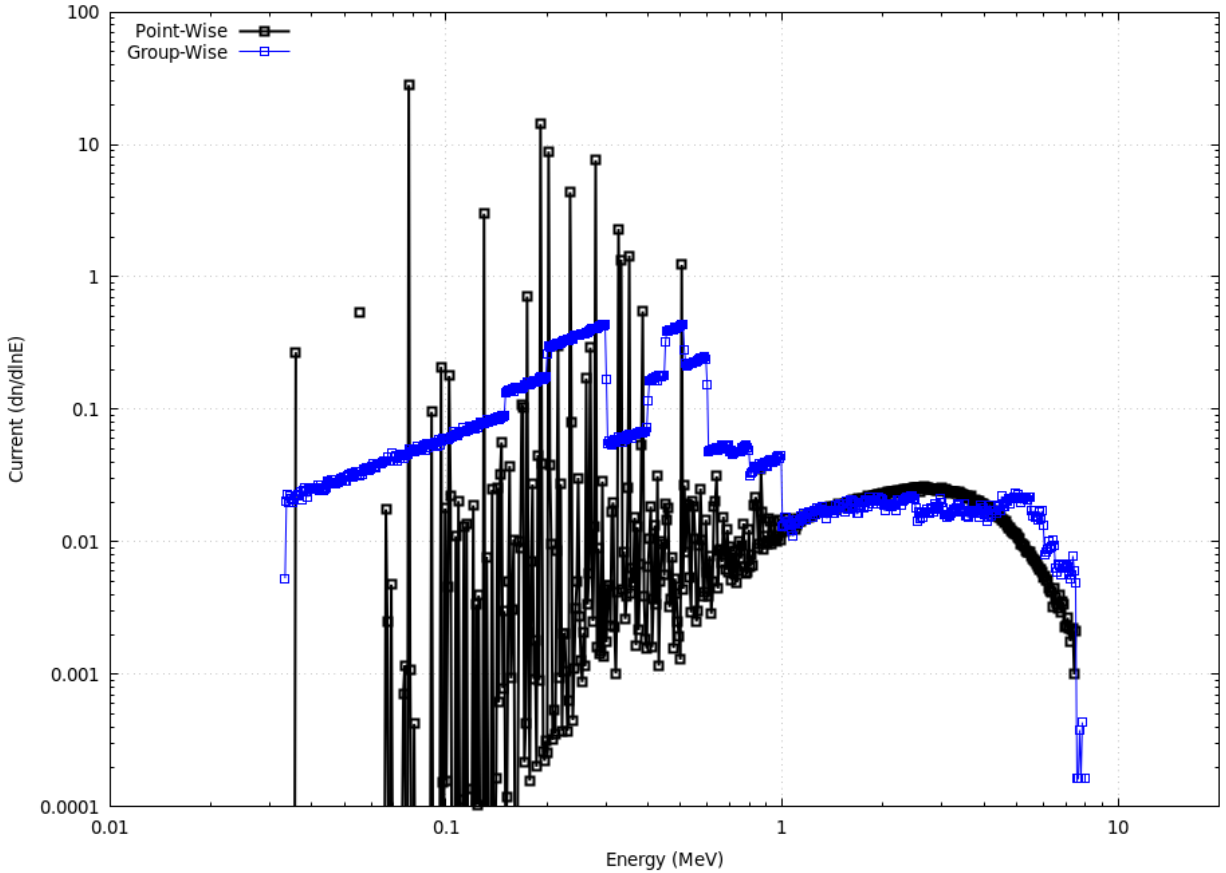


Point-wise (n,γ) in FLUKA

- The neutron is absorbed leading to an excited nucleus
  → standard FLUKA de-excitation module

- All known γ lines will be reproduced
- **Currently all isotopes de-excite to the ground state**
- Work is ongoing to properly use the probability to end in an isomeric state if the information is available in the database
- The recoil is properly generated

^{197}Au(n,γ)

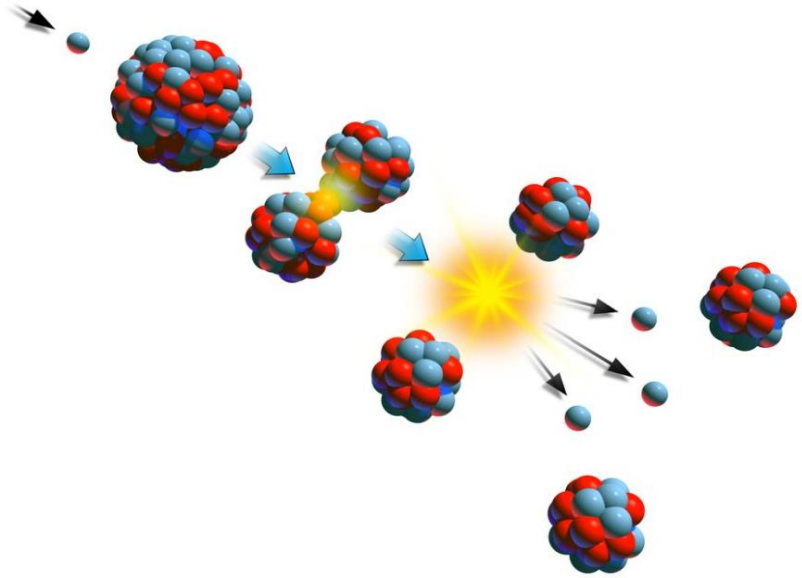


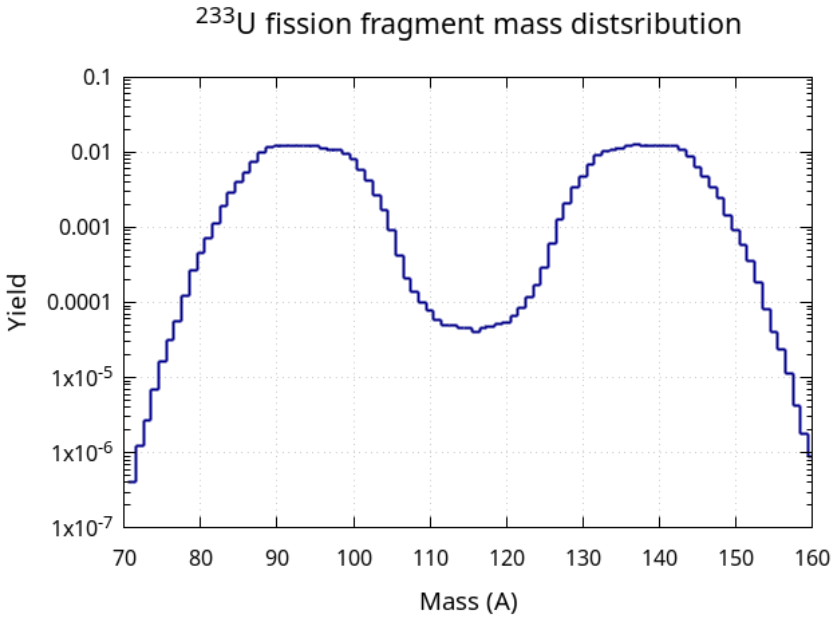
Inelastic interaction channels

- FLUKA selects a sub-channel based on the cross section
- It then samples the secondaries (including the residual nucleus) according to database information on the final state
- It will sample the secondaries (except the photons) one-by-one from the database distributions, getting back the Energy and cosθ of the ejectile, either in LAB or in CMS
- Excited residual nucleus is de-excited with the standard FLUKA modules (see Hadronics lecture)

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 (only two in FLUKA)
- 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 $S(\alpha,\beta,T)$ (1/2)

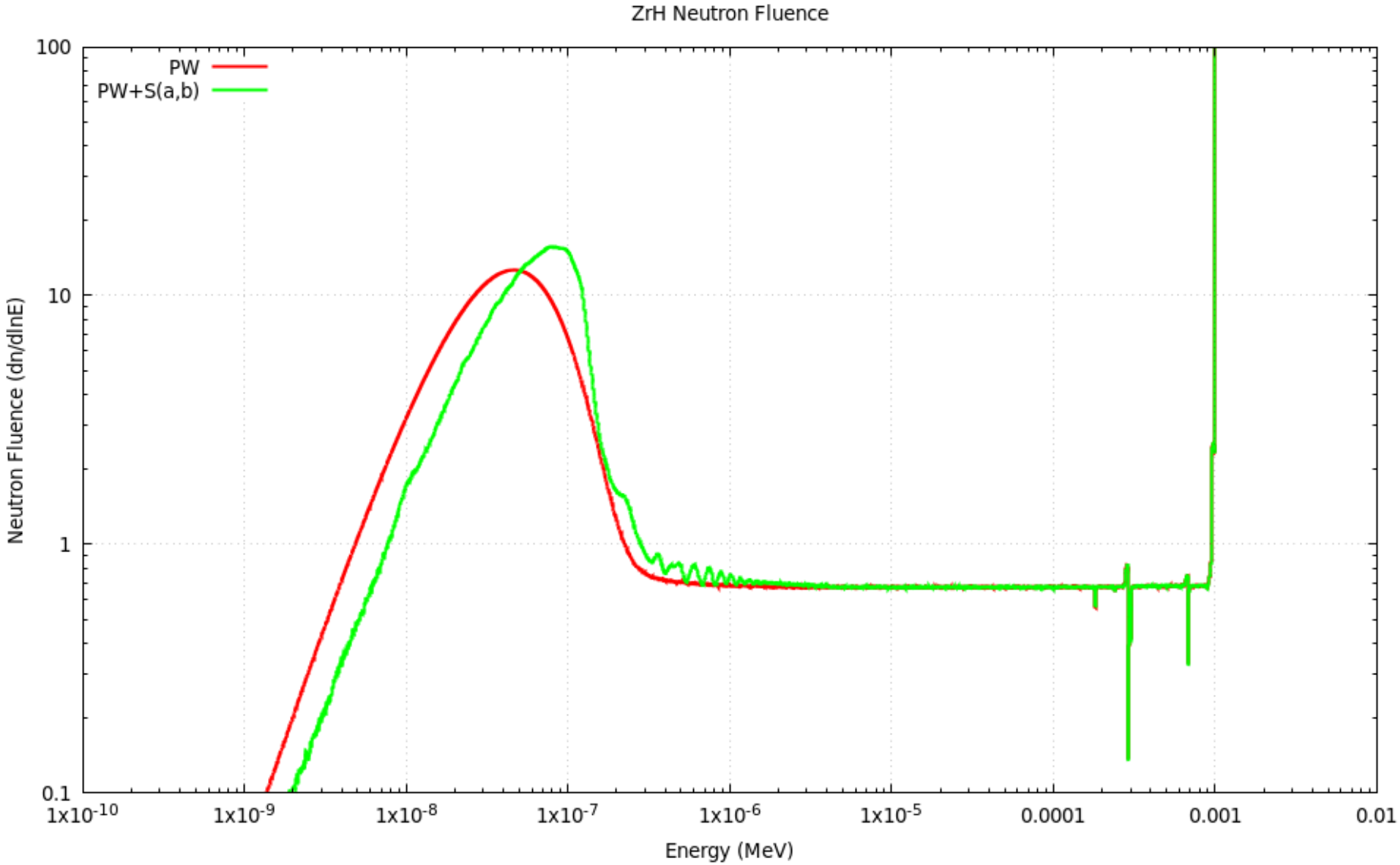
- For thermal neutrons, generally with energies less than ~4 eV, scattering cross sections are affected by the chemical/molecular/crystalline binding environment of the active target isotope
- If binding effects are not accounted for in a simulation, the reported results may be highly inaccurate

- 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 $S(\alpha,\beta,T)$ (2/2)

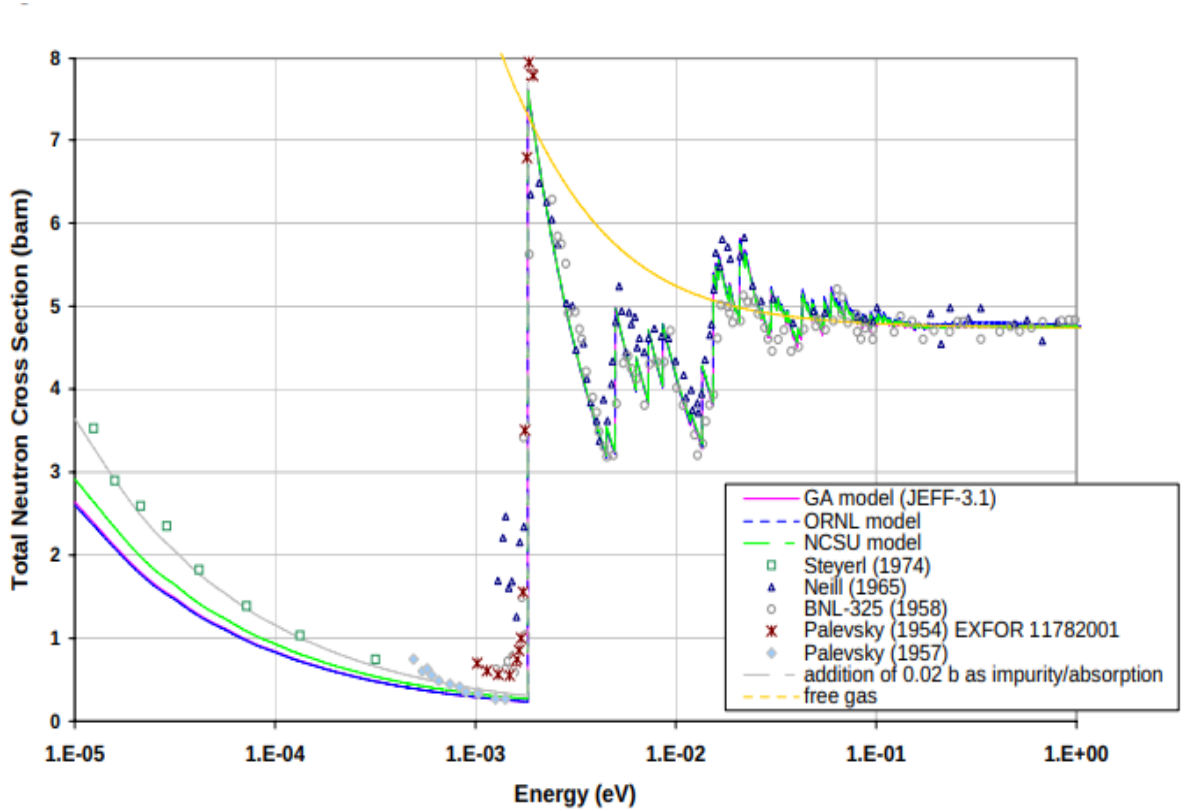
- Channels (nomenclature refers to state in which target system is left):
  - **Elastic** – the neutron energy remains the same, the angle changes
    - **Coherent** – discrete angles depending on the crystal direction vs neutron direction and Bragg edge selected, on crystal lattice
    - **Incoherent** – 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, …
- In addition, any S(α,β,T) ACE library with point-wise data can be used
- At various fixed temperatures per material: 4 .. 800 K
- Must be requested explicitly on a per-isotope basis (see **LOW-PWXS** card below)
- Exception: H is always assumed bound to H_2O

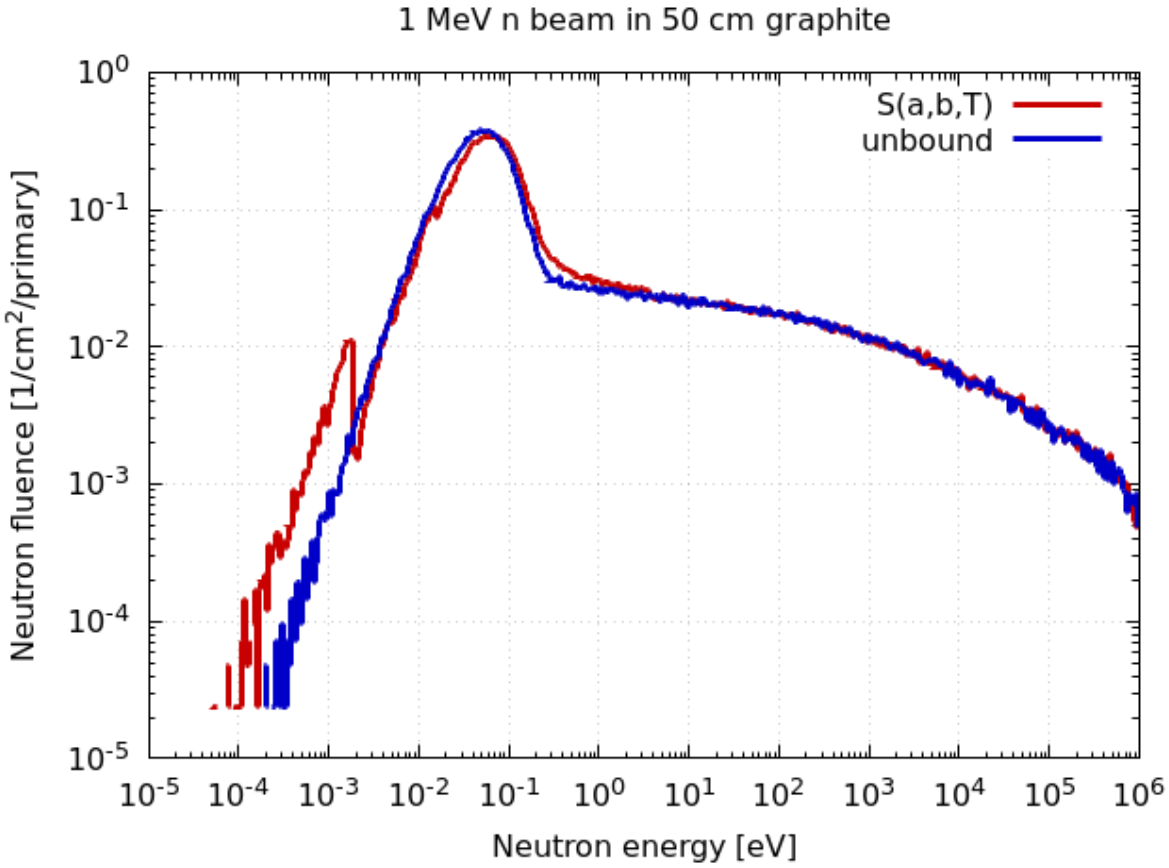
Example $S(\alpha,\beta,T)$ on ZrH



Binding effects of n scattering in graphite

- First Bragg edge of graphite: 1.82 meV





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

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

Usage: `LOW-PWXS` card

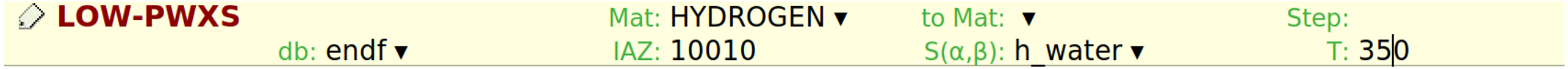
- `LOW-PWXS` card controls the new point-wise treatment in FLUKA
- WHAT(1):
  - **empty/0** = use PW treatment for this isotope (default)
  - **>0** Isotope code **Z*10000 + A*10 + iso**
  - **-1** = switch to OLD behavior, use GW/Old PW treatment for this isotope
- WHAT(2):
  - **S(α,β,T)** tabulation to associate with this isotope (list of isotopes in various binding environments)
- 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 v4-4 default = JEFF-3.3)

LOW-PWXS: examples

- Without any argument: enable PW treatment for all (available) isotopes

- With WHAT(1) = -1 to use GW supplemented by PW for a handful of channels

- Example:
  - 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 1H



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

Group-wise:

- When scoring of low-energy neutrons is requested, FLUKA will use the FIXED energy group structure of 260 groups, independently of what is supplied in the card

Point-wise:

- FLUKA will honor the user histogram settings:
  ONLY IF the materials of the regions involved have ALL constituents declared as point-wise
- Special attention to VACUUM which can be operationally declared as point or group-wise with the **`LOW-PWXS`** card
- E.g. USRBDX on a boundary between a point-wise material and VACUUM declared as group-wise, will still show group binning (!)

FLUKA output

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

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

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

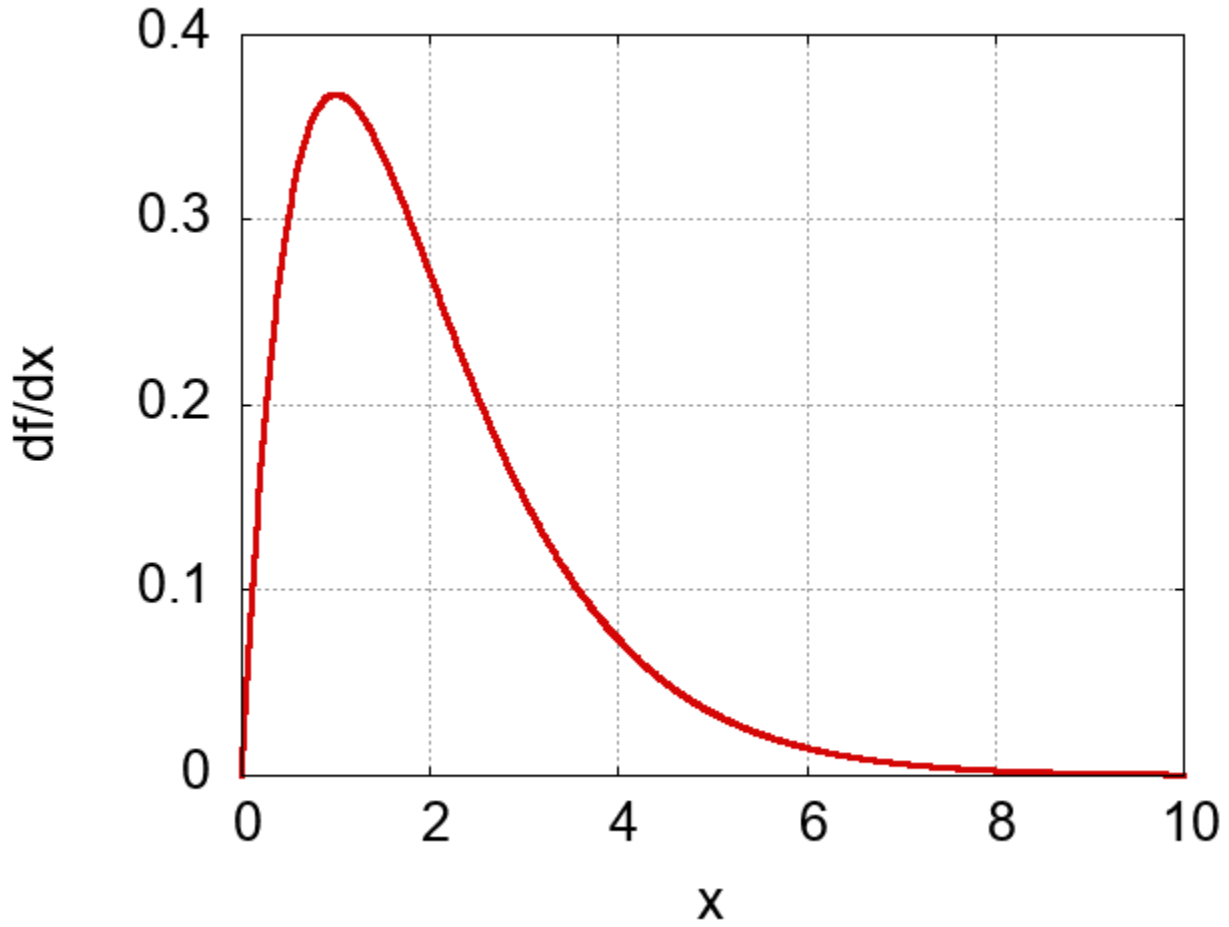
```
*** Low energy neutron Point Wise materials
  ###  Material   Z   A m     T(K)    Dataset
    3  HYDROGEN   1   1 0    296.0    default
         S(a,b)   1   1 0             h_water
    6  CARBON     6   0 0    296.0    default
                   12 0    0.9893
                   13 0    0.0107
    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
```

Lethargy units

An important reminder from the scoring lecture

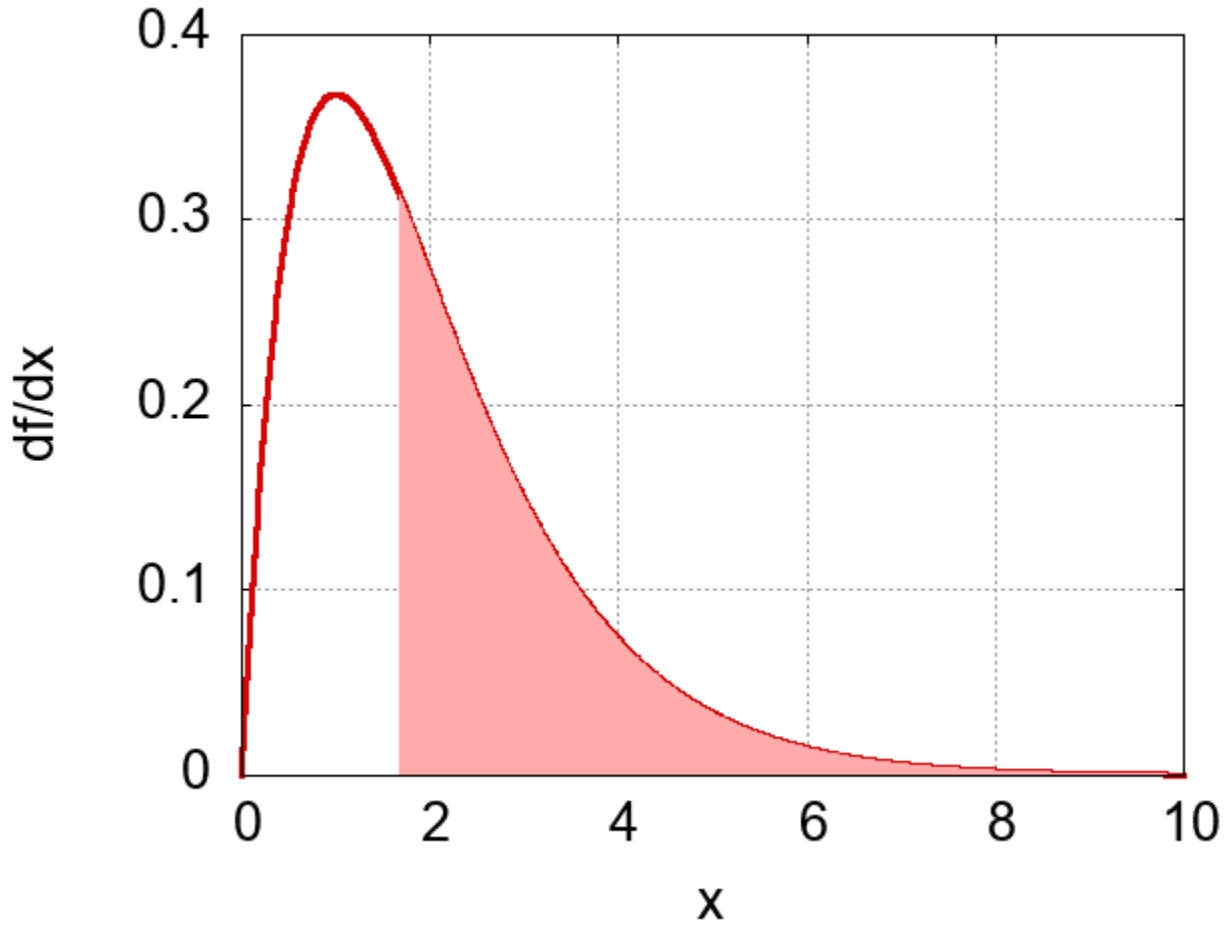
An important reminder from the scoring lecture

- Consider the (unnormalised) distribution $\frac{df}{dx} = x\,\mathrm{e}^{-x}$, where x is dimensionless:



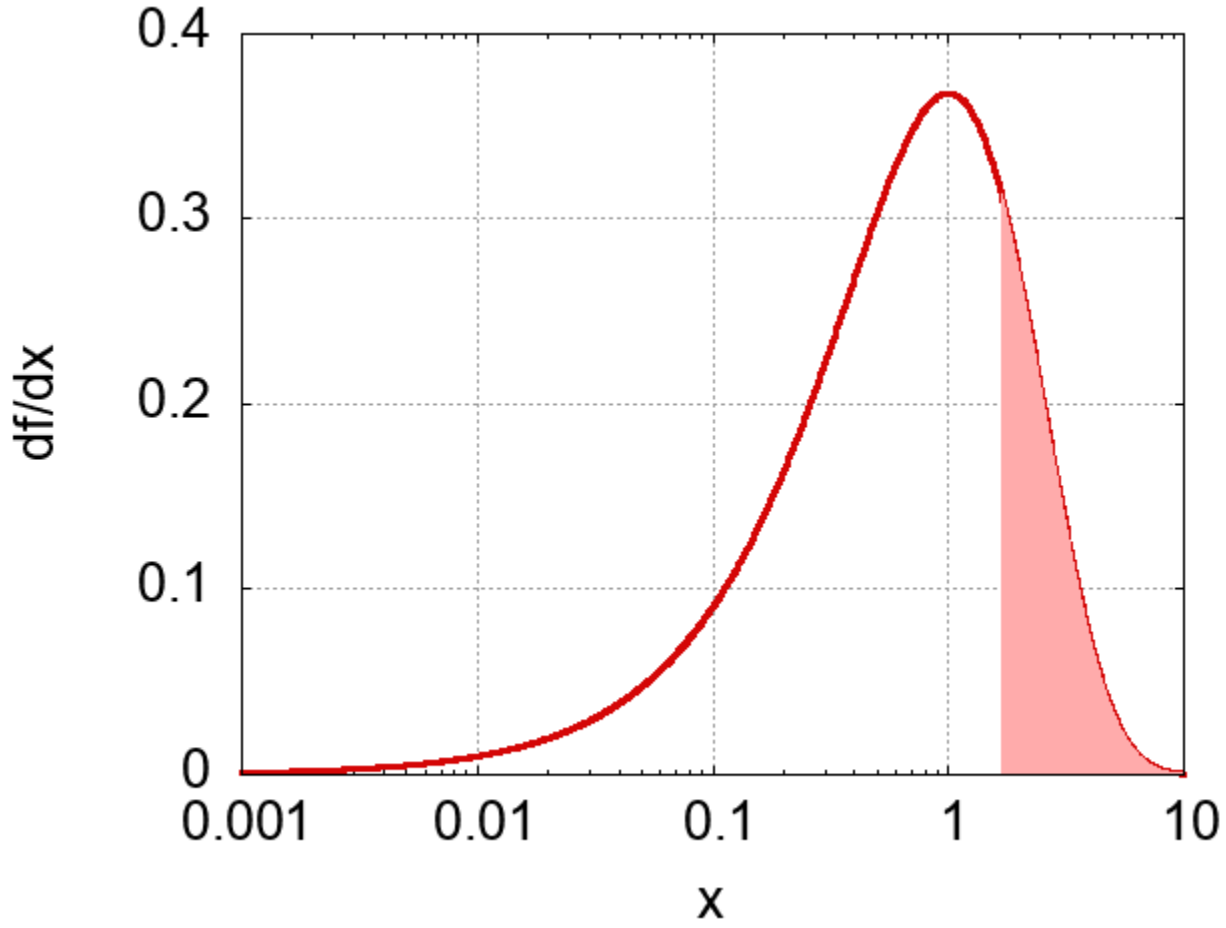
An important reminder from the scoring lecture

- We now shade in 50% of the area under the curve:



An important reminder from the scoring lecture

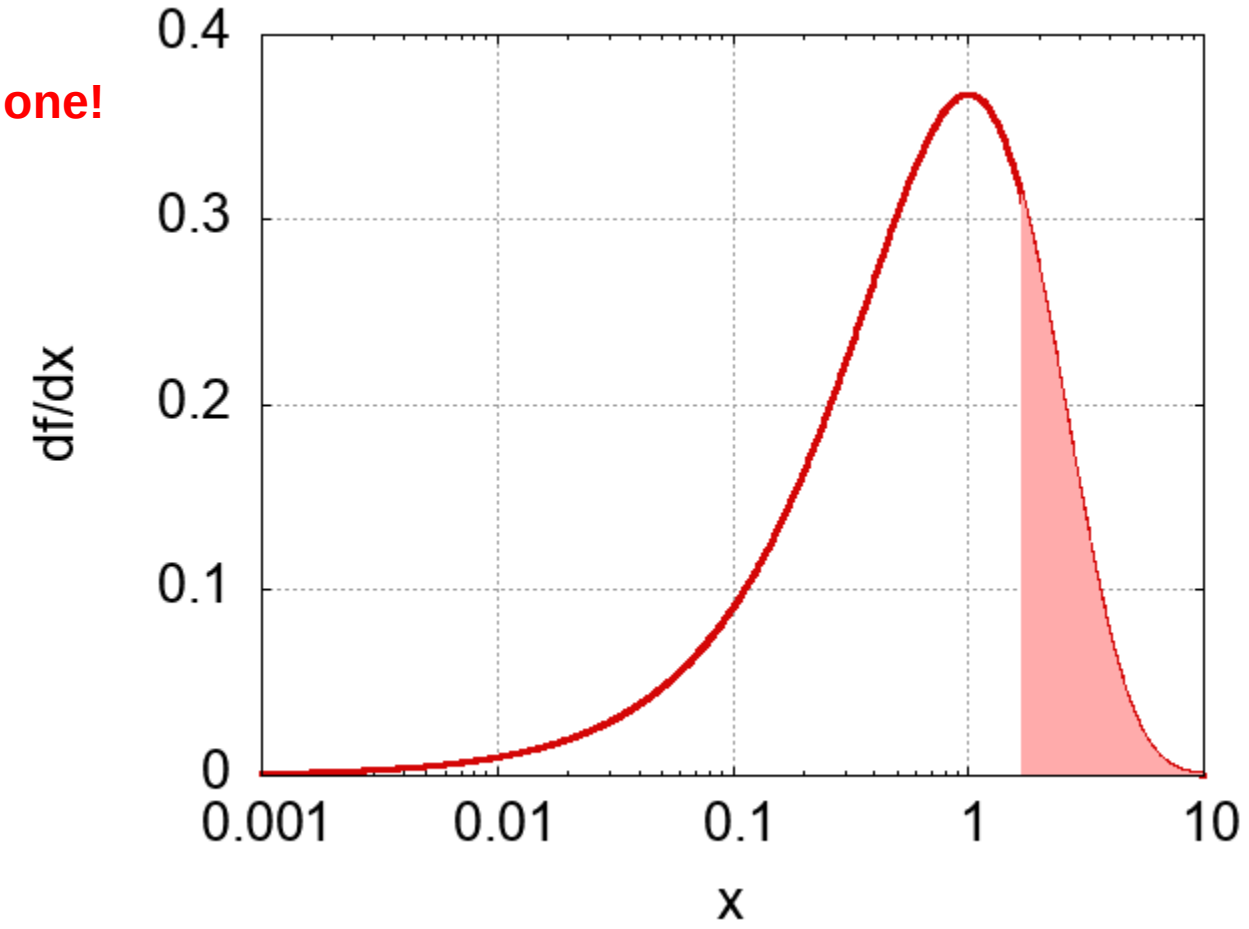
- Suppose you want to legitimally resolve what happens at small x in more detail
- So you naturally plot the **horizontal axis in logarithmic scale, don't you?**



An important reminder from the scoring lecture

- Suppose you want to legitimally resolve what happens at small x in more detail
- So you naturally plot the **horizontal axis in logarithmic scale**:

Careful! Achtung! Attenzione!

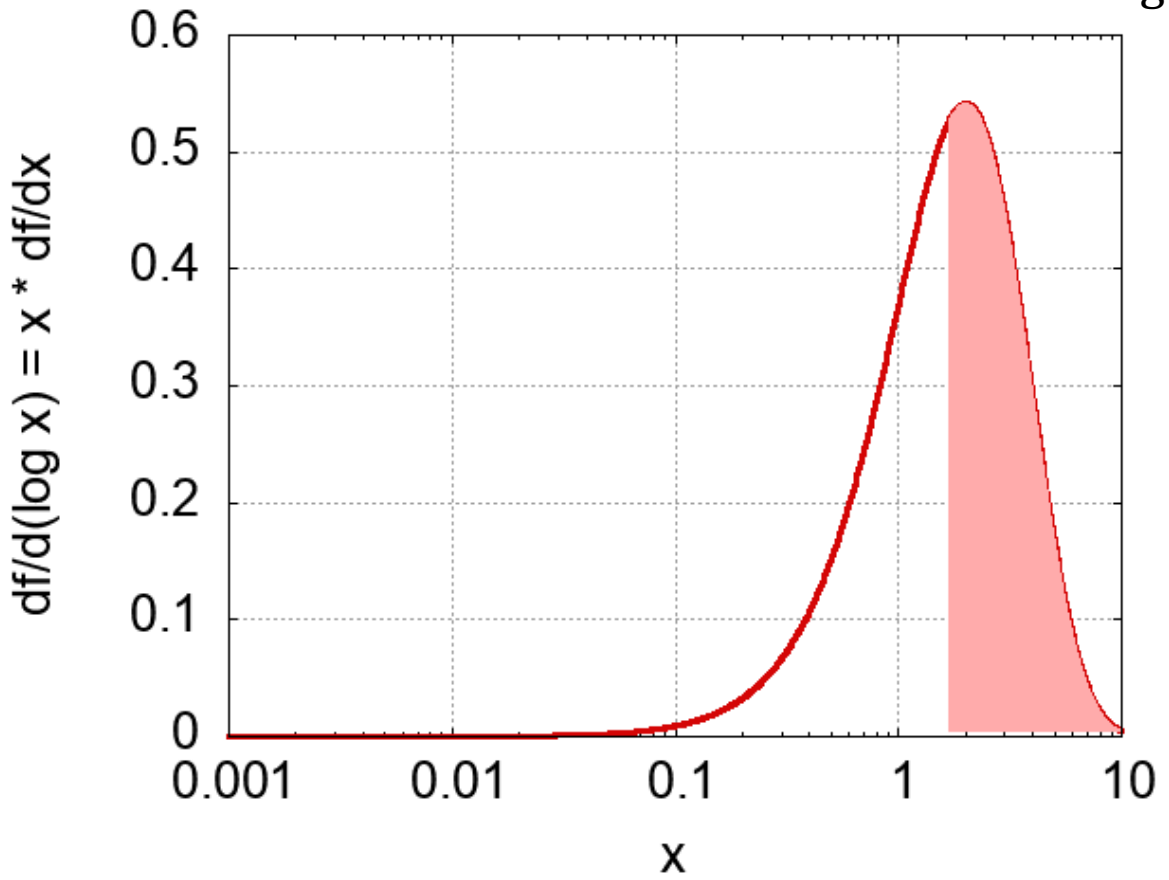


With this careless action you are severely distorting information!

The shaded area appears almost irrelevant in front of the unshaded region, while in reality both regions represent 50% of the distribution (!!!)

Lethargy units

- What happened? **You forgot a Jacobian**: $\frac{df}{d\log(x)} = \frac{df}{dx}\frac{dx}{d\log(x)} = x\,\frac{df}{dx}$
- Embrace ***lethargy* units***, the proper representation of $\frac{df}{d\log(x)}$:



* neutronics term (neutron lethargy)

lethargy: slowness, sluggishness, from Greek lēthargīa (ληθαργία)

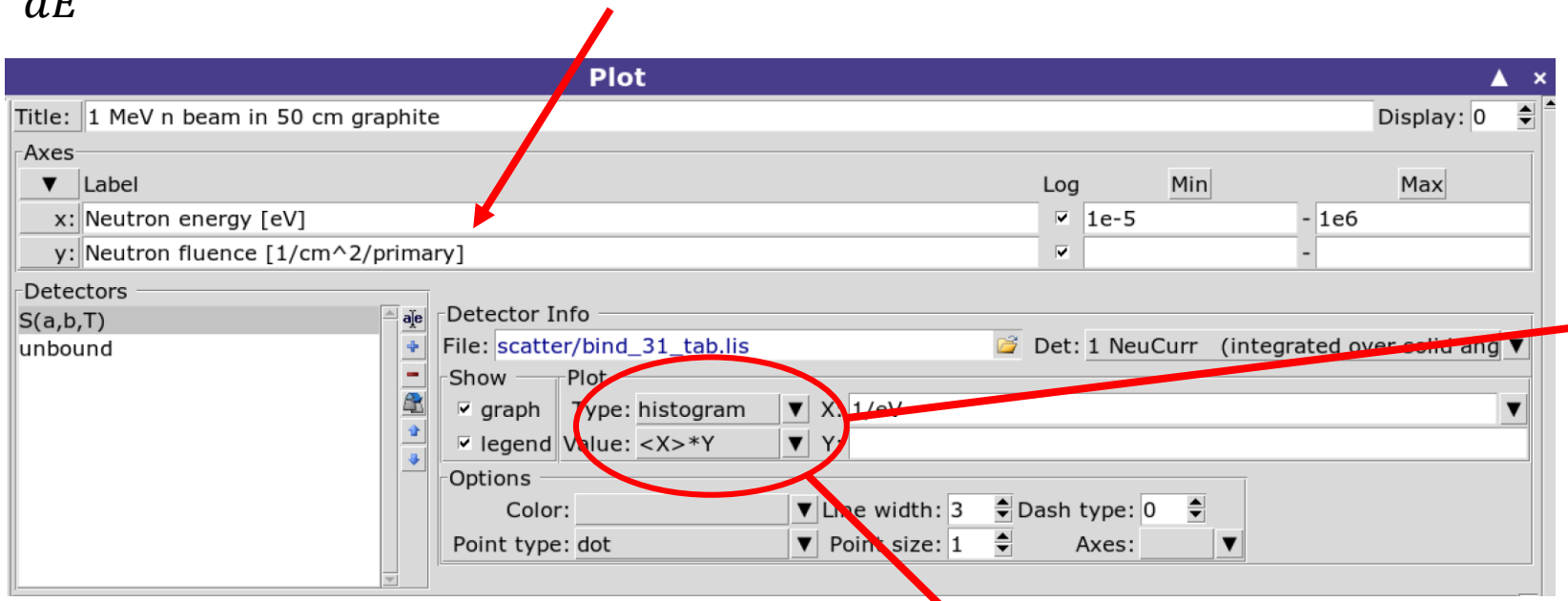
In this representation, integrals are respected

You are now representing information in a faithful way

(NB: taking a logarithmic scale in the vertical axis is harmless)

Flair helps you out (but you are responsible for axis labels)

- Do you need to worry? Yes. Be fully conscious when you plot histograms and distributions with logarithmic abscissas (horizontal axes) – **needed for low energy n**
- $\frac{df}{d\,\log(E)} = E\,\frac{df}{dE}$ → Indeed, the resulting spectrum does not have units of "1/GeV"



Regardless of whether you request **lin** or **log** spacing in your scoring cards

- What about histograms? Which *X* is taken? X_i? X_{i+1}?

$$\log X = \frac{1}{2}\left(\log X_{i+1} + \log X_i\right) = \frac{1}{2}\log(X_{i+1}X_i) \quad \Rightarrow \quad X = \left[e^{\log(X_{i+1}X_i)}\right]^{1/2} = \sqrt{X_{i+1}X_i}$$

Summary

- Low energy neutrons ≤20MeV receive special treatment in FLUKA
- Two methods are available:
  - Group-wise: coarse, but fast treatment. Few isotopes/channels are in point-wise.
  - Point-wise: superior model, highly optimised, giving access to all latest available neutron data, explicit treatment of interactions in fully correlated way
- What to use:
  - Prefer the use of point-wise
    - **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 point-wise to properly take all physical effects into account
  - Group-wise can work nicely for shielding applications
  - Optionally you can mix point- and group-wise treatment in the same problem


FLUKA