FLUKA

Low energy (≤20MeV) neutron interactions

Outline

(1/3)
- Neutron interactions below 20 MeV
  (small reminder above 20 MeV in passing)

(1/3)
- *Group-wise* treatment:
  - Legacy treatment
  - Default at present

(1/3)
- *Point-wise* treatment:
  - Introduced in v4-3.0
  - Soon to be made default

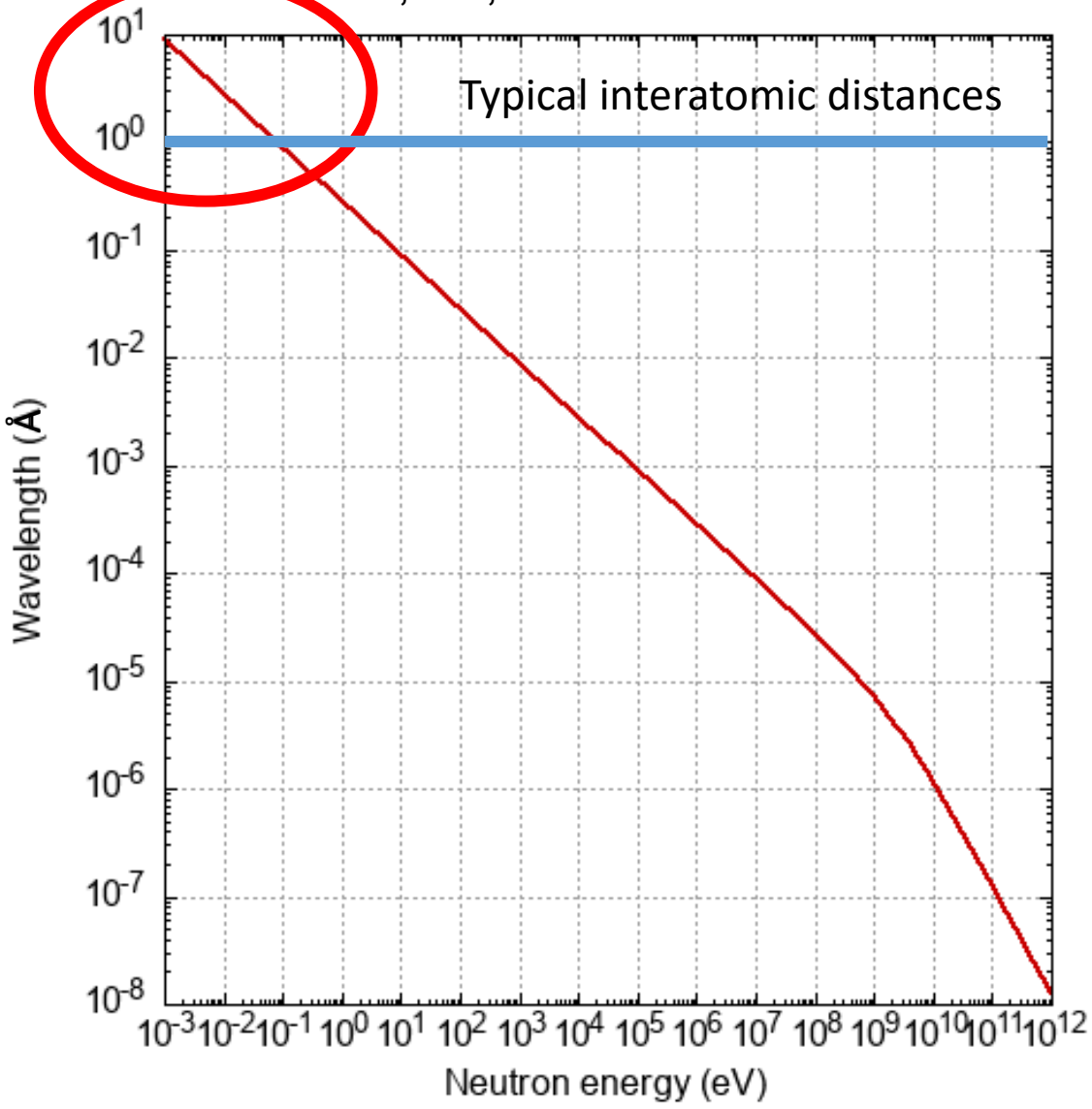
Low-energy neutron interactions

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
- **n 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: n 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 a nutshell

- Above 20 MeV, neutrons are treated in FLUKA on equal footing with other hadrons:
  - **Nuclear elastic** scattering: based on the Ranft model [1]
  - **Nuclear inelastic** interactions: FLUKA's hadron-nucleus reaction model (PEANUT)

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

- In addition, n **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*

[1] Ranft J., Part Acc 3 129-161 (1972)

Neutron energies

Neutron energy range names

Neutron energy	Energy range
0.0 – 0.025 eV	Cold (slow) neutrons
0.025 eV	Thermal neutrons (at 20°C)
0.025–0.4 eV	Epithermal neutrons
0.4–0.5 eV	Cadmium neutrons
0.5–10 eV	Epicadmium neutrons
10–300 eV	Resonance neutrons
300 eV–1 MeV	Intermediate neutrons
1–20 MeV	Fast neutrons
> 20 MeV	Ultrafast neutrons

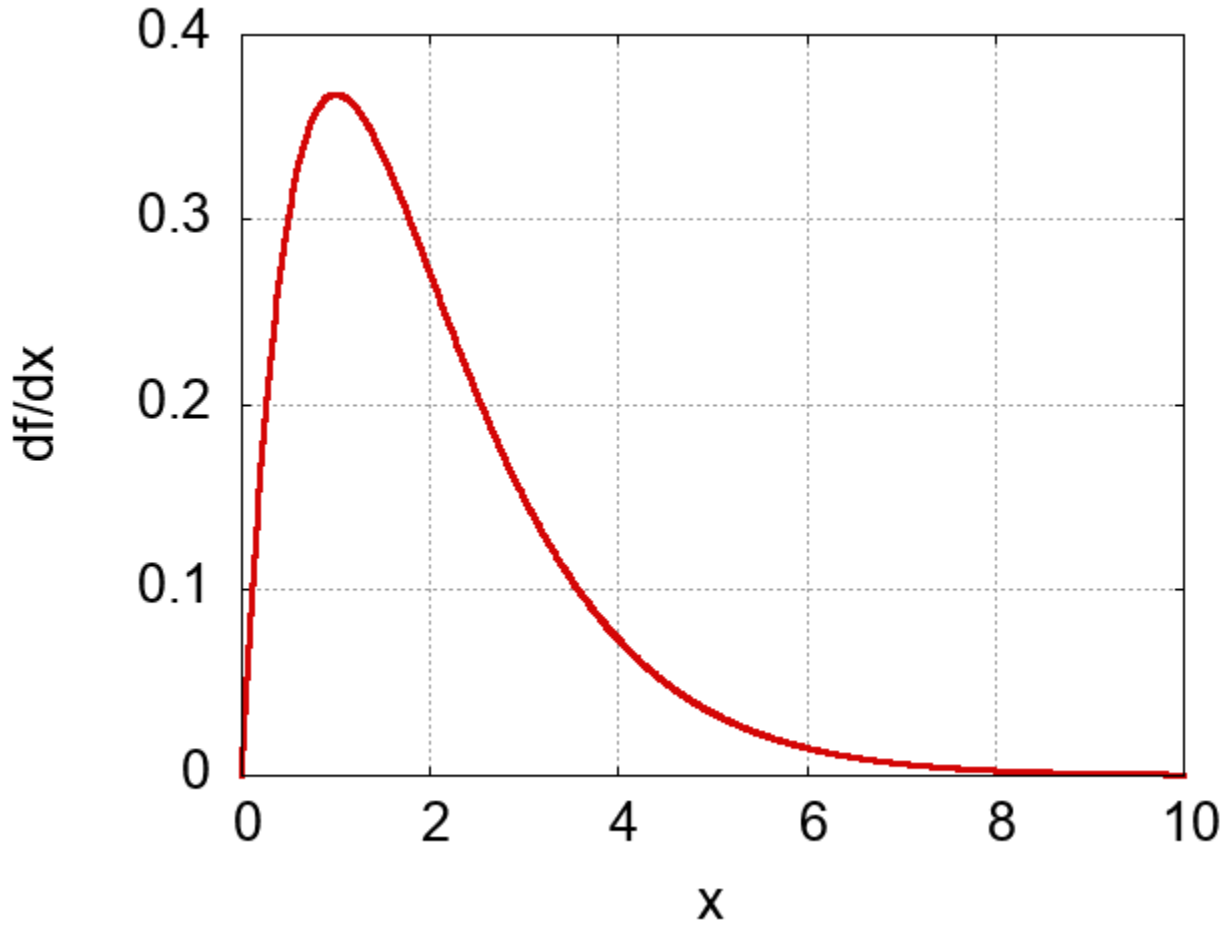
"Thermal energies": loosely for neutrons below O(1) eV

"Low energy neutron": FLUKA slang for neutrons below 20 MeV

Ref: https://en.wikipedia.org/wiki/Neutron_temperature

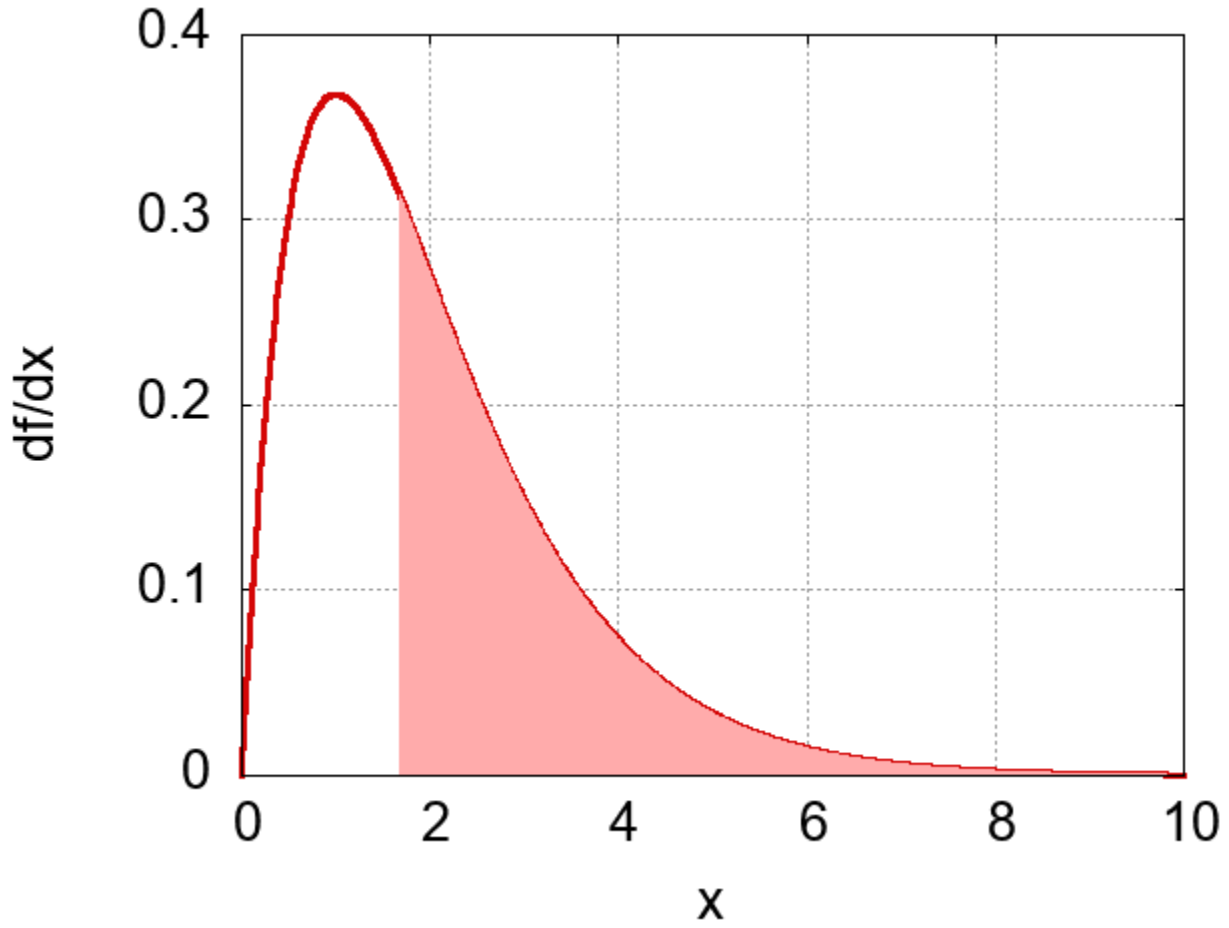
An important reminder from the scoring lecture

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



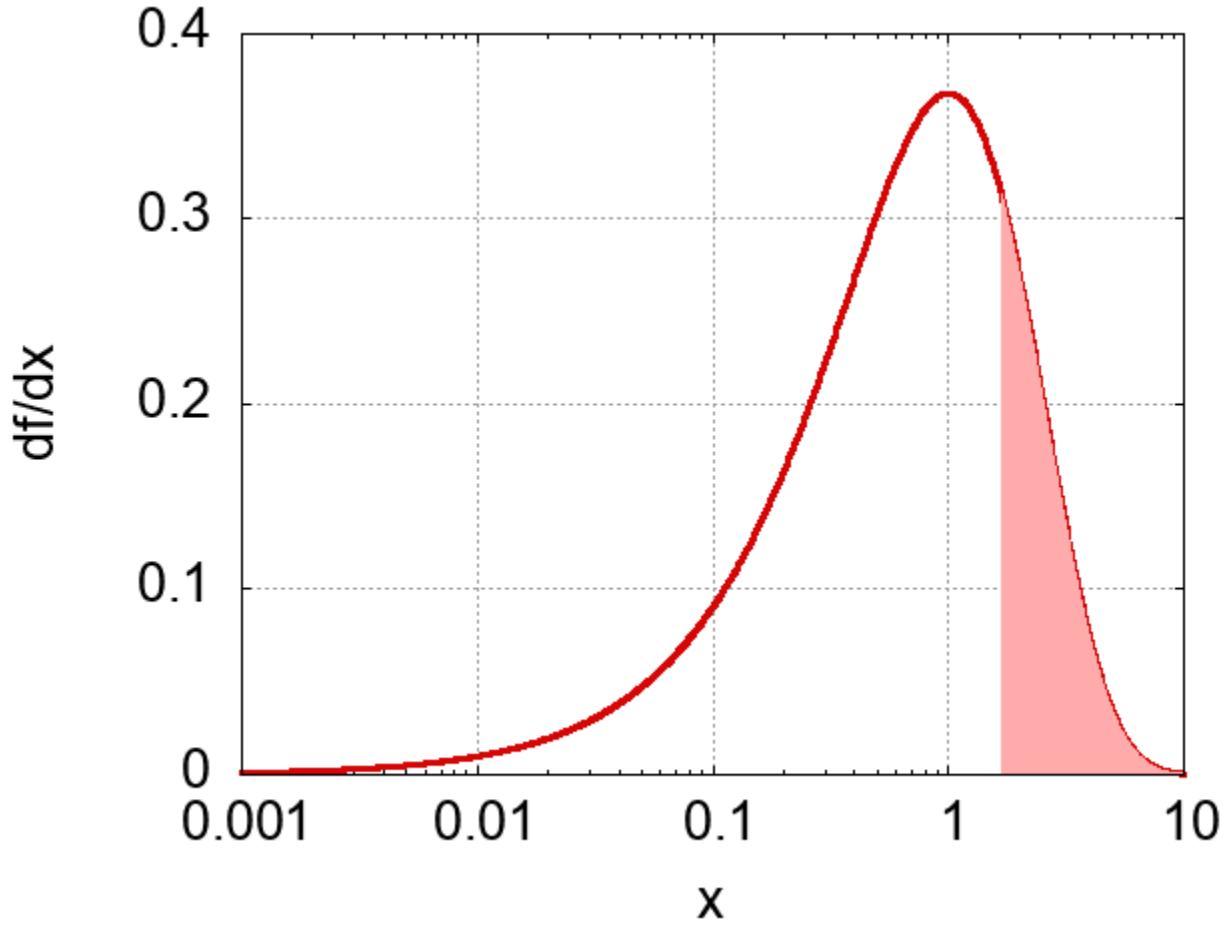
An important reminder from the scoring lecture

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



An important reminder from the scoring lecture

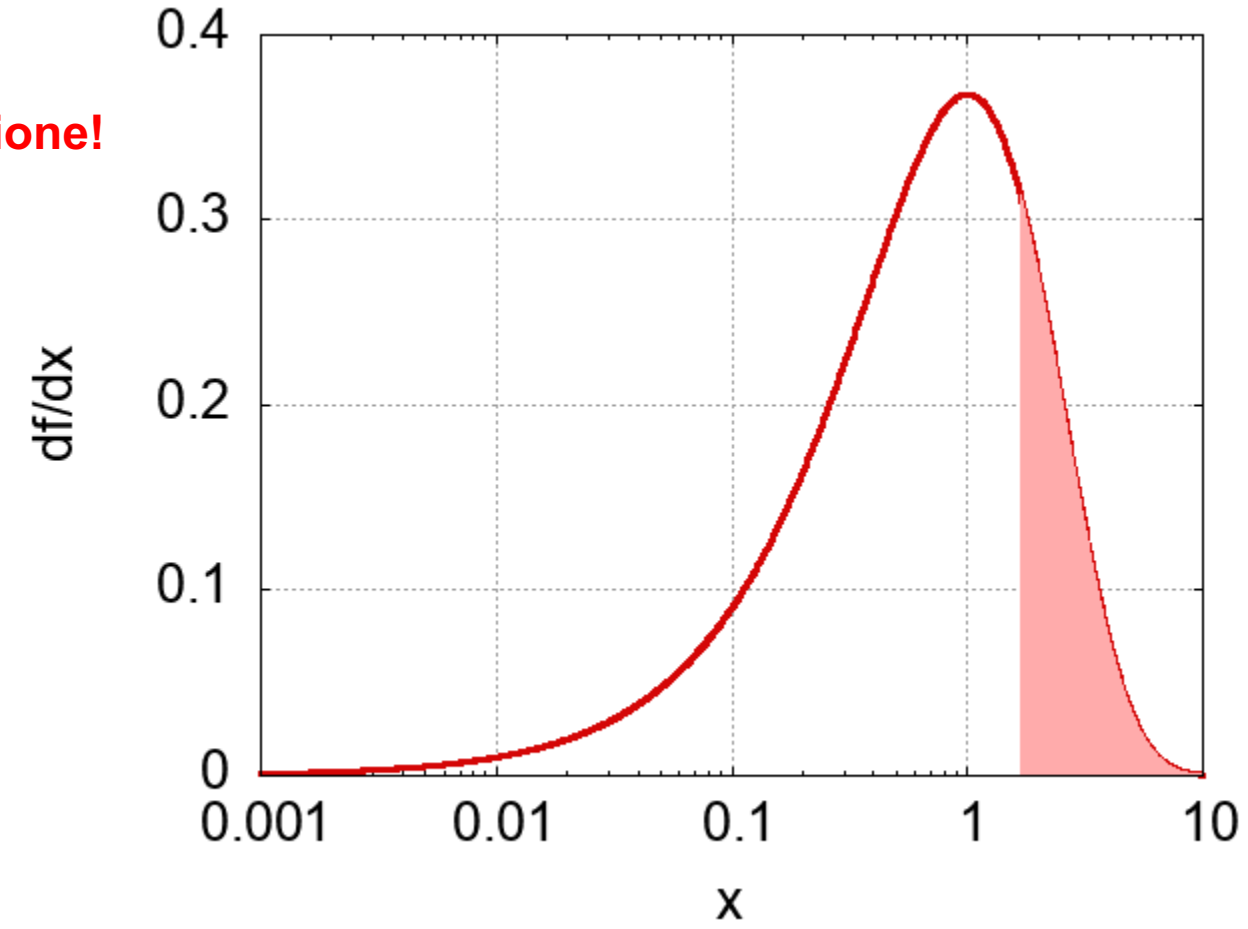
- Suppose you want to legitimally resolve what happens at small x in more detail
- So you naturally plot the **horizontal axis in logarithmic scale, don't you?**



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!

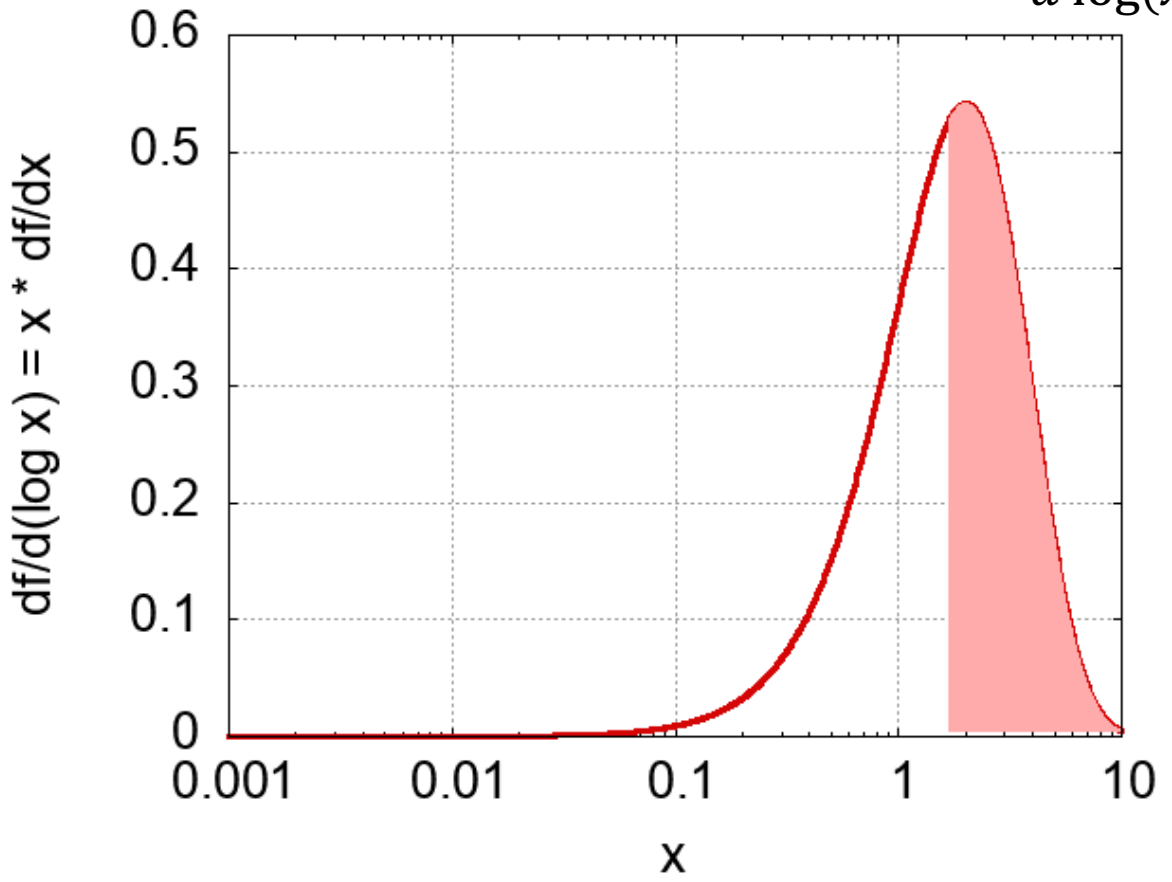


With this careless action you are severely distorting information!!!

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

An important reminder from the scoring lecture

- 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 $\frac{df}{d\log(x)}$:



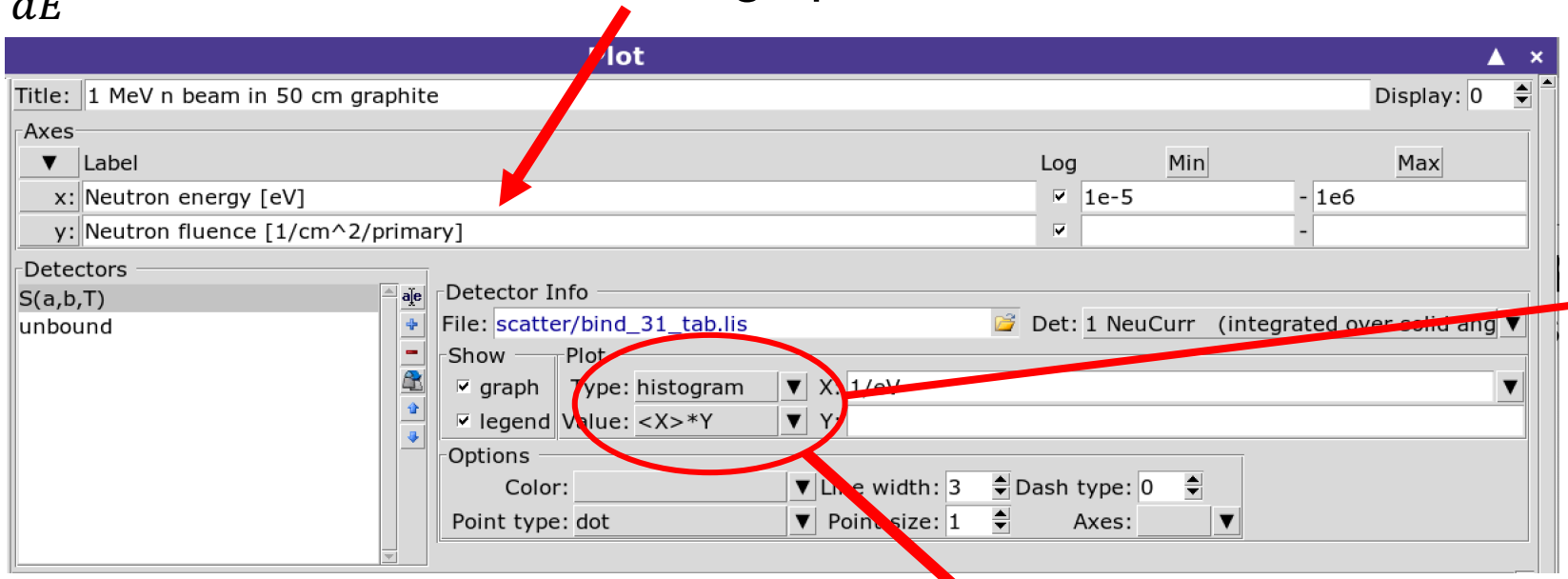
In this representation, integrals are respected

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 axes 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}?

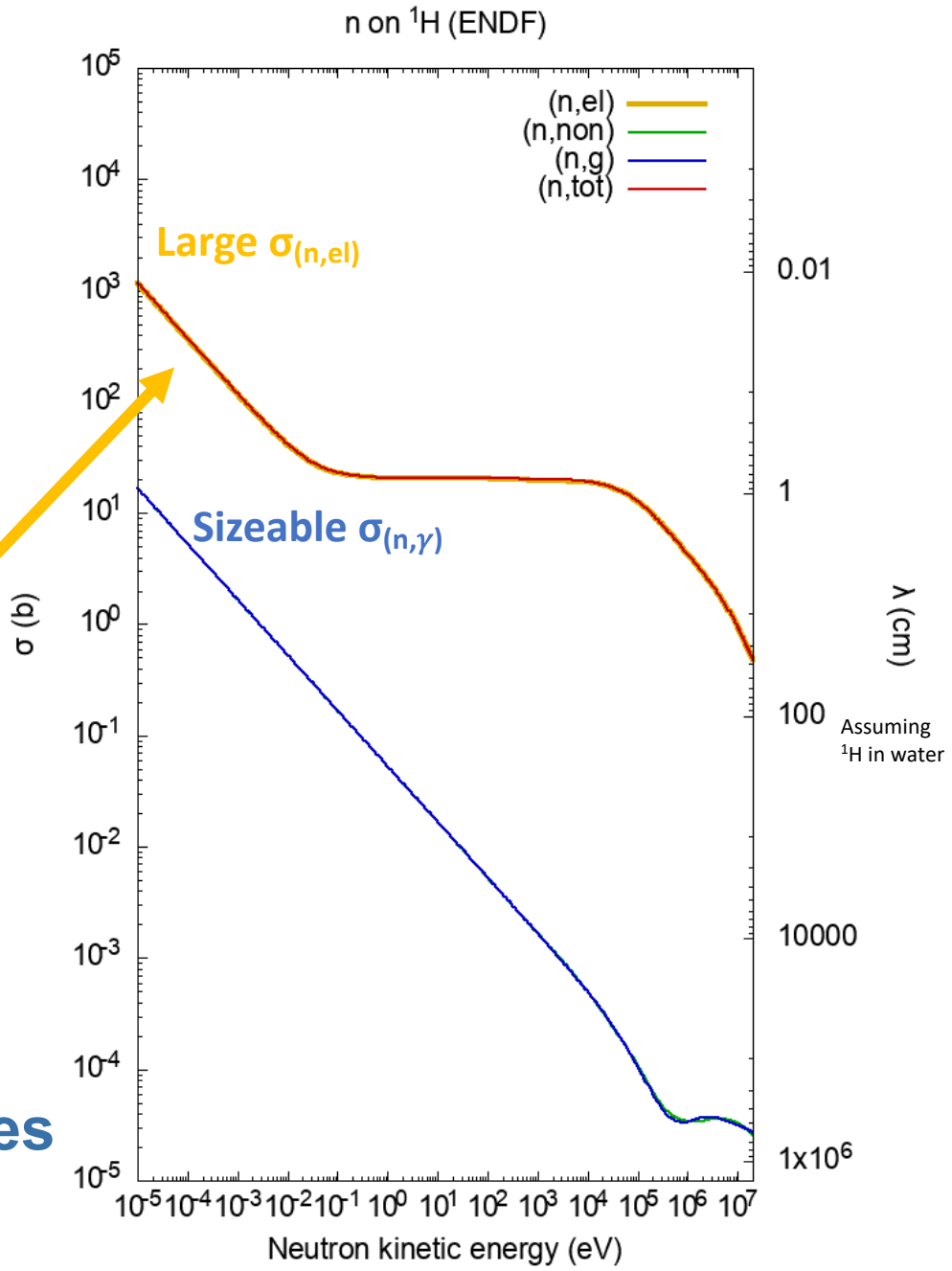
$$\log X = \frac{1}{2}\left(\log X_{i+1} + \log X_i\right) = \frac{1}{2}\log(X_{i+1}X_i) \quad \Rightarrow \quad X = \left[e^{\log(X_{i+1}X_i)}\right]^{1/2} = \sqrt{X_{i+1}X_i}$$

^{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 this energies, $\sigma_{(n,\gamma)}$ becomes sizeable: capture depletes the neutron flux in favor of MeV photons (!)
- **One must track neutrons down to thermal energies**

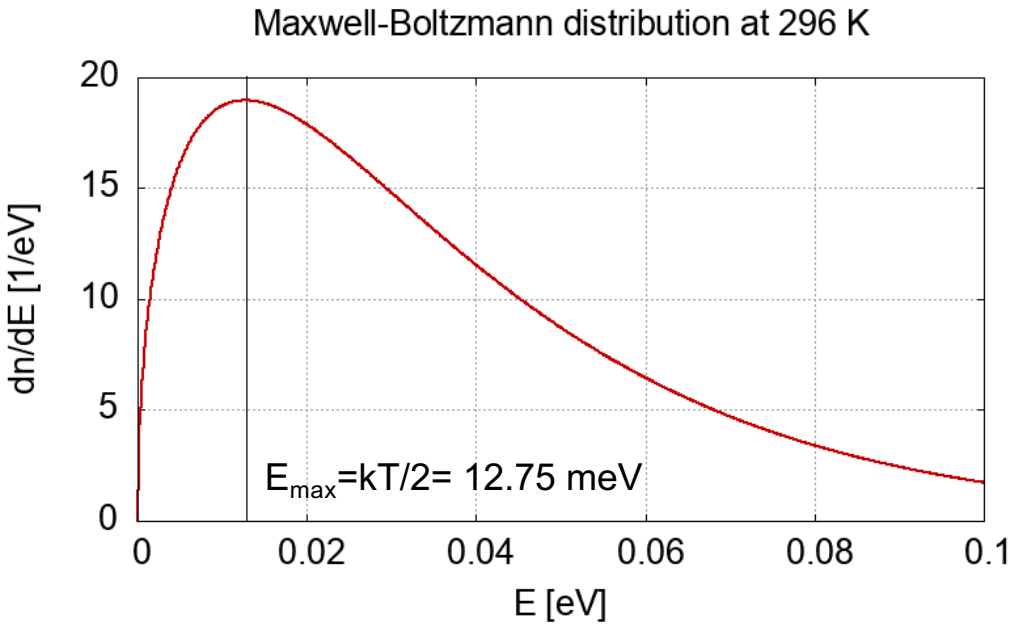


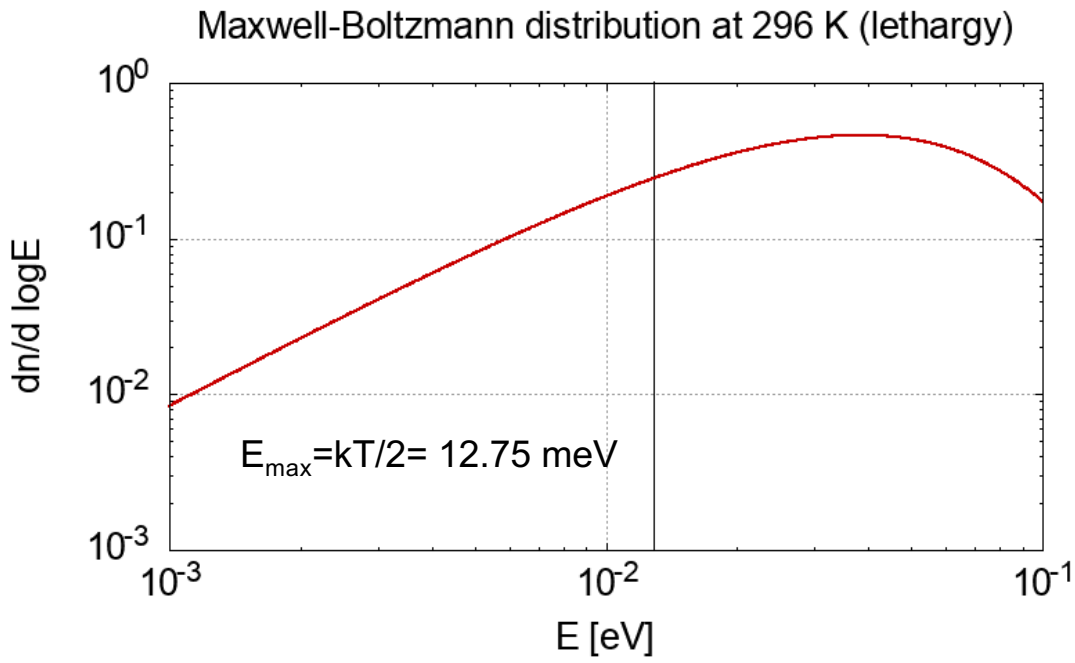
Neutron thermalization

- Thermal motion energy: O(*kT*)
- **At 296 K, *kT*=25.5 meV**
- At/near these energies, neutrons collide elastically* 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



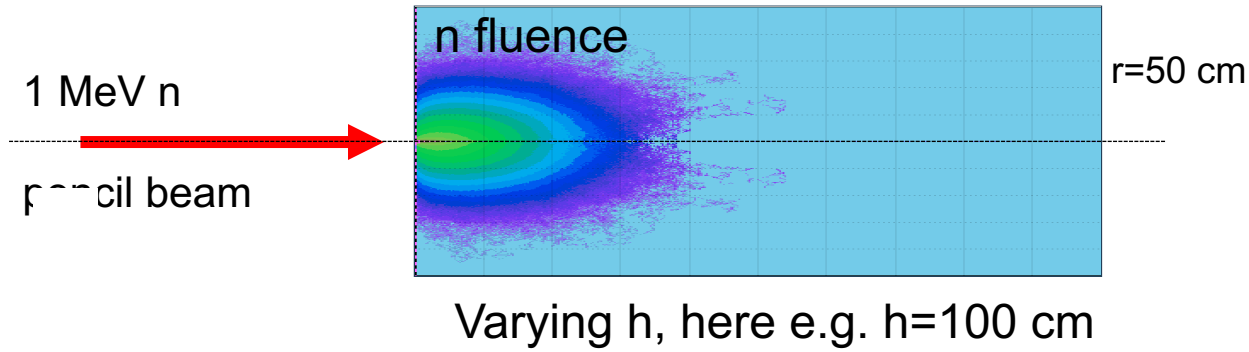


Thermalization in H_2O

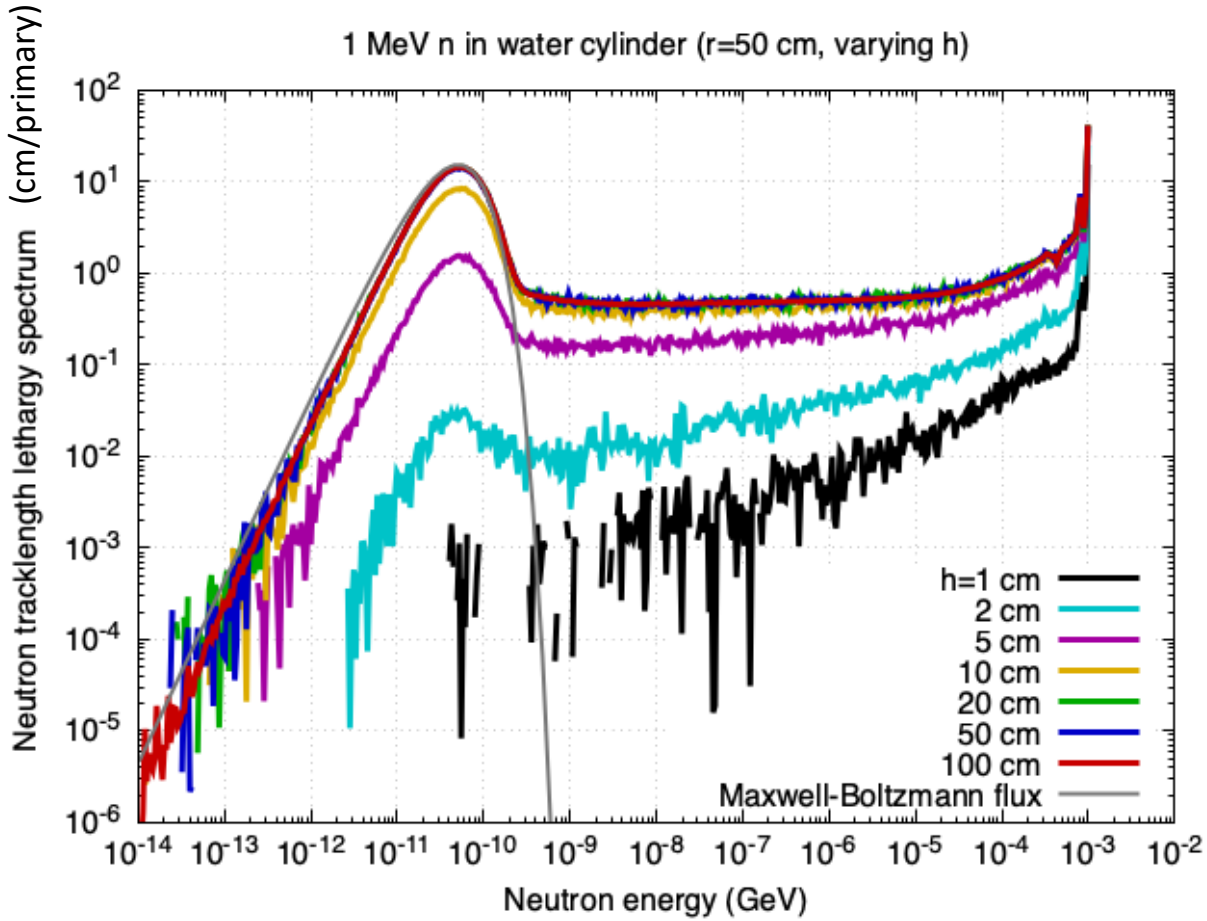
- Example: n pencil beam, E=1 MeV, impinging on a water cylinder (r=50 cm, varying h)
- $\lambda_{(n,el)}$(1 MeV) = 3.5 cm (in water)
- **For h≪$\lambda_{(n,el)}$, n barely scatter**
- **For h~ $\lambda_{(n,el)}$, n start to scatter elastically:**
  - Change direction (possibly staying longer in the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

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

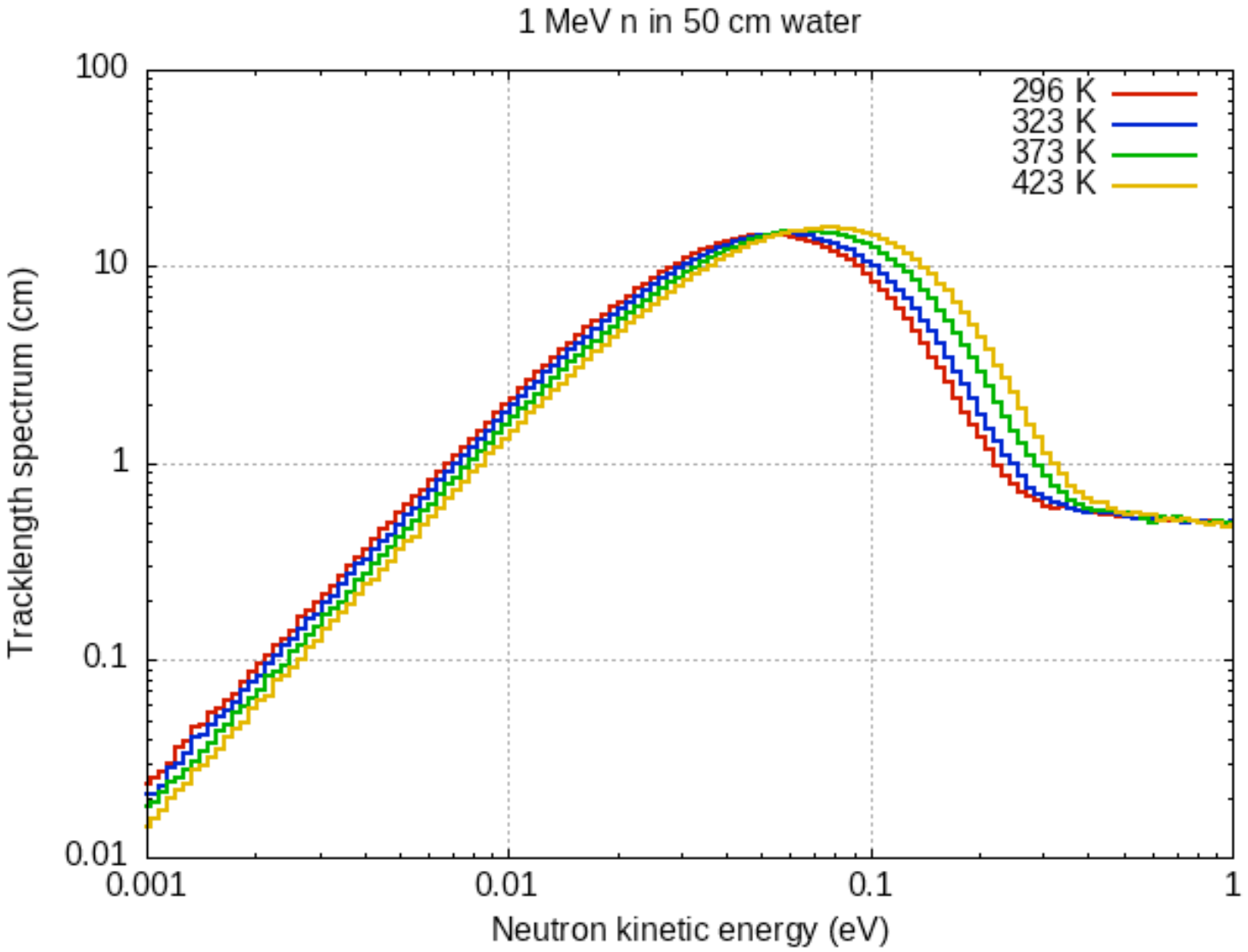
- (n,γ) on either ^{1,2}H or ^{16,17,18}O eventually consumes the neutron flux in favor of MeV photons



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



Thermalization at different temperatures

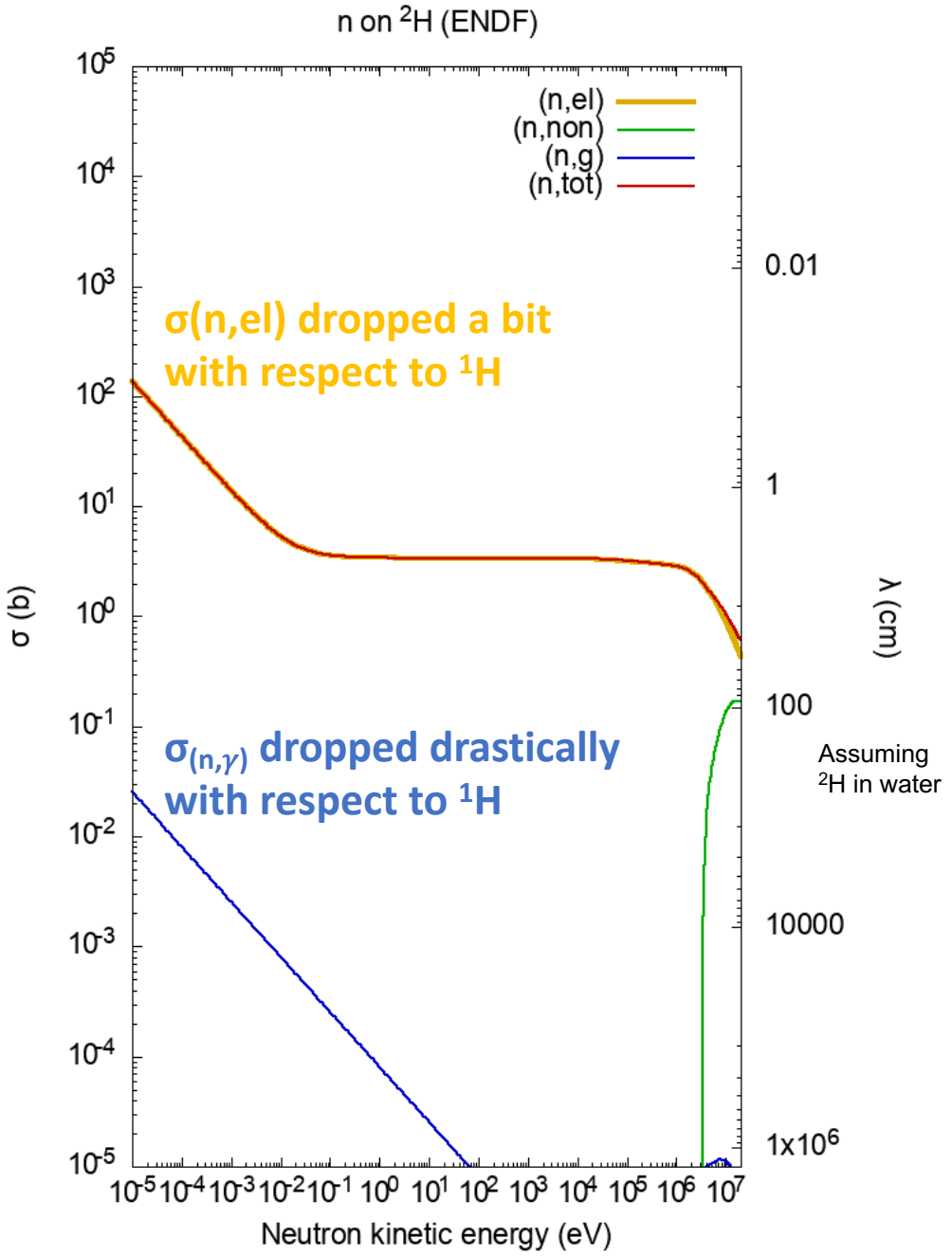


The thermal peak indeed shifts linearly with the temperature

^{2}H(n,el)

- Foregoing analysis: compounds containing ^{1}H are good neutron moderators
- But ^{1}H has a sizeable (n,γ) cross sections. 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 n lost to capture on the way to thermalization)
- ^{2}H still has good moderator properties:

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



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

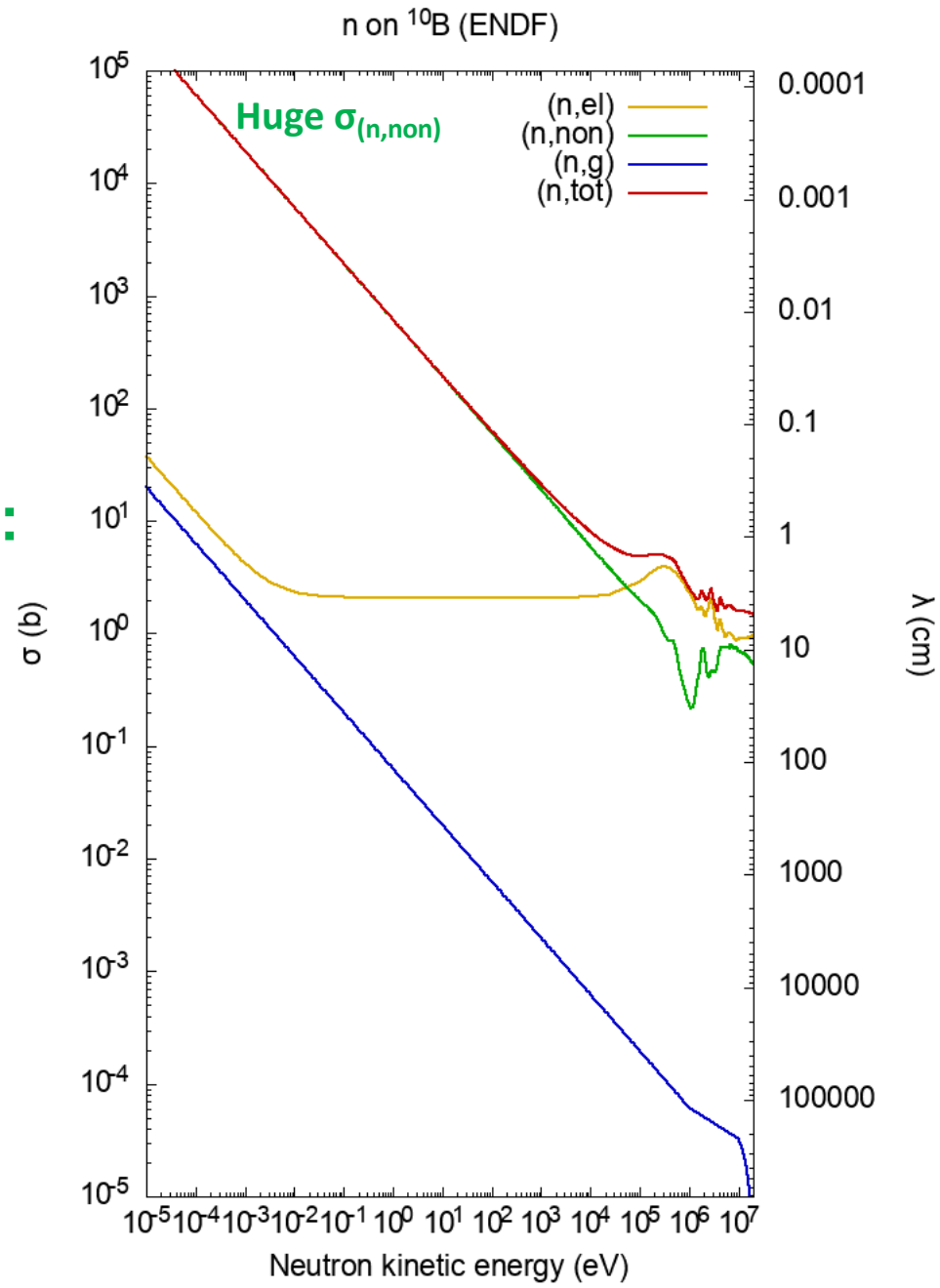
- $\sigma_{(n,el)}$ is only slightly lower than for $^{1,2}H$
- But: $E_{rec,max}$(n on ^{10}B) $\ll E_{kin}$
- ^{10}B is not as effective a moderator as $^{1,2}H$
- **However, ^{10}B has a reaction channel with large σ:**

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

- **10^3-10^5 b, i.e. mean free paths $\ll$ 100 μm**
- ^{7}Li and α have short range (< 10 μm).

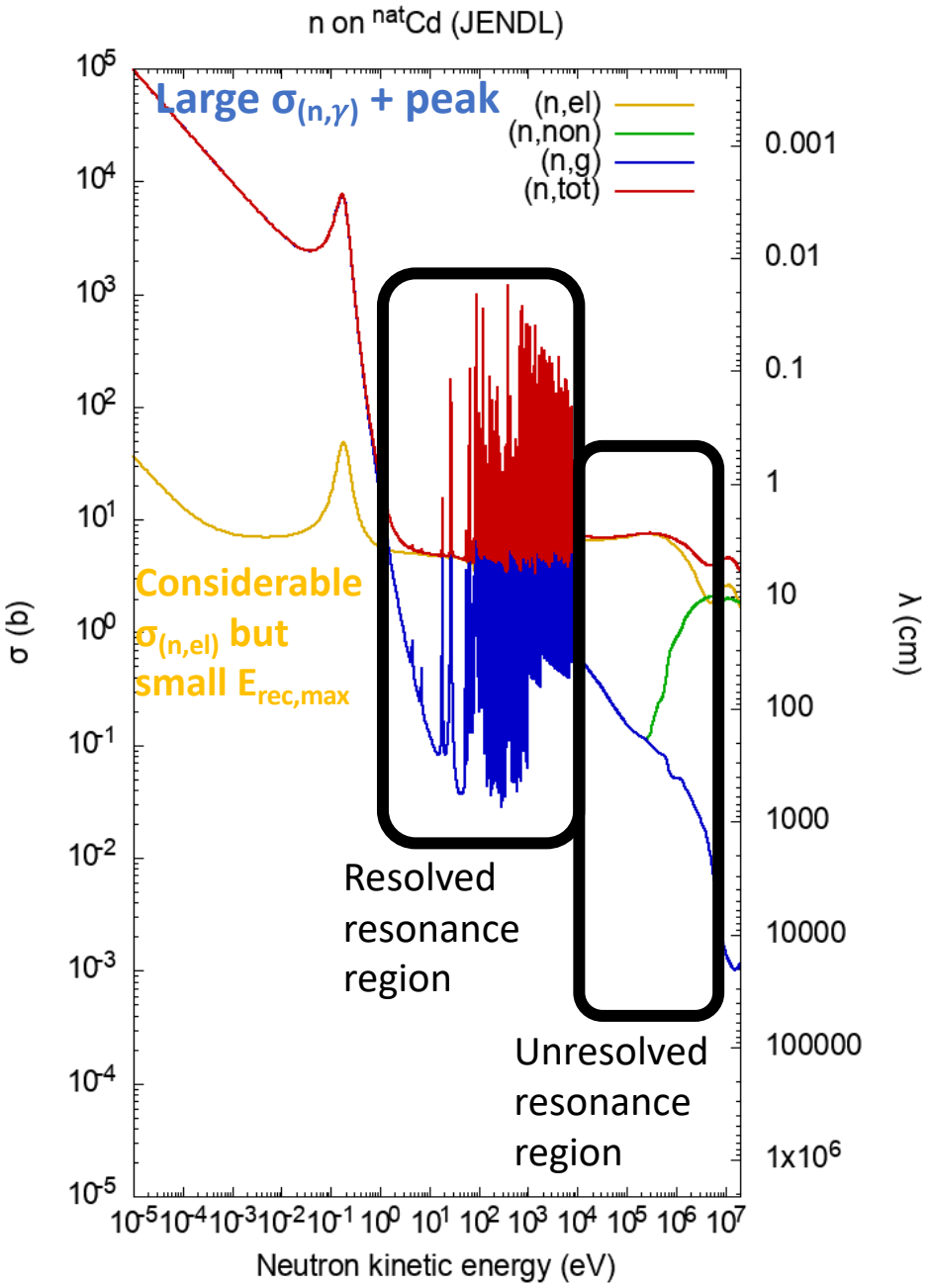
- Basis for various applications:
  - boron neutron capture* therapy (BNCT)
  - boron rods in nuclear power plants to control n flux

**should rather be "absorption"*



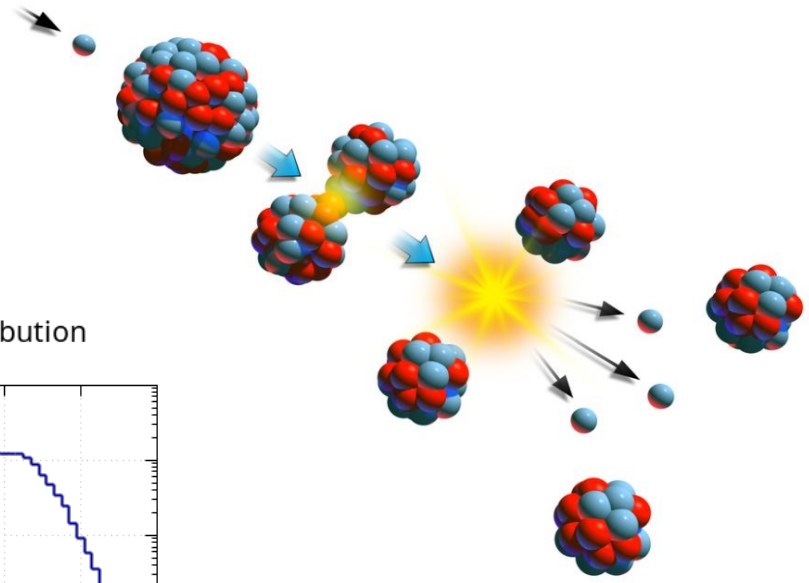
$^{nat}Cd(n,\gamma)$

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

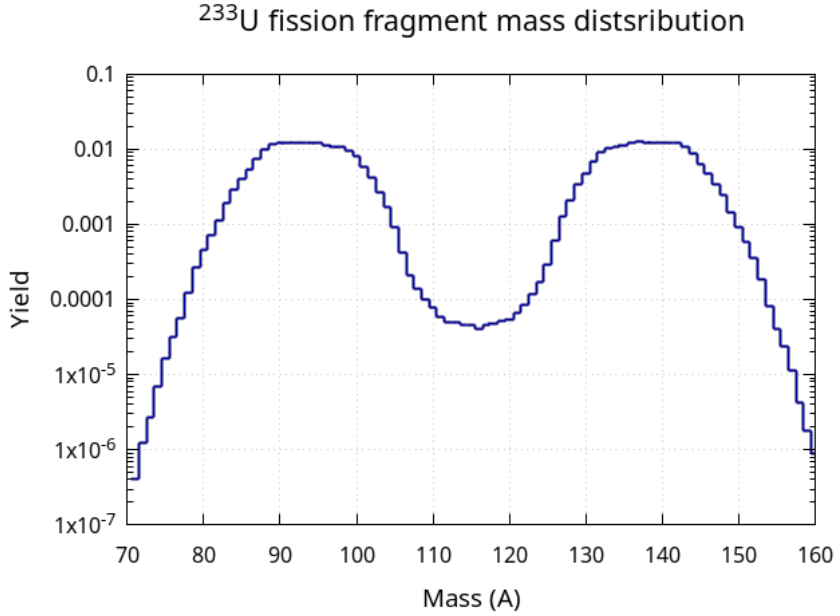


^{235}U(n,f)

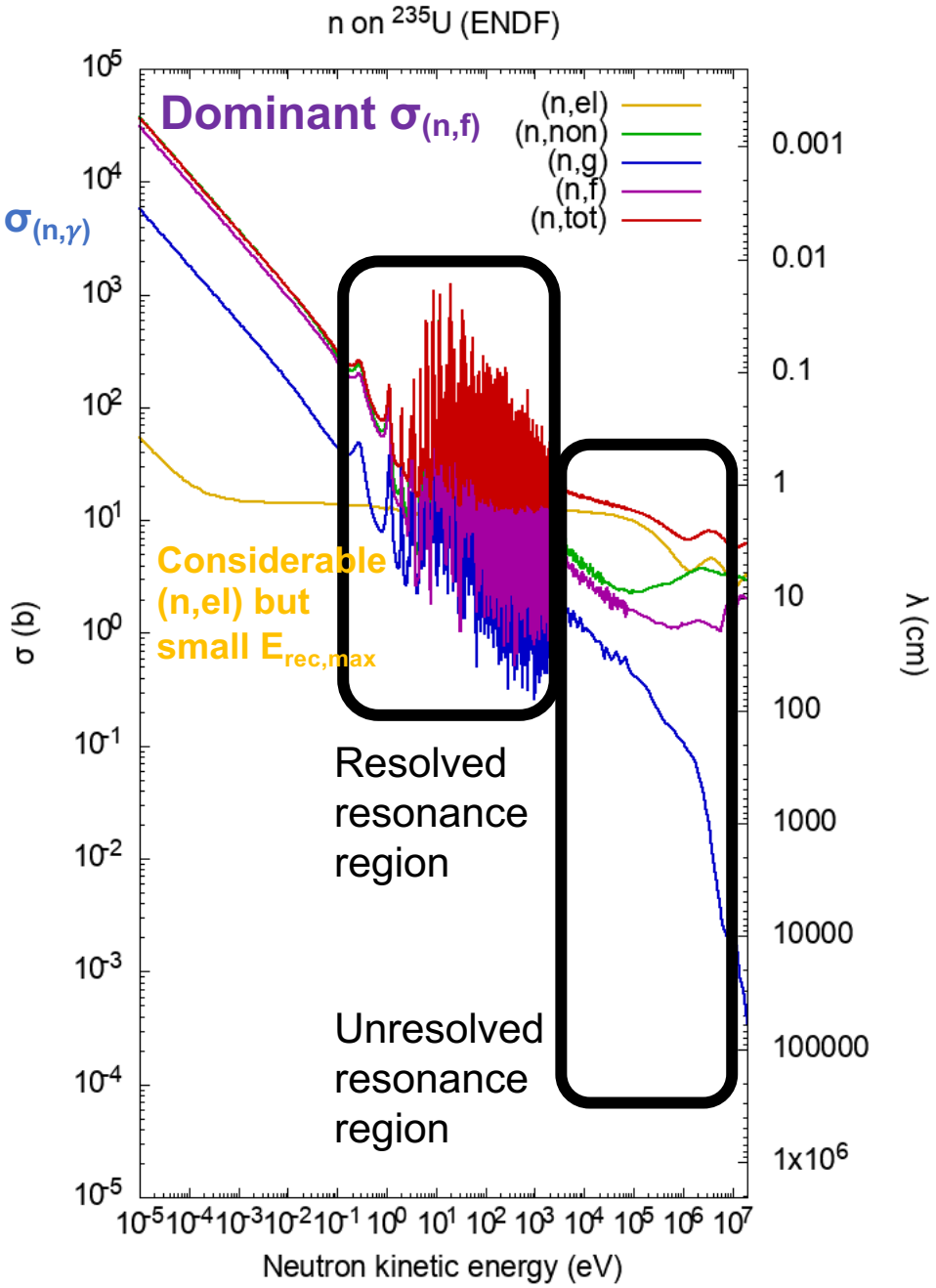
- For heavy targets, (n,f) tends to dominate at thermal energies



Fission neutrons with energies O(1) MeV



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



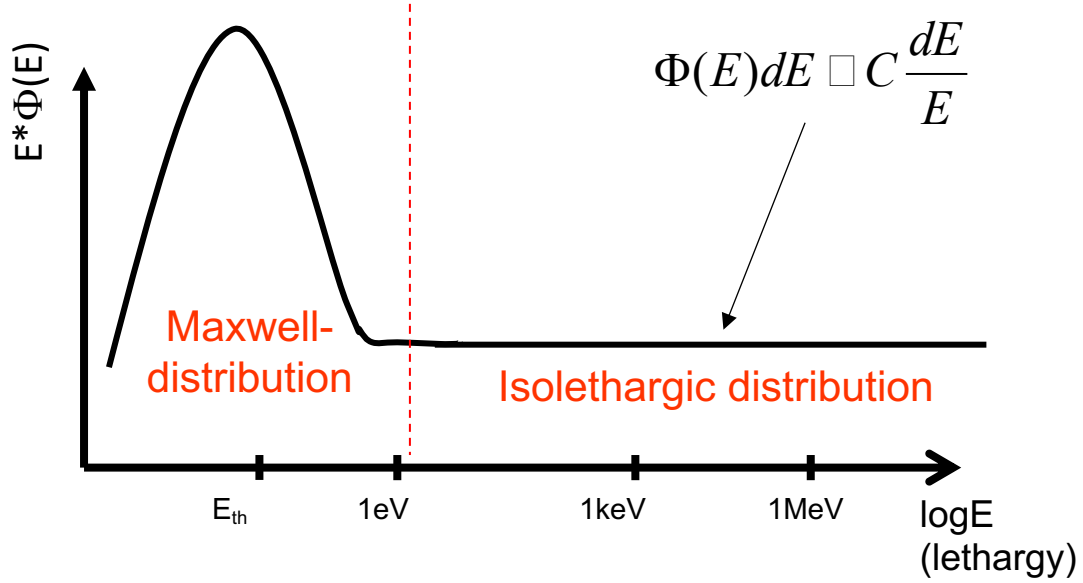
Group-wise treatment of neutron interactions below 20 MeV in FLUKA

Legacy approach, still the default as of FLUKA v4-3.4

Future FLUKA versions will adopt point-wise approach by default
Group-wise interactions still supported

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:



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

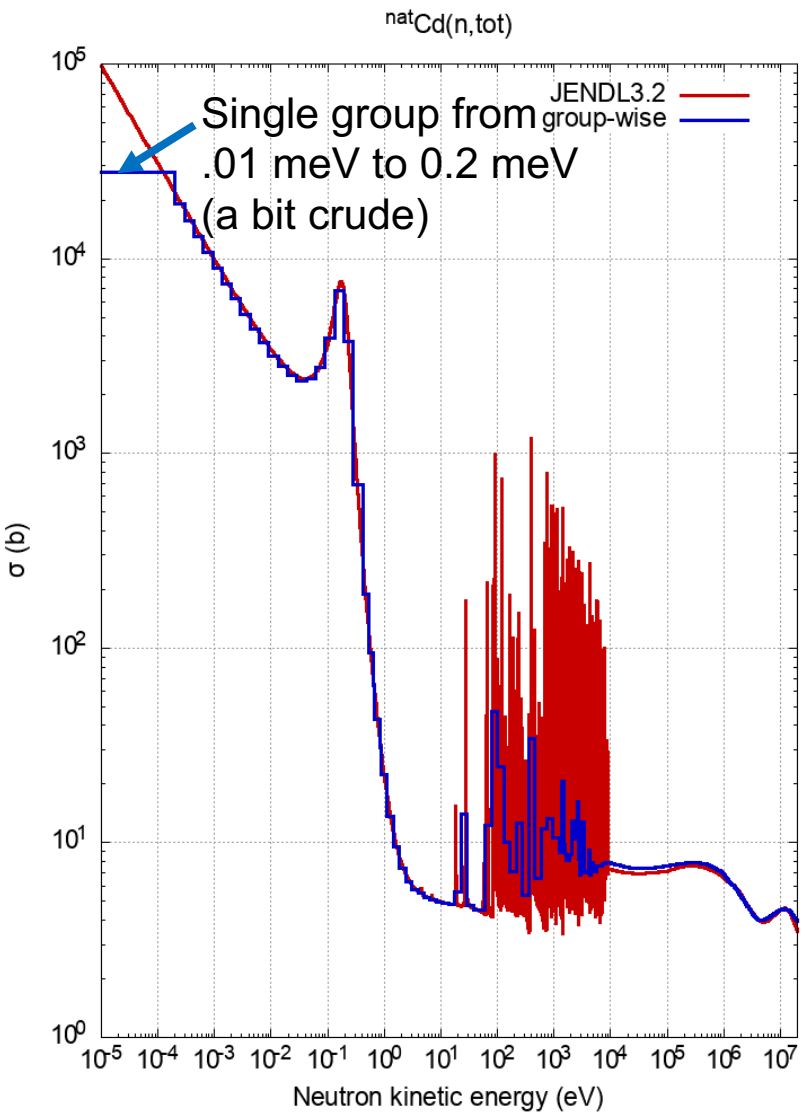
- Energy (**continuous variable**) becomes a group index *g* (**discrete variable**)
- Effect: continuous cross sections become histograms

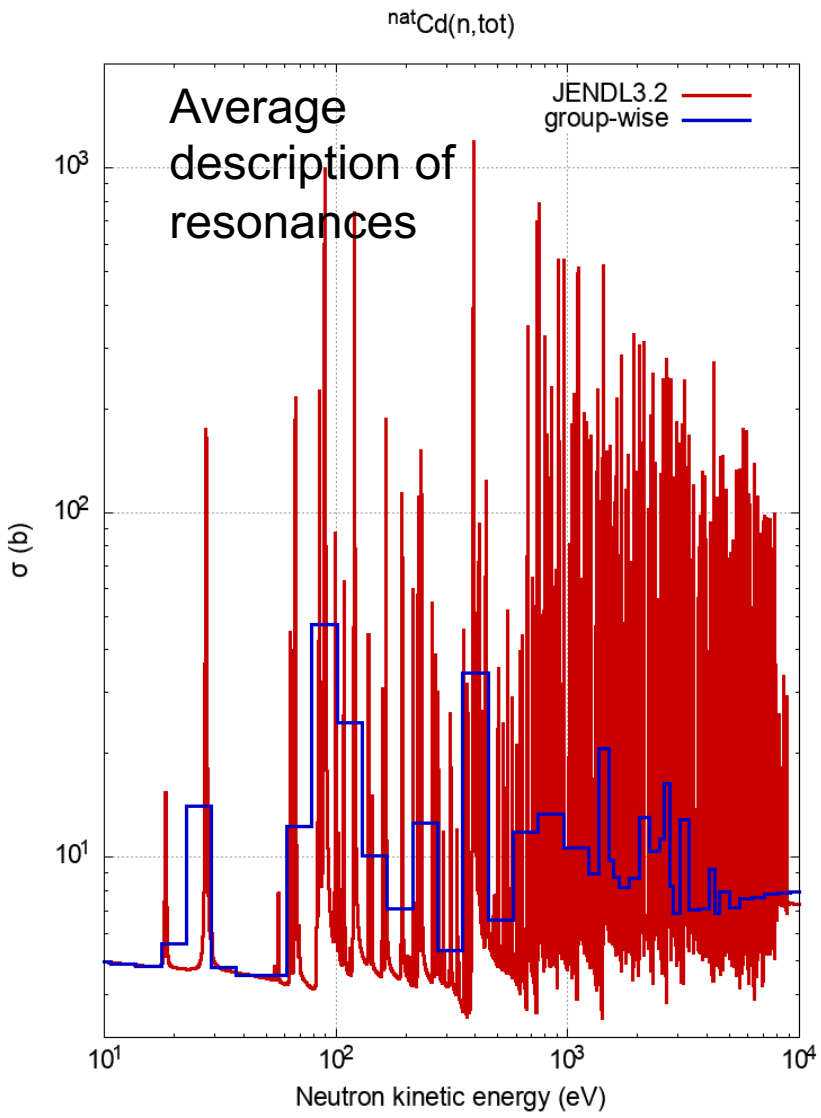
Low-energy neutron groups in FLUKA

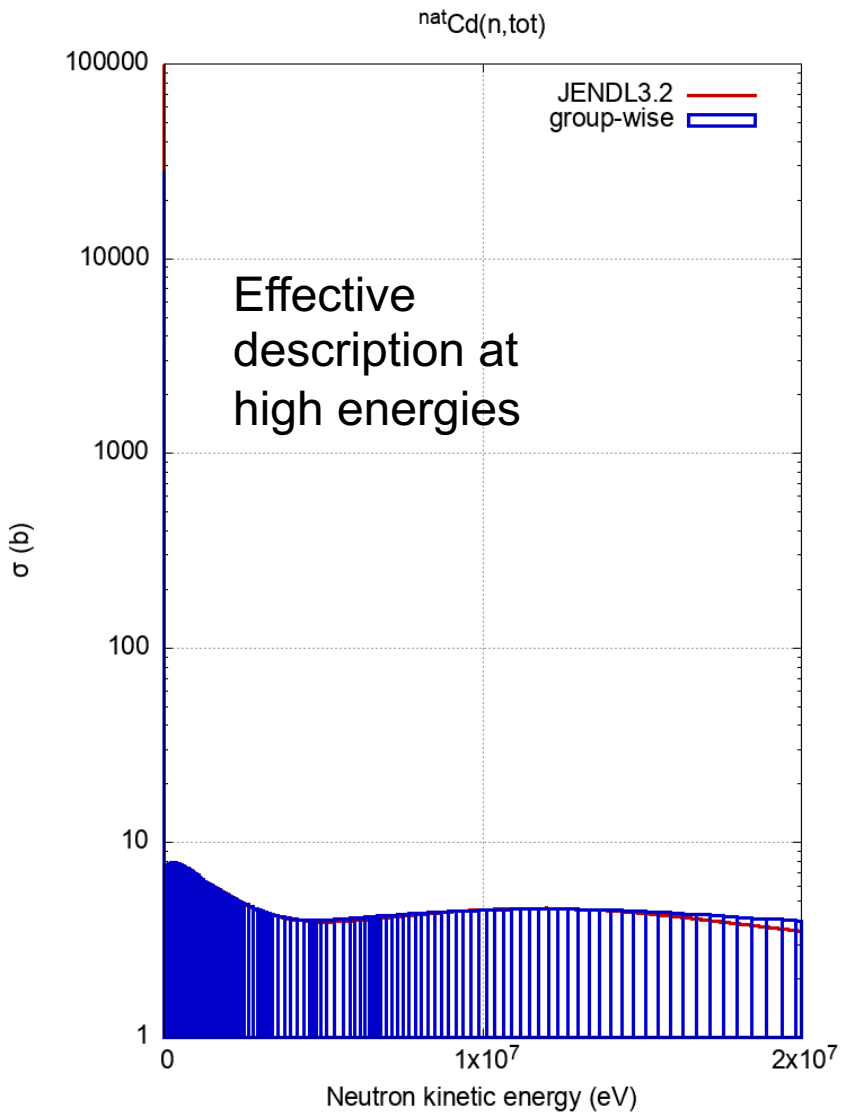
- Highest considered energy group index: 1
- Lowest considered energy group index: 260
- All energy-resolved quantities involving low-energy neutrons default to this fixed binning
- This affects USRTRACK, USRBDX, USRYIELD, USRCOLL

#	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

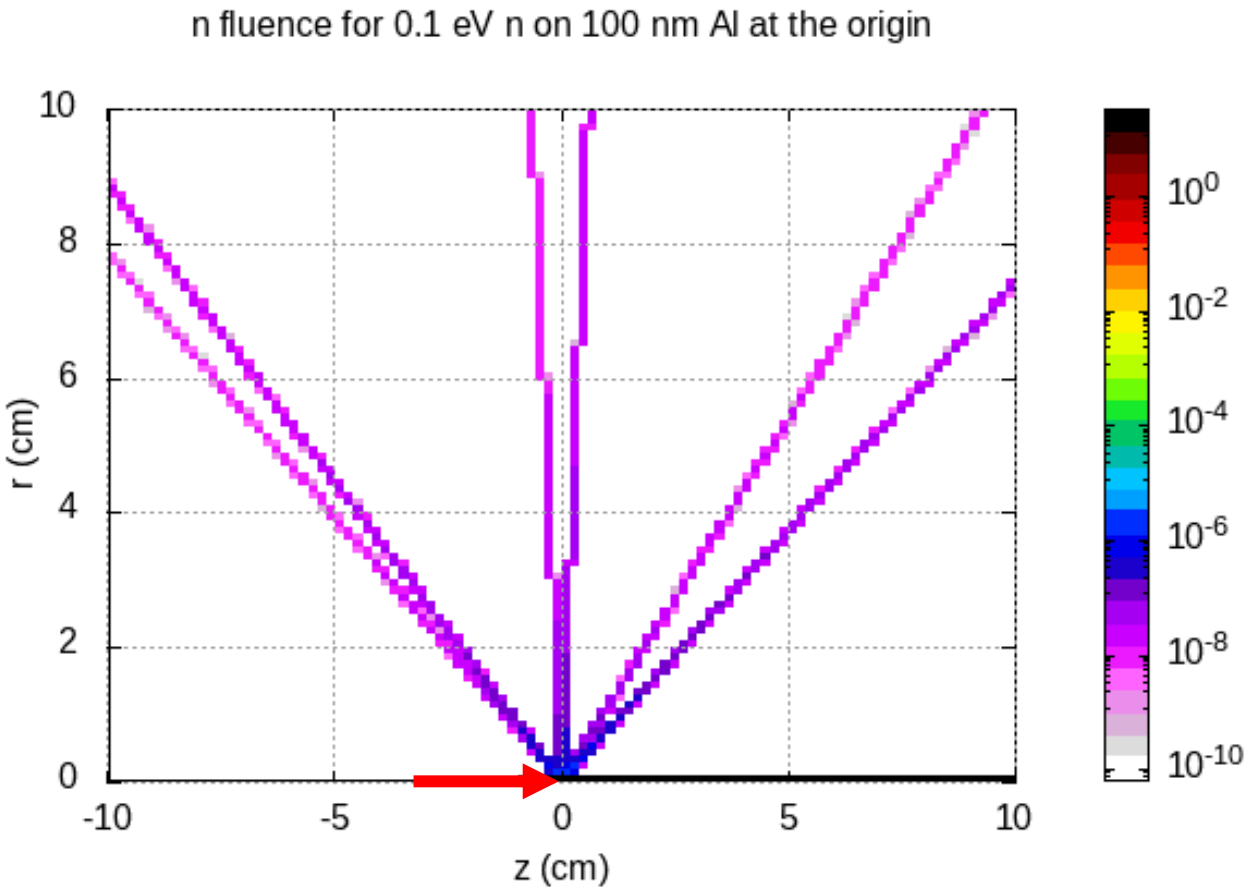






Angular distributions

- (n,el) and reaction channels with secondary n are described in terms of an **up/down-scattering matrix $M_{gg'}$** providing the likelihood for a n to transition from a group *g* to a 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 discretized onto 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 isotope. 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** for 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 merit:
  - It is **fast** and has **small memory requirements**
  - It is sufficient for some applications, e.g. to score energy deposition in thick materials
- As of v4-3.4 it is still the default

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

- As of v4-3.4, group-wise treatment is the default for all FLUKA DEFAULTS
- Every FLUKA material* 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 ▼	

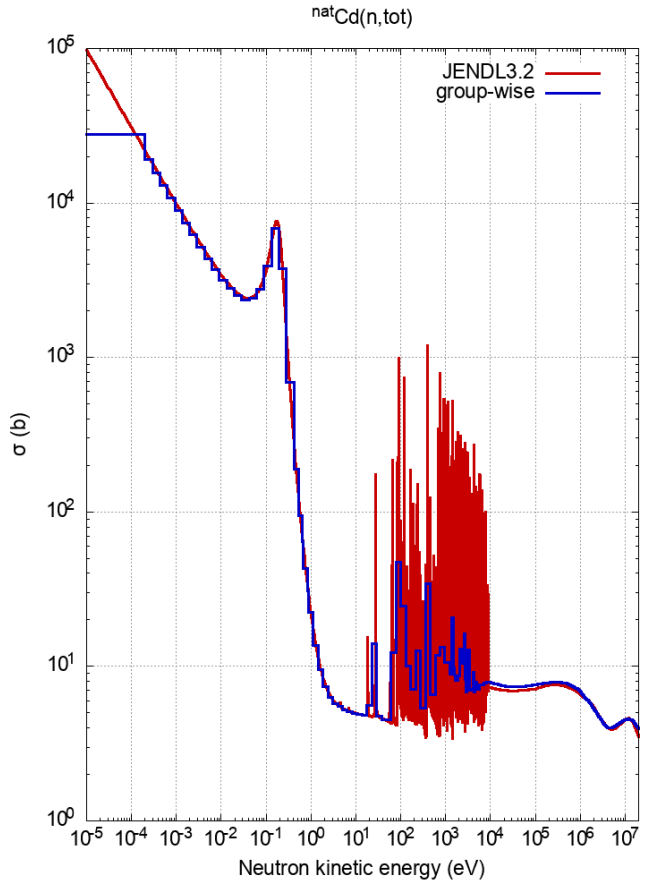
- The first match of FLUKA material name to group-wise library material name is taken

** besides VACUUM and BLCKHOLE…*

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

General treatment introduced in FLUKA v4-3.0

Soon to be the default in FLUKA
(stay tuned to release announcements)



Point-wise interactions in FLUKA

- Nearly direct sampling from evaluated nuclear data libraries:
  - **ENDF** (Evaluated Nuclear Data Files): https://www-nds.iaea.org/exfor/endf.htm
  - **JEFF** (Joint Evaluated Fission and Fusion library): https://www.oecd-nea.org/dbdata/jeff/
  - **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
- FLUKA's implementation relies on G4NDL:

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

- Requires download of additional packages:

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

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 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 fission channel

FLUKA point-wise data libraries

- Due to huge size, the neutron data libraries are provided as separated 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 v4-3.4 is **JEFF-3.3**
- Older evaluations are provided as well for comparison purposes
- Thermal Scattering Law S(α,β,T) for several materials

- 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

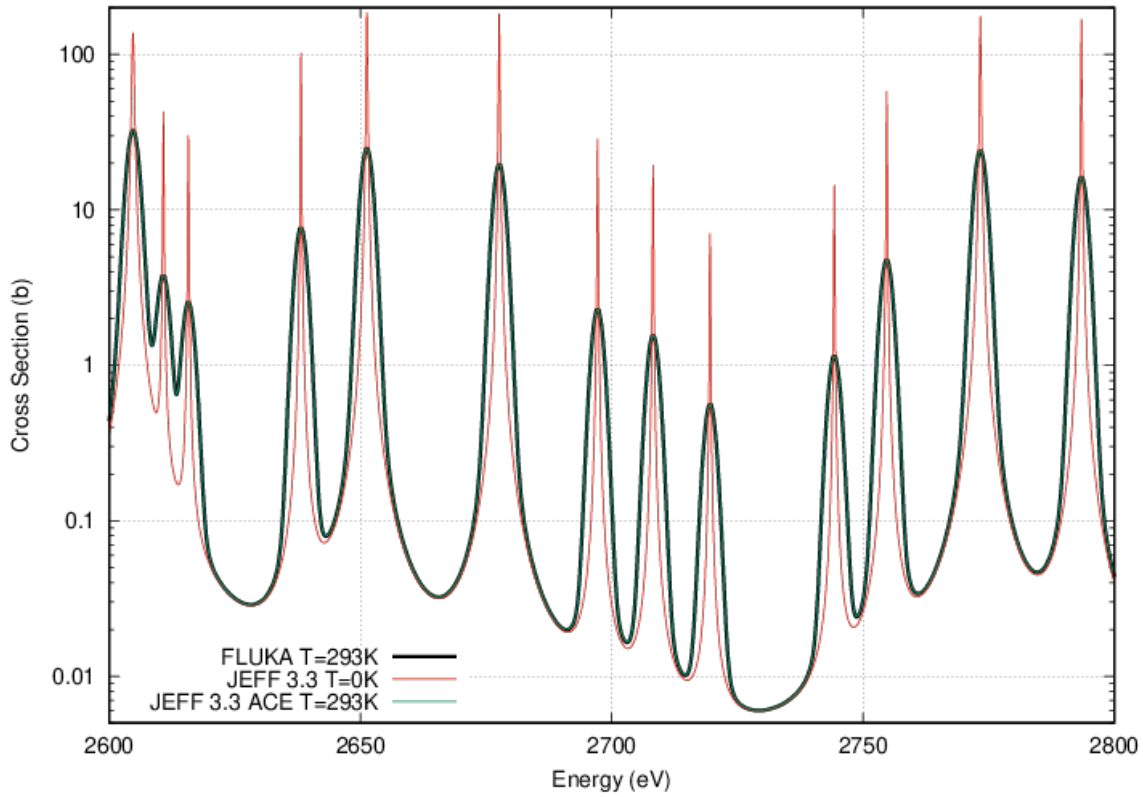
Pointwise interactions in FLUKA: key features

- Nearly direct sampling from evaluated nuclear data libraries
- (E_i,σ_i) tables with accuracy < 0.1%
- Modern C++ implementation
- Heavily 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
- Fast Doppler broadening at arbitrary temperature performed at initialization
- "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 T required using an adaptive numerical integration
- Performed at initialization
- Fast: CPU time reported in output file (see below)

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

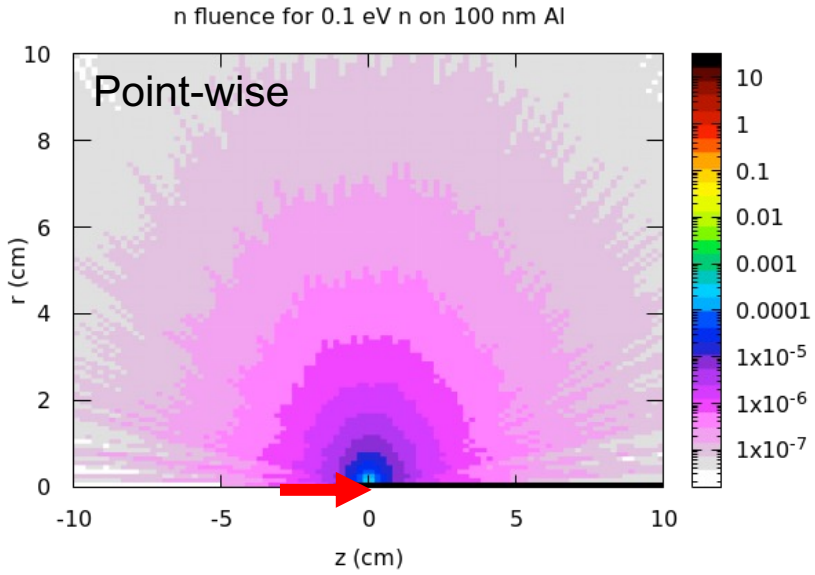


Online Doppler broadening example at 293 K for ^{113}Cd(n,g):

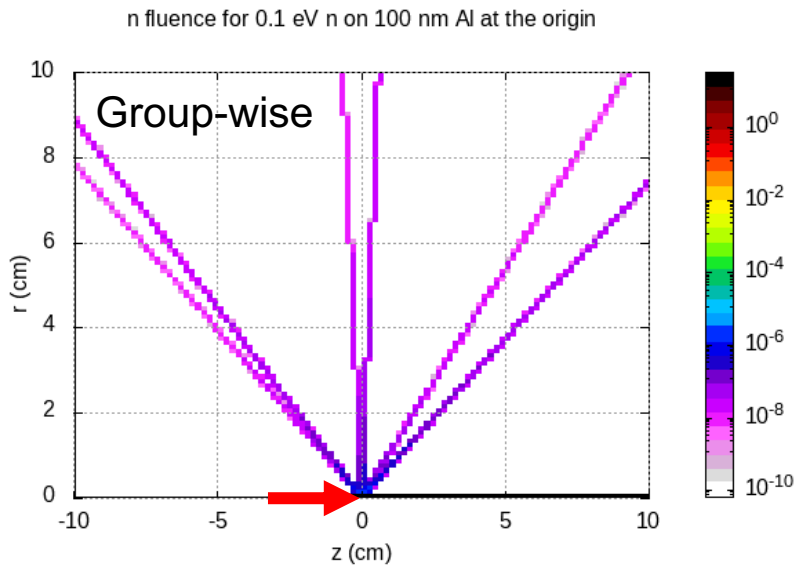
- FLUKA
- JEFF (T=0 K)
- JEFF processed with NJOY

Point-wise (n,el) in FLUKA

- Above ~5eV the **target nucleus is effectively at rest**
- Below ~5eV the **target nucleus motion** is sampled from a Maxwell Boltzmann distribution (using the constant cross section model)
- Recoils are explicitly calculated and pushed in the stack



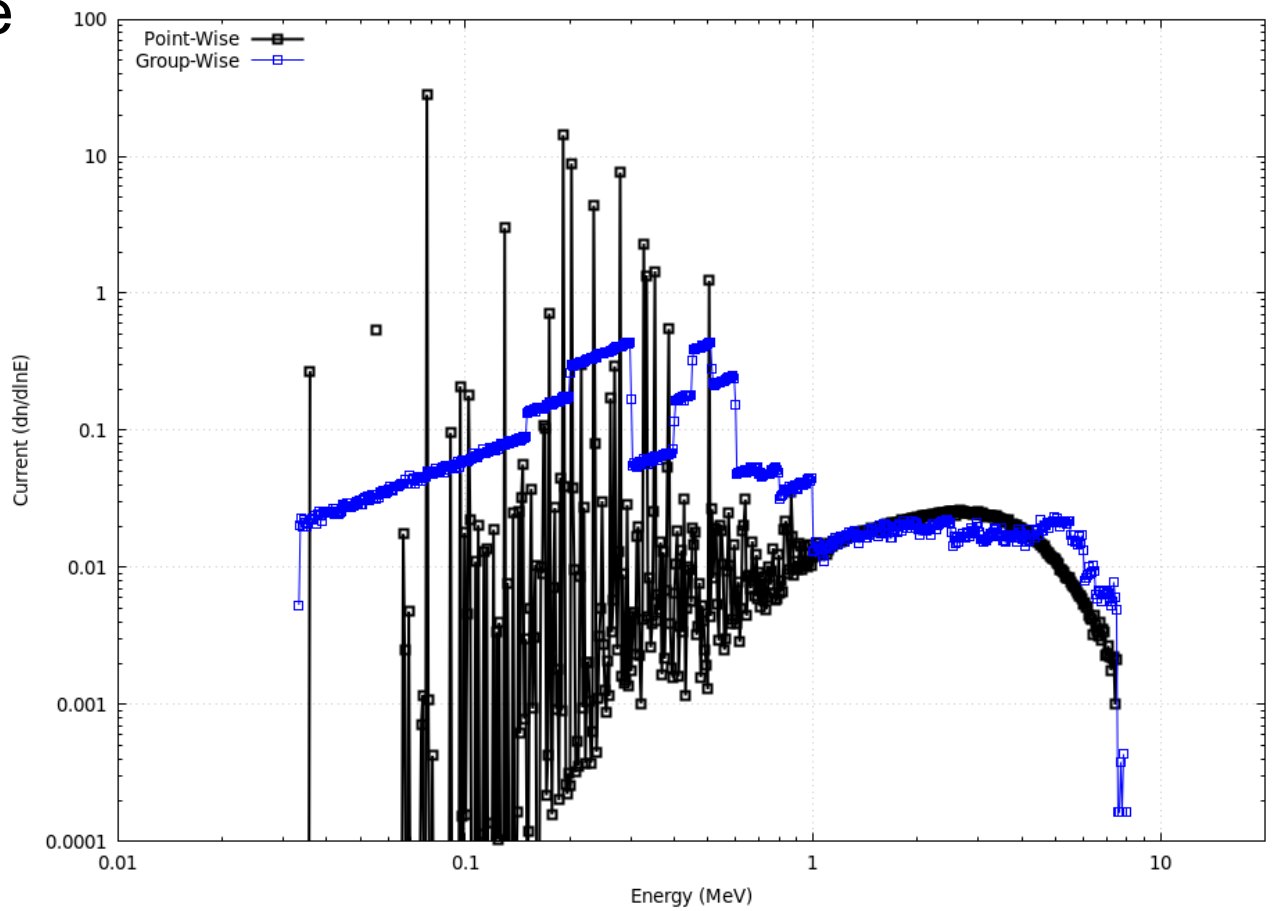
- Below ~eV, neutron wavelength spreads over several atoms. Neutron scattering cross sections are sensitive to the specific molecular/crystalline binding of the active target isotope.
  - H(n,el) will be different depending on whether H is bound in H_2, H_2O, ZrH, etc.
- To account for binding effects, 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 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

^{197}Au(n,γ)

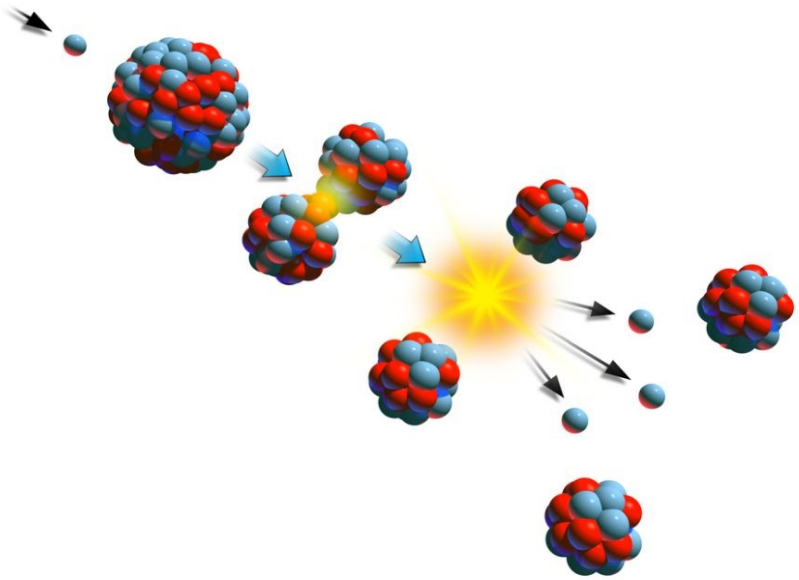


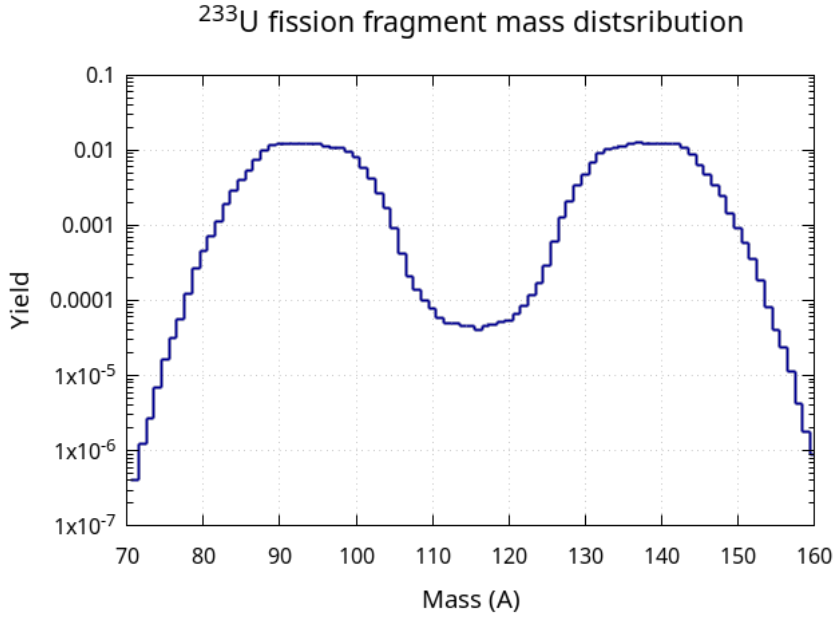
Inelastic interaction channels

- 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 one-by-one the secondaries (except the photons) 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 later)

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)

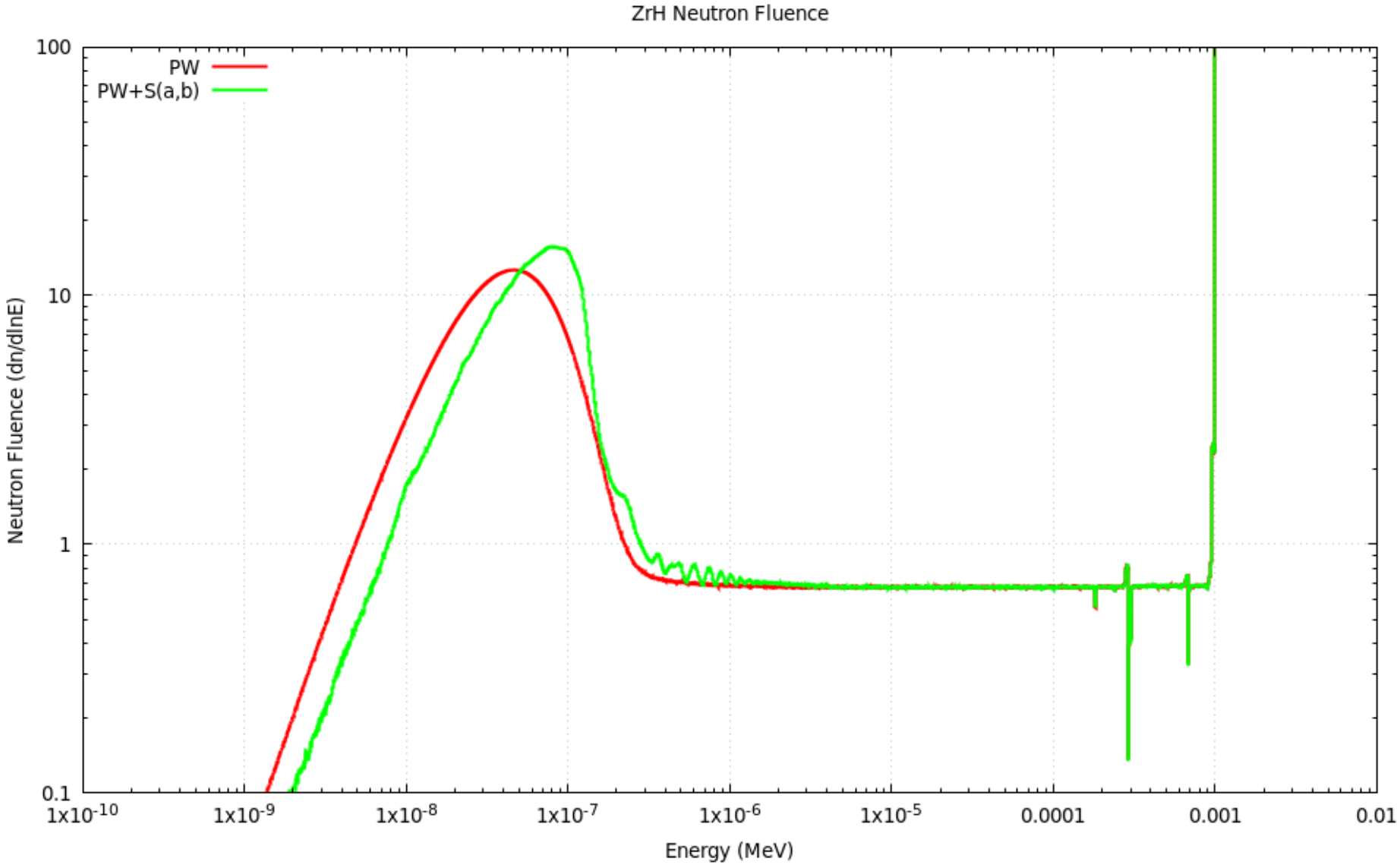
- For neutrons with thermal energies, generally less than ~4 eV, scattering cross sections are affected by the chemical/molecular/crystalline binding environment of the active target isotope.
- If binding effects are not accounted for in a simulation, the reported results may be highly inaccurate.

- 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(α,β,T) (2/2)

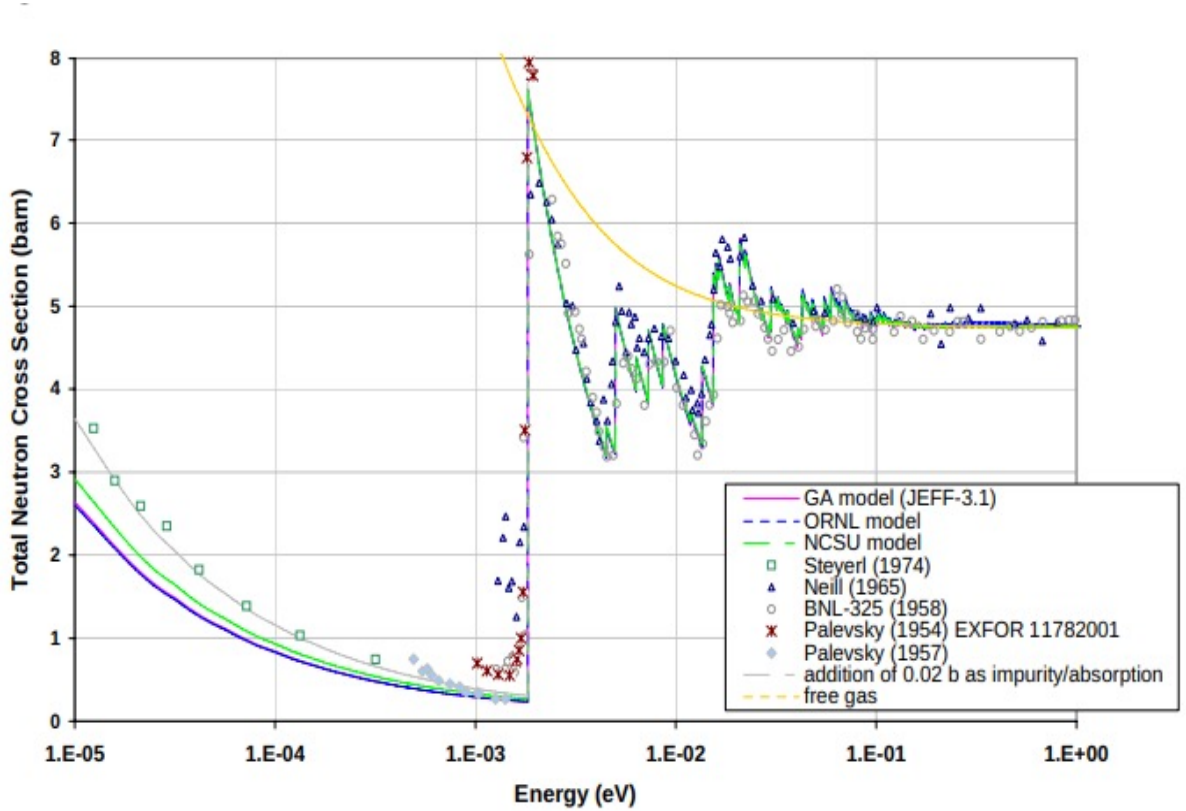
- Channels (nomenclature refers to state in which target system is left):
  - **Elastic** – the neutron energy remains the same, the angle is changing
    - **Coherent** – discrete angles depending on the crystal direction vs neutron direction and Bragg edge selected, on crystal lattice
    - **Incoherent** – 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
- Must be requested explicitly on a per-isotope basis (see LOW-PWXS card below)
- Exception: H is always assumed bound to H_2O

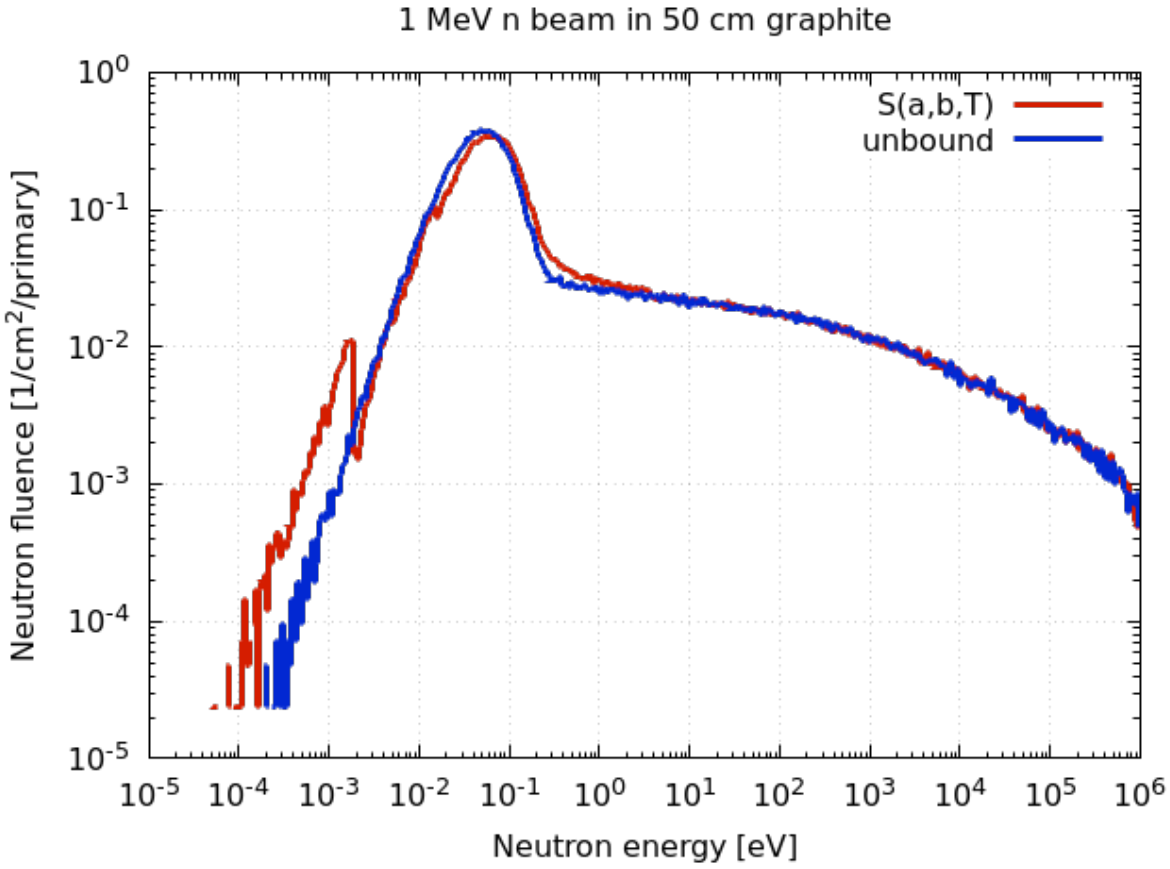
Example S(α,β,T) on ZrH



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

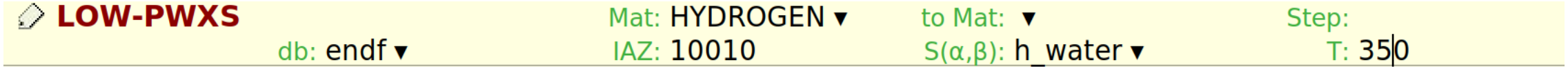
- `LOW-PWXS` card controls the new point-wise treatment in FLUKA
- WHAT(1):
  - **empty/0** = use PW treatment for this isotope (default)
  - **>0** Isotope code **Z*10000 + A*10 + iso**
  - **-1** = switch to OLD behavior, use GW/Old PW treatment for this isotope
- WHAT(2):
  - **S(α,β,T)** tabulation 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 v4.3 default = JEFF-3.3)

LOW-PWXS: examples

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

- With WHAT(1) = -1 to use OLD way, i.e. GW supplemented by PW for a handful of channels

- 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**



- *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 operationally declared as point or groupwise with the `LOW-PWXS` card.
- E.g.: USRBDX with a pointwise material and VACUUM 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 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**: 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