Low-Energy Neutron Treatment in FLUKA

Beginners' FLUKA Course

Introduction

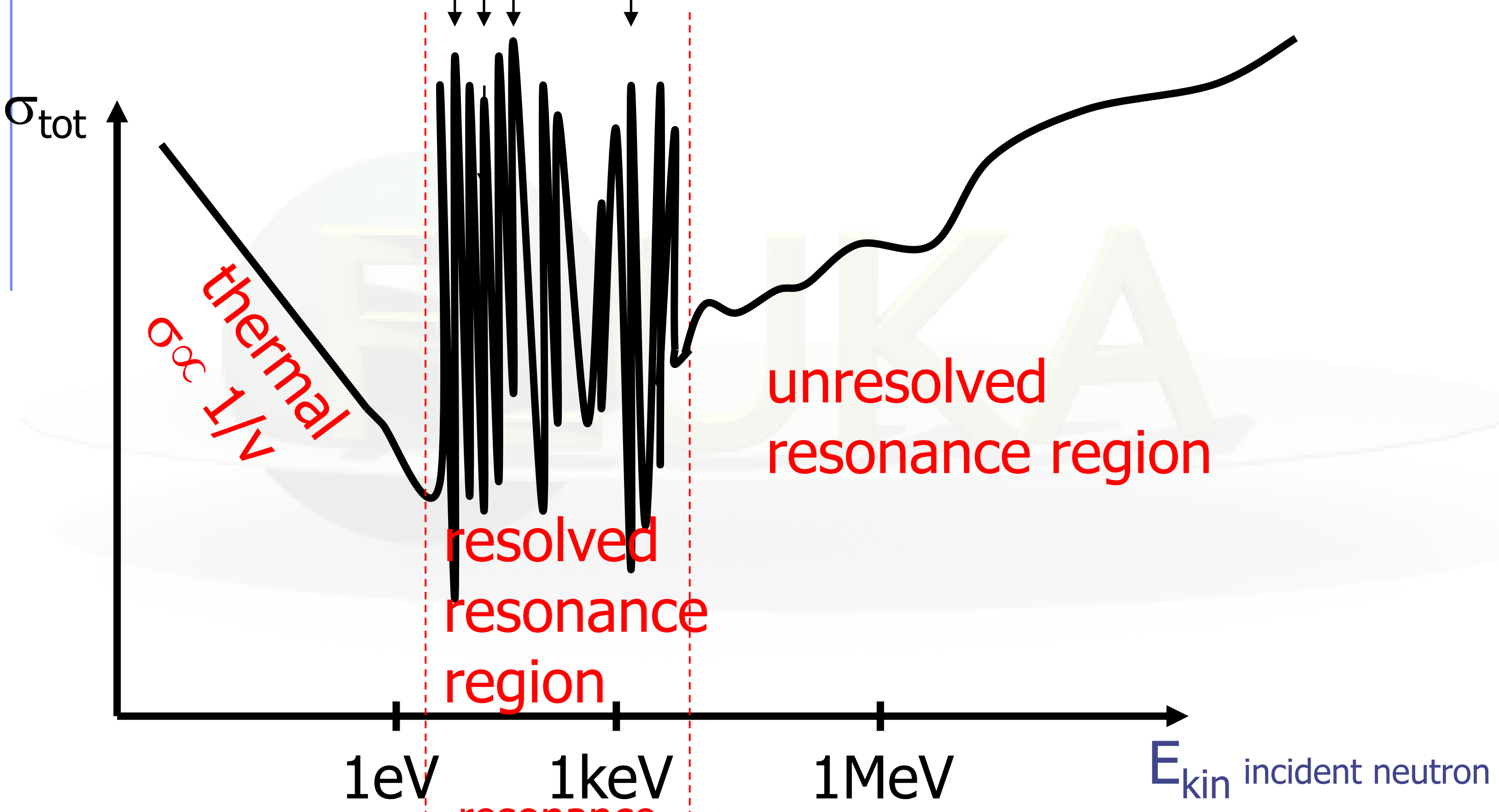
- In FLUKA we call neutrons below 20 MeV low energy neutrons
- Neutron interactions at higher energy are handled by FLUKA nuclear models
- Transport and interactions of neutrons with energies below 20 MeV are handled by a dedicated library

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 ➔ cannot be calculated by models ➔ we rely on data files

Typical neutron cross section

Resonances ⇒ energy levels in compound nucleus $^{A+1}Z^*$



resonance spacing few eV

Resonance spacing too dense ⇒ overlapping resonances

Evaluated Nuclear Data Files

- Evaluated nuclear data files (ENDF, JEFF, JENDL...)
  - typically provide neutron σ (cross sections) for E<20MeV for all channels
  - σ are stored as continuum + resonance parameters
  - Complex programs like NJOY, PREPRO convert the ENDF file to P-ENDF (point-wise cross sections), or G-ENDF (group-wise) including Doppler broadening etc.

Point-wise and Group-wise cross sections

- In neutron transport codes in general two approaches used: point-wise ("continuous" cross sections) and group-wise transport
- Point-wise follows cross section precisely but is can be time and memory consuming
- Group approach is widely used in neutron transport codes because it is fast and gives good results for most applications

Group Transport Technique

- The energy range of interest is divided in a given number of discrete intervals ("energy groups")
- Elastic and inelastic reactions simulated not as exclusive processes, but by group-to-group transfer probabilities (downscattering matrix)
- Downscattering matrix: if a neutron in a given group undergoes a scattering event and loses energy, it will be transferred to a group of lower energy (each of the lower energy groups having a different probability)
- If the neutron does not lose enough energy to be in another group, it will stay in the same group (in-scattering).
- In thermal region neutrons can gain energy. This is taken into account by an upscattering matrix, containing the transfer probability to a group of higher energy

Angular distribution

- The probability distribution of the scattering angle for each group-to-group transfer is represented by a Legendre polynomial expansion truncated at the $(N+1)^{th}$ term:

$$\sigma_s(g \rightarrow g', \mu) = \sum_{i=0}^{N} \frac{2i+1}{4\pi} \mathrm{P}_i(\mu)\, \sigma_s^i(g \rightarrow g')$$

where $\mu = \overline{\Omega} \cdot \overline{\Omega}' =$ scattering angle

$\mathsf{N} =$ chosen Legendre order of anisotropy

Angular distribution

- In FLUKA, N=5
- The scattering angular probabilities are obtained by a discretization of a P5 Legendre polynomial expansion of the actual scattering angular distribution which preserves its first 6 moments.
- Result of this P5 expansion is a set of 3 discrete polar angle cosines and 3 corresponding probabilities, i.e. for a given transfer $g \rightarrow g'$ only three values are possible for the polar angle
- The azimuthal angle is sampled from a uniform distribution and can have any value between 0 and 2π

Group wise treatment

- Convert σ to energy groups like histograms, the energy width is different for each group in order to better represent resonances
- Each group contains the <average> σ:

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

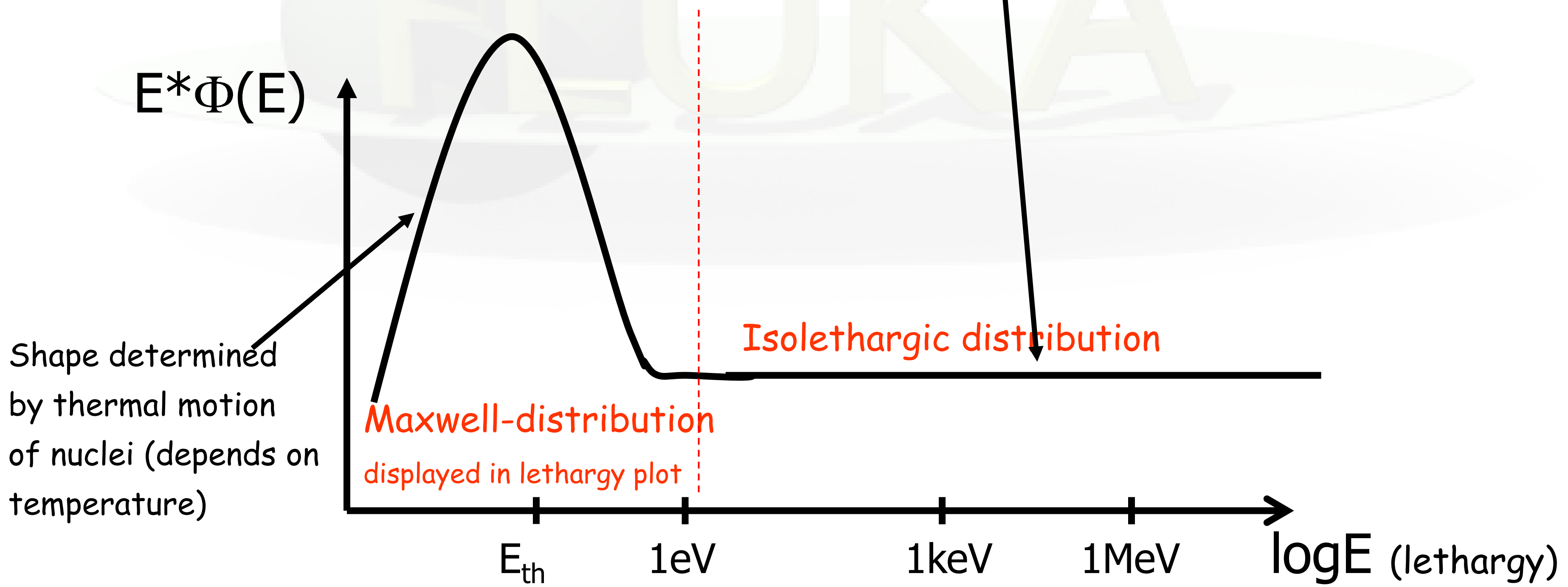
- Advantage: fast
- Disadvantage: effects like self shielding are not accurately reproduced (see later), angular distributions replaced by a discrete number of angles (3 in FLUKA) conserving their first n moments (6 in FLUKA)

Fluence

- An assumption is needed about the neutron spectrum to be used as a weighting function for calculating the average cross section on each group
  For instance it can be shown that in most cases, between 1 eV and 1 MeV:

$$\Phi(E)dE = C\frac{dE}{E} \quad (\frac{1}{E}\text{ spectrum})$$

- In any case, the error is small if the group width is small



Self shielding

- The group structure is necessarily coarse with respect to the resonance structure in many materials
- A resonance in a material present in a dilute mixture or as a small piece cannot affect much a smooth neutron flux (so-called "infinite dilution'')
- But if an isotope exhibiting large resonances is very pure or is present with a large fractional abundance, it can act as a "neutron sink", causing sharp dips in the neutron spectrum corresponding to each resonance ➔ an apparent decrease in σ
- This effect, which results in a lower reaction rate $\sigma\Phi$, is called *self-shielding* and is necessarily lost in the process of cross section averaging over the width of each energy group, unless a special correction is made

The FLUKA Low Energy Neutron Library

- FLUKA uses the multigroup transport technique
- The energy boundary below which multigroup transport takes over depends in principle on the cross section library used. In the present library it is 20 MeV.
- Both fully biased and semi-analog approaches are available
- Number of groups: 260 of approximately equal logarithmic with, the actual energies limits of each group can be found in the manual (or can be printed to *.out file)
- N.B. the group with the highest energy has the number 1, the group with the lowest energy has number 260
- 31 thermal groups, with 30 upscattering groups
- Energy range of library: 0.01 meV - 20 MeV

The FLUKA Low Energy Neutron library

- Based on recent versions of evaluated nuclear data files: ENDF/B-VI.8, ENDF/B-VII.0, Jendl-3.3, Jendl-3.4, Jeff-3.1,…
- About 270 isotopes/materials available
- Almost all materials available at 2 temperatures: 87K, 296K
- Some also at 4K, 120K, 430K
- Doppler broadening at the relevant temperature is taken into account
- The library handles also gamma generation, energy deposition by kerma factors, residual nuclei production, secondary neutrons, fission neutrons
- For some isotopes/materials: self-shielding, molecular binding, correlated gamma generation, point-wise transport
- NB: Because of the group technique the energy of a transported neutron below 20 MeV is only defined within the accuracy of the groups

The FLUKA Low Energy Neutron library

Energy weighting:

- Averaging inside each energy group according to the following weighting function. In order of increasing energy:
  - a Maxwellian at the relevant temperature in the thermal range
  - a 1/E spectrum in the intermediate energy range
  - a fission spectrum
  - again a 1/E spectrum

But it is important to realize that the groups in the present library are very narrow! Therefore the energy weighting is not very important

Gamma generation

- Gamma generation from $(n,x\gamma)$ reactions is possible only for the elements where data is available in the evaluated nuclear data files (see manual for a complete list)
- Gamma generation too is done by a multigroup scheme
- Number of gamma groups: 42
  - NB number of γ groups different from number of neutron groups!
- Energy range: 1keV - 50 MeV
  - NB γ energy range different from neutron energy range!
- The actual energy of the generated photon is sampled randomly in the energy interval corresponding to its gamma group
- Exception: 2.2 MeV from $H(n,\gamma)^2H$ reaction, 478 keV photon from $^{10}B(n,\alpha)$ and gamma cascades from $Cd(n,\gamma)$ and $Xe(n,\gamma)$
- Capture gammas as well as gammas from inelastic reactions like (n,n') are included
- The neutron library only creates gammas, the transport is done by the EMF module (like all other gammas in FLUKA)

Energy deposition

- Energy deposition by neutrons below 20 MeV is estimated by means of kerma factors
- For some materials with gamma production the kerma values of some groups (mainly at high energies) are problematic (see manual). The reason is inconsistent data in the evaluated data files. Effort was addressed to apply corrections to improve the situation but there are still some materials with problematic kermas.
- The user should check carefully the results of simulations with these materials. However, the effect should vanish in a typical simulation.

Secondary and Fission Neutrons

- Neutrons from (n,xn) reactions are taken into account implicitly by a group-dependent non-absorption probability, i.e. a factor by which the weight of a neutron is multiplied after a collision
- If the only possible processes are scattering and capture the non-absorption probability is smaller than 1. If also (n,2n) is possible, the factor is bigger than 1
- Fission neutrons are treated separately by a group-dependent fission probability
- Fission neutrons are emitted isotropically with an energy sampled from a fission spectrum appropriate for the isotope and neutron energy
- The fission neutron multiplicity was obtained separately from the evaluated data files
- The fission fragments are not transported, their energy is deposited at the spot

Charged particle generation

- Recoil protons from hydrogen and protons from $^{14}N(n,p)$ are produced and transported explicitly (i.e. like other protons)
- That means that detailed kinematics of elastic scattering, continuous energy loss with energy straggling, delta ray production, multiple and single scattering, are all taken into account
- If point-wise transport has been requested, α and ^{3}H fragments from neutron capture in ^{6}Li and ^{10}B can also be transported explicitly
- All other charged secondaries produced in low energy neutron reactions, including fission fragments, are not transported but their energy is deposited at the point of interaction using kerma factors

Residual nuclei production

- Residual nuclei: nuclei that are the result of a reaction and are at rest, e.g. ^{28}Al after a neutron capture reaction of ^{27}Al
- For all materials data are available for estimating residual nuclei production by low energy neutrons. Command RESNUCLEi allows to request separately residual nuclei from low energy neutrons and from high energy particles
- For Ti, Ga the residual nuclei information is based on different evaluations than the transport

Using the Low Energy Neutron Library

Available Materials

- Section 10.4.1.2 of manual gives a list of available materials
- Example:

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

RN: residual nuclei

Gam: Gamma production

Name: name to be used in LOW-MAT card

Identifiers: to be used in LOW-MAT card

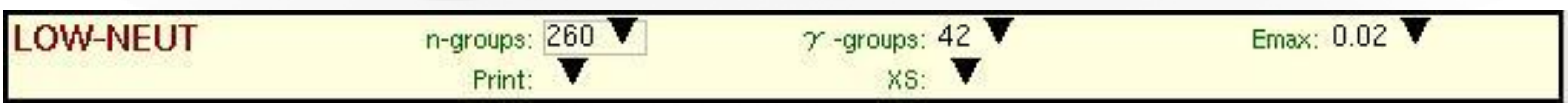
Using the Low Energy Neutron Library

- How to activate low energy neutron transport?
  - Explicit: giving a LOW-NEUT card
  - Implicit: giving a DEFAULTS cards (except with default EM-CASCA), or not giving a DEFAULTS card at all
  - That means: you are using the library in almost any simulation (unless you are using the default EM-CASCA or you have switched it off explicitly with a LOW-BIAS card)
- What must the user do?
  - To set correspondence between the actual material and the material in the low neutron library (LOW-MAT card), if not done by default.
    - NB you don't need it in most practical cases!
  - To set transport thresholds with PART-THR, if defaults are not ideal for the actual problem
  - To request special features like point wise cross sections (LOW-NEUT)

Input Cards: LOW-NEUT [1/4]

This card activates low-energy neutron transport.

- WHAT(1): number of neutron groups of the library
  - Default: 260
- WHAT(2): number of gamma groups of the library
  - Default: 42
- WHAT(3): maximum energy (in GeV) of the library
  - Default: 0.02
- WHAT(5): number of thermal groups
  - Default: 31

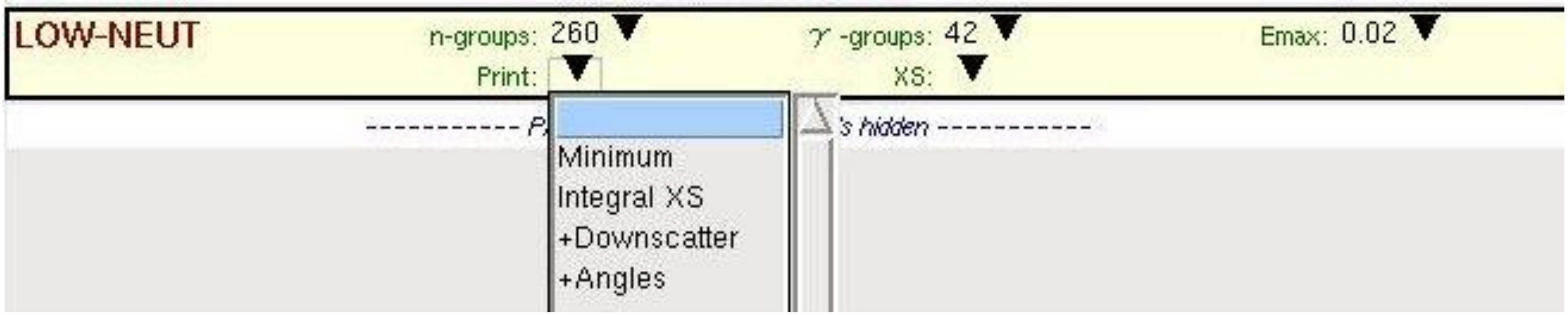


- The defaults for WHAT(1) – WHAT(3) and WHAT(5) are fine. The only reason for changing them would be if using a different library (there was one until recently, but it has been suppressed)

➔ Don't use them!

Input Cards: LOW-NEUT [2/4]

- WHAT(4): printing flag, neutron cross section information is written to *.out file
    - 0.0 Minimum
    - 1.0 integral cross sections, kerma factors and probabilities
    - 2.0 additionally downscattering matrices and gamma matrices
    - 3.0 additionally scattering probabilities and angles
    - 4.0 residual nuclei information
  - Default: 0.0 (minimum)

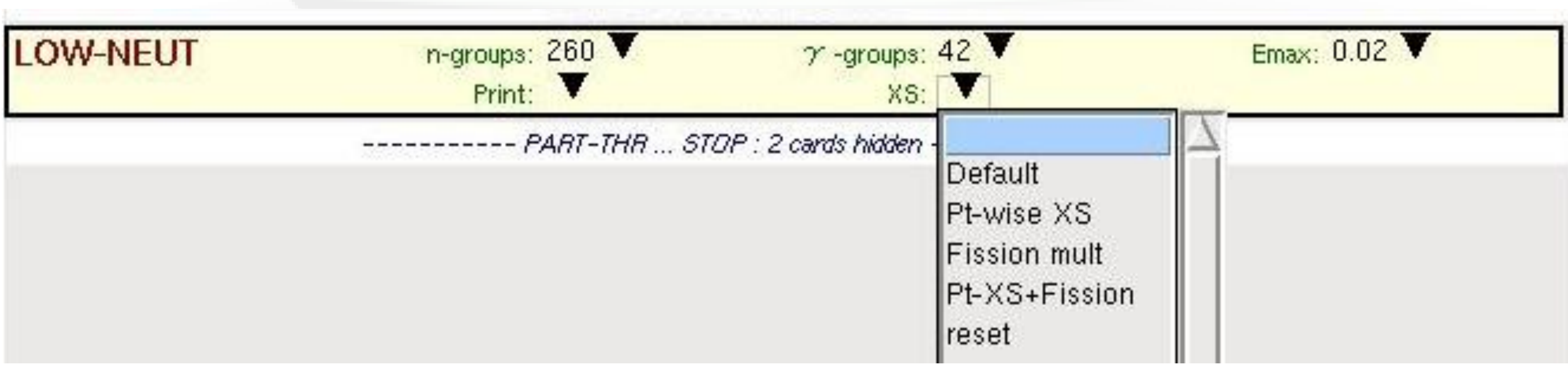


Input Cards: LOW-NEUT [3/4]

- The output for WHAT(4) = 1
  - Group energy limits, average energies, velocities and momenta, thermal velocities, gamma group limits
  - For each material: availability of residual nuclei information (the line: “RESIDUAL NUCLEI INFORMATIONS AVAILABLE” indicates the possibility to use option RESNUCLEi with WHAT(1)= 2.0
  - for each neutron energy group in each material:
    - SIGT = total cross section
    - SIGST = “scattering” cross section: s(n,n) + 2s (n,2n) + 3s (n,3n)
    - PNUP = upscatter probability, is 0.0 in non thermal groups
    - PNABS = Probability of Non-ABSorption (= scattering)
      PNABS = SIGST/SIGT, and can sometimes be> 1 because of (n,xn) reactions
    - GAMGEN = GAMma GENeration probability = gamma production cross section divided by SIGT and multiplied by the average number of g per (n, g) reaction
    - NU*FIS = fission neutron production = fission cross section divided by SIGT and multiplied by ν, the average number of neutrons per fission
    - EDEP = Kerma contribution in GeV per collision
    - PNEL, PXN, PFISS, PNGAM = partial cross sections, expressed as probabilities (*i.e.*, ratios to SIGT). In the order: non-elastic, (n,xn), fission, (n,gamma)

Input Cards: LOW-NEUT [4/4]

- WHAT(6): $i_0 + 10 * i_1$:
  - i_0 = 1: available point wise cross sections used and explicit and correlated ^{6}Li(n,γ)^{7}Li, ^{6}Li(n,t)^{4}He, ^{40}Ar(n, γ) ^{41}Ar, ^{x}Xe(n, γ) $^{x+1}$Xe and ^{113}Cd(n, γ)^{114}Cd photon cascade requested
    - = 0: ignored
    - =<-1: resets to the default (point wise cross sections are not used)
  - i_1 = 1, fission neutron multiplicity forced to 1, with proper weight to compensate for the "wrong" multiplicity
    - = 0, ignored
    - =<-1: resets to the default (normal fission multiplicity)
  - Default = -11., unless option DEFAULTS is present with **SDUM** = CALORIME, ICARUS, NEUTRONS or PRECISIO, in which case the default is 1.0 (point wise cross sections are used when available and fission multiplicity is not forced)



Input Cards: LOW-MAT [1/3]

- The LOW-MAT card sets the correspondence between FLUKA materials and the low energy neutron transport

- If a material has the same name as the name given in the list of low neutron material, the correspondence between material and low energy neutron transport is set automatically, a LOW-MAT card is not necessary. The first material with the right name is taken. This is always a material at room temperature.

- That means for the predefined material HYDROGEN hydrogen bound in water is used, not the free gas one

- If you want to use low energy neutron transport in H_2 gas you have to do this explicitly by a LOW-MAT card

Input Cards: LOW-MAT [2/3]

- WHAT(1): Name of the material (single element only!)
    - In flair this can be chosen from a pull down menu
- WHAT(2), WHAT(3) and WHAT(4): the 3 identifiers from table 10.4.1.2 of the manual
- SDUM: name of the material from table 10.4.1.2 of the manual
- In flair there is only one pull down menu for all identifiers and the name
- If you want to use the predefined materials at a temperature different from 296K, it is mandatory to give a LOW-MAT card with the proper identifiers

Input Cards: LOW-MAT [3/3]

- Setting the correspondence between a material and low energy neutron transport cross sections:
  - First create the material with a MATERIAL card and give it a name in SDUM
  - Give a LOW-MAT card with WHAT(1) = the name you gave in the SDUM of the MATERIAL
  - Give in WHAT(2), WHAT(3) and WHAT(4) of the LOW-MAT card the numerical identifiers (table 10.4.1.2 in manual) of the material you want to use, be careful to use the one with the right temperature
  - Give in SDUM of the LOW-MAT card the name provided in the same table

Example compound at 87K

- Example: water at 87K
  - Create a material hydrogen and give it some name (HYDR_87), do the same with oxygen (OXYG_87)
  - Give a LOW-MAT card for HYDR_87, chose the right cross sections identifiers (those for 87K) and name (see list in manual), do the same for oxygen
  - Create a material WATER_87 by giving first a MATERIAL card and then a corresponding COMPOUND card with the right composition

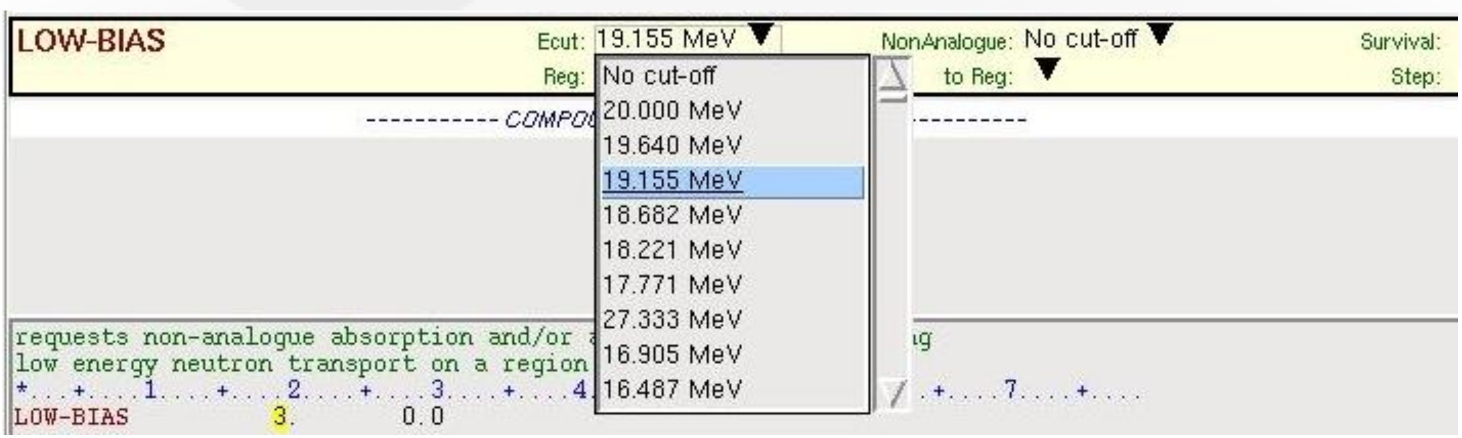
MATERIAL	Name: HYDR_87	#	ρ: 8.988E-5
Z: 1.	Am: 1.00794	A:	dE/dx: ▼
LOW-MAT	Mat: HYDR_87 ▼	LowMat: H. Free gas natural Hydrogen, 87K ▼	
MATERIAL	Name: OXYG_87	#	ρ: 0.001492
Z: 8.	Am: 15.9994	A:	dE/dx: ▼
LOW-MAT	Mat: OXYG_87 ▼	LowMat: 16O. Oxygen 16, 87K ▼	
MATERIAL	Name: WATER_87	#	ρ: 1.
Z:	Am:	A:	dE/dx: ▼
COMPOUND	Name: WATER_87 ▼	Mix: Atom ▼	Elements: 1..3 ▼
f1: 2.0	M1: HYDR_87 ▼	f2: 1.0	M2: OXYG_87 ▼
f3:	M3: ▼		

Input Cards: LOW-BIAS [1/2]

This card sets an energy cut-off during low-energy neutron transport on a region by region basis and/or non-analogue absorption.

<u>However it is preferable to use PART-THR</u>

- WHAT(1): number of the group to apply a transport cut-off, i.e. neutrons in groups with numbers >= WHAT(1) are not transported. Remember that the groups with the highest energy has the number 1.
  - Default: 0.0 (no cut-off)
  - *flair* automatically matches the group number to the upper energy boundary of each group



Input Cards: LOW-BIAS [2/2]

- Analogue absorption: a neutron does not exist any more after an absorption process
- Non-analogue absorption: the neutron is not killed after an absorption process but lives on with a lower weight, capture gammas are created with a weight corresponding to the surviving neutron
- WHAT(2): Group limit for non-analogue absorption (neutrons in groups >= WHAT(2) undergo non-analog absorption)
  - Default: 230
- WHAT(3): non-analogue survival probability
- WARNING: Only experts should modify the non-analogue absorption survival probability!
- If no LOW-BIAS card is given non-analogue absorption depends on the DEFAULTS card (see manual)
- The change of weight of the particle is taken into account (see lecture about biasing)

Transport cut-offs

- Transport cut off: a particle is not transported if its energy is lower than a cut off energy
- Transport cut offs for neutrons can be set to save CPU time
- Use cut offs with care, you could miss important effects like activation, dose, secondary particles,…
- For activation thermal neutrons are very important. If you are interested in activation never cut off low energy neutrons!
- To set a transport cut off for neutrons give the energy of the cut off in the PART-THR card, no matter if high or low energy neutrons. That was different in previous versions: the card LOW-BIAS was needed.

Self shielding [1/3]

- Self-shielded materials in FLUKA:
  - ^{27}Al at 296K, 87K, 4K, 430K
  - ^{nat}A, ^{40}Ar at 296K, 87K
  - ^{nat}Fe at 296K, 87K, 4K, 430K
  - ^{nat}Cu at 296K, 87K, 4K, 430K
  - ^{181}Ta at 296K, 87K
  - ^{nat}W at 296K, 87K, 4K, 430K
  - ^{197}Au at 296K, 87K
  - ^{nat}Pb at 296K, 87K
  - ^{208}Pb at 296K
  - ^{209}Bi at 296K, 87K
    - Special case: cast iron (Fe +5%C) at 296K, 87K, 4K, 430K (see example further on)

Self shielding [2/3]

- When to use these materials?
  - Bulky (huge) pieces that are very pure (containing only one isotope)
- When not to use self shielded materials?
  - "small" iron, copper, lead, aluminum pieces
  - Thin gold foils (but a self-shielded 100μm Au foil is available)
  - Diluted materials
- How to use self shielded materials?
  - Define your material with a MATERIAL card
  - Give additionally a LOW-MAT card and give the proper identifiers in WHAT(2)-WHAT(4) and SDUM
  - If you have to use self shielded and non self shielded materials of the same element you need to define 2 different materials
  - Attention: predefined materials like iron, copper and lead are not self shielded, you have to give a LOW-MAT card to use self shielded

Self shielding [3/3]

- Cast iron is iron with a significant amount of carbon
- There is a self-shielded material cast iron in the low energy neutron library which is prepared to be used for creating a compound of iron and roughly 5% carbon. The amount of carbon doesn't need to be exactly 5%.
- How to create self shielded cast iron?
  - Define a material iron called FeCarbSS (or any other name you like) with a MATERIAL card
  - Give additionally a LOW-MAT card and give the proper identifiers for cast iron in WHAT(2)-WHAT(4) and SDUM
  - Give a MATERIAL card to create a material called CastFe (or any other name you like)
  - Give a COMPOUND card for CastFe to composed a compound of FeCarbSS and CARBON (predefined)

Artifacts of discrete angular distribution

- Artifacts can arise when a neutron is likely to scatter only once (thin foil, regions of low density like gases), due to the discrete angular distribution (only 3 angles are possible for each g→g')
- The user should be aware of such artifacts and interpret results of scattering at thin foils and gases carefully
- Because the 3 angles are different for each g→g' and the azimuthal angle is sampled from a discrete distribution, the artifact disappears when the neutrons have the possibility of scattering two or more times.
- Information about which angles and probabilities are used for each group can be obtained by setting WHAT(4) = 3 in the LOW-NEUT card. The information is then written to the *.out file (see manual chapter 9: Output)

Materials with molecular binding

- Available materials with molecular bindings at 296K:
  - H (natural isotopic amount) in H_2O, CH_2
  - ^1H in H_2O, CH_2
  - ^2D in D_2O
  - C in graphite
- Use of these materials makes the thermal neutron calculation more realistic and can affect the energy and spatial distributions
- Example: CH_2 (polyethylene) including molecular binding
  - Create a material hydrogen and give a corresponding LOW-MAT card that refers to H bound in CH_2
  - Give a COMPOUND cart that creates CH_2 as a compound of bound H and normal carbon
- For hydrogen H bound in water is the default, because it is the first in the list of low energy neutron materials

Advanced low energy neutron features:

- The LOW-DOWN card biases the downscattering probability during low-energy neutron transport on a region by region basis
  - It can be useful for very particular problems
  - If not used properly it can lead to big errors
  - Only recommended for experts!

Summary

- Most of the simulations in FLUKA use the low energy neutrons, implicitly via the DEFAULTS card
- Low neutron transport in a material is enabled by a LOW-MAT card, only needed if the material's name is not one of those in the neutron cross section library, or temperature, self-shielding or molecular binding are different from the default ones
- Use self shielded materials properly for "bulky" and "pure" (in isotopic composition) materials
- Don't give a LOW-MAT card for compounds