Materials & Related Scorings

Advanced FLUKA Course

Material under irradiation

- The prediction of the structural damage to materials under irradiation is essential to evaluate consequences due to long term employment of construction materials in nuclear reactors and charged particle accelerators.
- There are several effects and quantities that are important for studying the material behavior under irradiation and FLUKA is capable in predicting several of them:
  - Heating total energy deposition
    → could be used for temperature rise, stresses, deformations …
  - Energy deposition due to EMF → radiolysis calculations …
  - Dose calculation → medical applications …
  - Gas production
  - Non Ionizing Energy Losses (NIEL)
  - Displacement per Atoms (dpa)
  - Silicon 1MeV Neutron Equivalent (Si1MeVEq)
  - Single Event Upsets to electronics (SEU)

Gas production, Non Ionizing Energy Losses (NIEL), Displacement per Atoms (dpa) → material damage …

Silicon 1MeV Neutron Equivalent (Si1MeVEq), Single Event Upsets to electronics (SEU) → electronics

For all the above you need to input the proper MATERIAL properties

Material definition

Single-element material definition

	atomic number Z	atomic weight	density (g/cm³)	material number	Alternate material to use for dE/dx	mass number (A)	name
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7....+...							
MATERIAL	24.0	51.9961	7.18	26.0	0.0	0.0	CHROMIUM

MATERIAL	Name: PHOSPHO	#	ρ: 2.2
Z: 15	Am: 30.973761	A:	dE/dx:

Notes:

- if $\rho<0.01$: gas at atmospheric pressure unless specified otherwise
- Atomic Weight is **calculated by the code** using the internal database: it is better to leave empty
- Material number use it **ONLY** if you want to **override** a predefined one
- Mass Number to define specific **ISOTOPES**
  Do not confuse with the Atomic weight
- Choose a name corresponding to the **LOW-ENERGY neutron database** Section 10.4 in the manual

Predefined ICRU materials

In the present version of FLUKA, the code contains several predefined materials with the composition suggested by ICRU

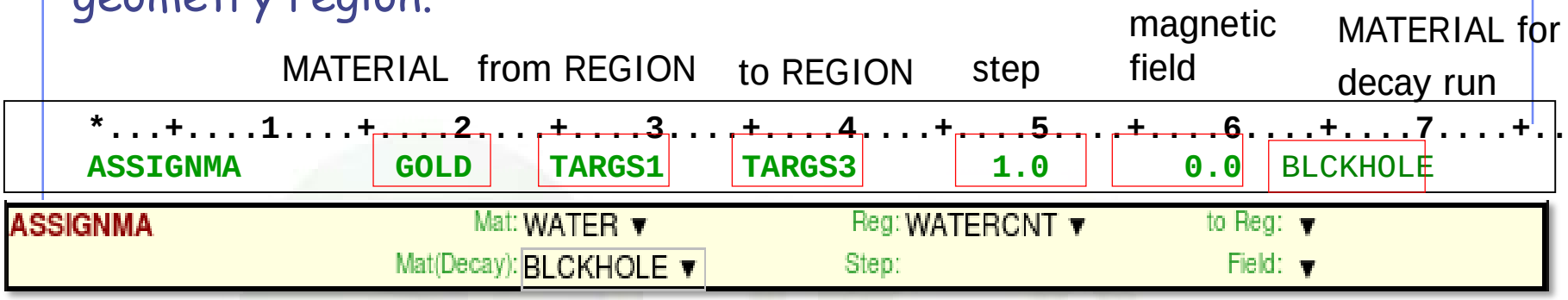
FLUKA	Material	FLUKA	Material
AIR	Dry air 20°C	BONECOMP	Compact bone
WATER	Water	BONECORT	Cortical bone
POLYSTYR	Polystyrene	MUSCLESK	Skeletal muscle
PMMA	Polymethyl methacrylate	MUSCLEST	Striated muscle
POLYETHY	Polyethylene	ADTISSUE	Adipose tissue
PLASCINT	Plastic scintilator	KAPTON	Kapton

- The materials can be used WITHOUT the need of an explicit MATERIAL / COMPOUND cards
- If the user defines a MATERIAL card in the input with the same name as the predefined ones IT WILL OVERRIDE THE PREDEFINED.

Material Assignment

Card: ASSIGNMat

A (single-element or compound) material is assigned to each geometry region.



In the new version of FLUKA:

- WHAT(5) is controlling the magnetic (& electric) field for the prompt and radioactive decay product transport
- WHAT(6) is permitting to assign a different material for the radioactive decay product transport.

MAT-PROP

Card: MAT-PROP

```
MATERIAL                          .00373654                          ELIO-KRY
COMPOUND    -.3333333  -KRYPTON -.6666667 -HELIUM-3                  ELIO-KRY
MAT-PROP          3.0                      ELIO-KRY
```

```
MAT-PROP                                78.0      WATER
```

MAT-PROP | Type: | Gas pressure: | RHOR:
Ionization: | Mat: | to Mat: | Step:

- Supply extra information on gaseous materials (pressure)
- Create materials with fictitious or effective density
- Override the default average ionization potential for dE/dx

```
MAT-PROP          25.                    LEAD                    DPA-ENER
```

MAT-PROP | Type: DPA-ENER | DPA Eth:
Mat: | to Mat: | Step:

- Set the DPA energy damage threshold (WARNING in eV)

```
MAT-PROP          1.0                    HYDROGEN   @LASTMAT     USERDIRE
```

MAT-PROP | Type: USERDIRE | Call: USRMED
Mat: | to Mat: | Step:

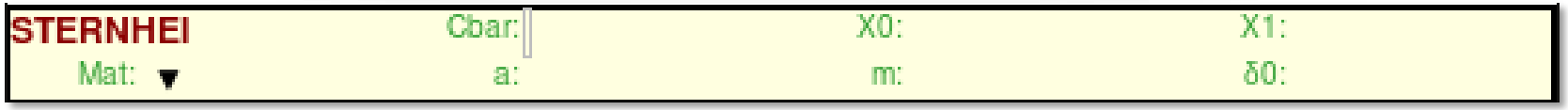
- Enable the call to USRMED routine when a particle enters in the desired materials

STERNHEIme card

- Below the δ-ray threshold, energy losses are treated as "continuous", with some special features:
  - Fluctuations of energy loss are simulated with a FLUKA-specific algorithm
  - The energy dependence of cross sections and dE/dx is taken into account exactly
  - Latest recommended values of ionization potential and density effect parameters implemented for elements (Sternheimer, Berger & Seltzer), but can be overridden by the user with (set yourself for compounds!) the

STERNHEI C X0 X1 a m δ0 MAT

STERNHEIME	3.5017	0.24	2.8004	0.09116	3.4773	WATER



- In addition, the card MAT-PROP can be used a to override the value of the average ionization potential used by the program

MAT-PROP Gasp Rhosc Iion Mat1 Mat2 Step

dpa: Displacements Per Atom

- Is a measure of the amount of radiation damage in irradiated materials
  For example, 3 dpa means each atom in the material has been displaced from its site within the structural lattice of the material an average of 3 times
- Displacement damage can be induced by all particles produced in the hadronic cascade, including high energy photons.
  The latter, however, have to initiate a reaction producing charged particles, neutrons or ions.
- The dpa quantity is directly related with the total number of defects (or Frenkel pairs)

$$dpa = \frac{1}{\rho} \sum_i N_i N_F^i$$

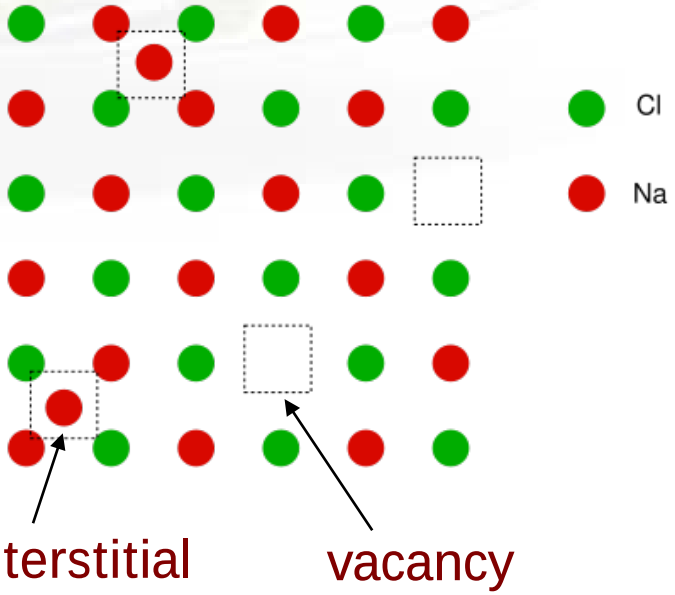
ρ atoms/cm^3
N_i particles per interaction channel i
N_f^i Frenkel pairs per channel

Frenkel pairs

- Frenkel pairs N_F (defect or disorder), is a compound crystallographic defect in which an interstitial lies near the vacancy. A Frenkel defect forms when an atom or ion leaves its place in the lattice (leaving a vacancy), and lodges nearby in the crystal (becoming an interstitial)

$$N_{NRT} \equiv N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

N_{NRT}	Defects by Norgert, Robinson and Torrens
$\kappa=0.8$	is the displacement efficiency
T	kinetic energy of the primary knock-on atom (PKA)
$\xi(T)$	partition function (LSS theory)
$\xi(T)$ T	directly related to the NIEL (non ionizing energy loss)
E_{th}	damage threshold energy



E_{th} Damage Threshold Energy

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

- E_{th} is the value of the threshold displacement energy averaged over all crystallographic directions or a minimum energy to produce a defect

Element	Eth (eV)	Element	Eth (eV)
Lithium	10	Co	40
C in SiC	20	Ni	40
Graphite	30..35	Cu	40
Al	27	Nb	40
Si	25	Mo	60
Mn	40	W	90
Fe	40	Pb	25

Typical values used in NJOY99 code

- FLUKA way

MAT-PROP *WHAT(1)* = E_{th} (eV)
WHAT(4,5,6) = Material range
SDUM = **DPA-ENER**

FLUKA Implementation [1/2]

Charged particles and heavy ions

- **During Interactions**
  - ✔ For all charged particles and Heavy Ions, calculate the recoil. Use recoil as a normal particle

- **During transport**
  - ✔ Calculate the restricted and unrestricted nuclear stopping power for the average energy at the middle of the step with calls to DEDXNU and SNRDFR and add it to TKNIEL and TKEDPA global variables
  - ✘ For electrons Bremsstrahlung, sample randomly a recoil energy from the distribution of the recoils (uncorrelated with the event) Treat the recoil as a normal particle (*work on progress*)

- **Below threshold**
  - ✔ Calculate the TKNIEL(=TKEDPA) by using the Lindhard partition function

FLUKA Implementation [2/2]

Neutrons

- **High energy E_n>20 MeV**
  - ✔ Like CP, calculate the recoil. Treat recoil as a normal particle

- **Low energy $E_n \leq 20$ MeV (group-wise)**
  - ✔ Calculate the NIEL from NJOY, then add it to TKNIEL and TKEDPA global variables

- **Low energy $E_n \leq 20$ MeV (point-wise)**
  - ✘✔ Calculate the recoil if possible Treat the recoil as a normal particle (available for those where point-wise exist)

Photons

- ✘ Pair production, sample randomly a recoil for a distribution (uncorrelated with the event) Treat the recoil as a normal particle

dpa: Recipe

FLUKA is using a more accurate treatment during the particle transport. While below the transport threshold is employing the Lindhard approximation with the NRT model, it is strongly advisable to use as low thresholds as possible:

Thresholds:

- All Hadrons 1 keV
- Neutrons down to thermal (1e-15 GeV)
- Leptons 50-100 keV would be ok

Material Damage:

Set with MAT-PROP the damage threshold for all materials under consideration. All other will use the default of 30eV!!!!

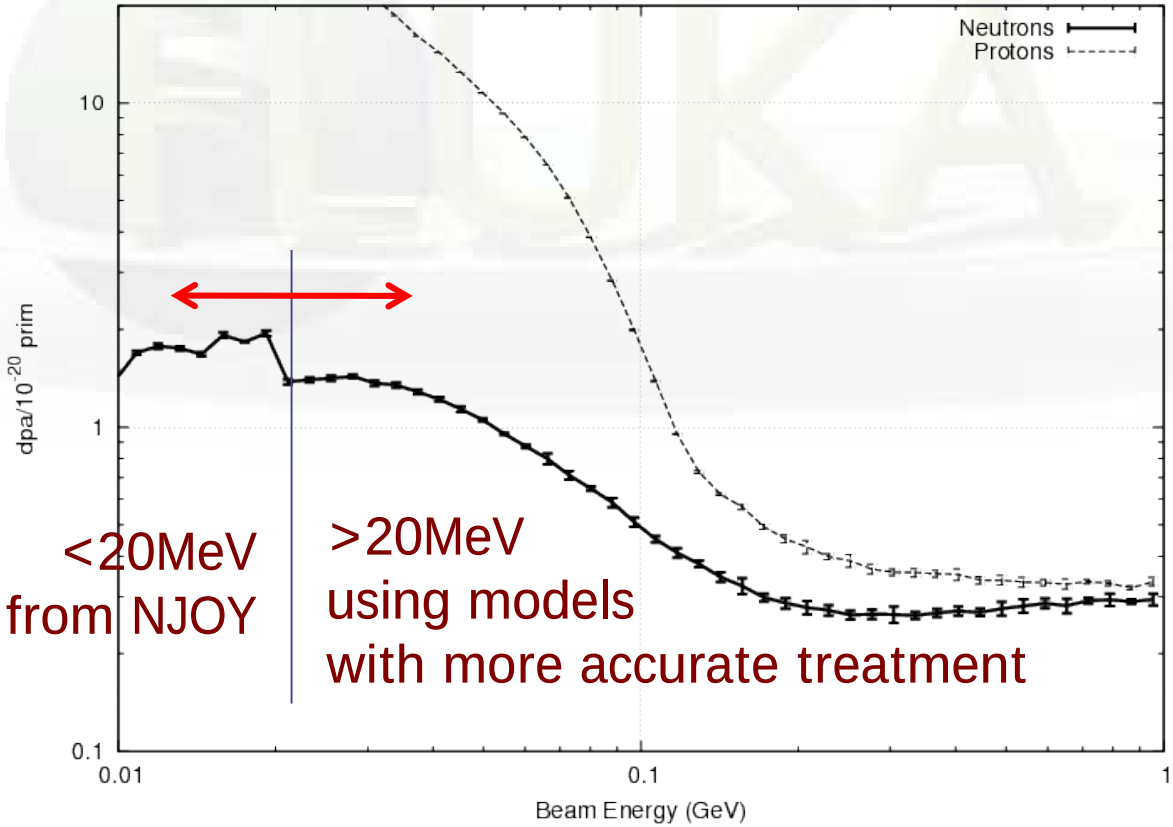
Scoring:

Use USRBIN with DPA-SCO or NIEL

DEFAULTS: DAMAGE

dpa: Artifacts

- Due to the group treatment of low-energy neutrons, there is no direct way to calculate properly the recoils.
- Therefore the evaluation is based on the KERMA factors calculated by NJOY, which in turn is based on the Unrestricted Nuclear losses from using the NRT model.



Cards Displacement Damage + Charge

For all charged particles and Heavy Ions FLUKA calculates the recoil as a normal particle. During transport it calculates the restricted and unrestricted nuclear stopping power, allowing to score dpa's and non-ionizing energy loss (NIEL):

NIEL-DEP Non Ionizing Energy Loss deposition

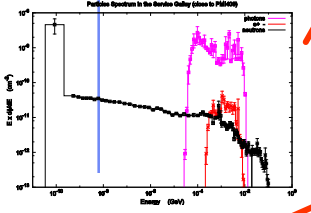
DPA-SCO Displacements per atoms

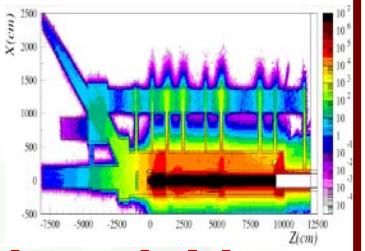
In addition (not necessarily linked to displacement damage) the following can be useful in order to get the net charge deposition in a given region:

NET-CHRG Net Charge

Radiation Physics/Effects/Monitoring

nuclear cascade





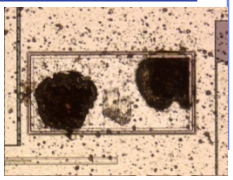
h > 20 MeV

Radiation Field

h, e,.. > 100 KeV

EM cascade

radiation damage in semiconductors



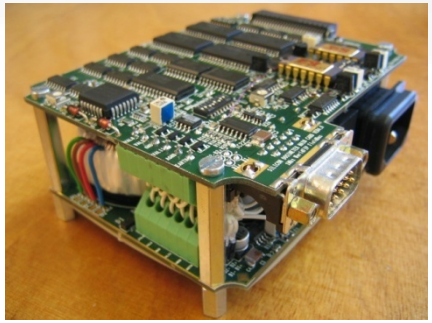
Single Events

Effect in the Device

Displacement

Dose

radiation monitor



SEU counter

Measurement

PIN Diodes

Radfet

Main Radiation Effects on Electronics

Category		Effect
Single Event effects (Random in time)	***Single Event Upset (SEU)***	Memory bit flip (soft error) Temporary functional failure
	Single Event Latchup (SEL)	Abnormal high current state Permanent/destructive if not protected
Cumulative effects (Long term)	***Total Ionizing Dose (TID)***	Charge build-up in oxide Threshold shift & increased leakage current Ultimately destructive
	Displacement damage	Atomic displacements Degradation over time Ultimately destructive

Radiation Damage to Electronics

- All important quantities to estimate risks of damage to electronics can be directly scored in FLUKA :

  Cumulative damage:

  - Energy deposition (total ionizing dose) by scoring **DOSE** with any 'energy deposition like estimator' (*e.g.*, **USRBIN**)
  - Si Lattice displacement (1-MeV neutron equivalent particle fluxes) with any 'fluence like estimator' (*e.g.*, **USRTRACK**)

  Stochastic failures (SEU):

  - "high" energy hadron fluences ("E>20 MeV") with any 'fluence like estimator' (*e.g.*, **USRTRACK**)

- The FLUKA scoring options together with the analysis of particle energy spectra allows studies aimed at selecting possible locations for electronics or efficiently design shielding implementations

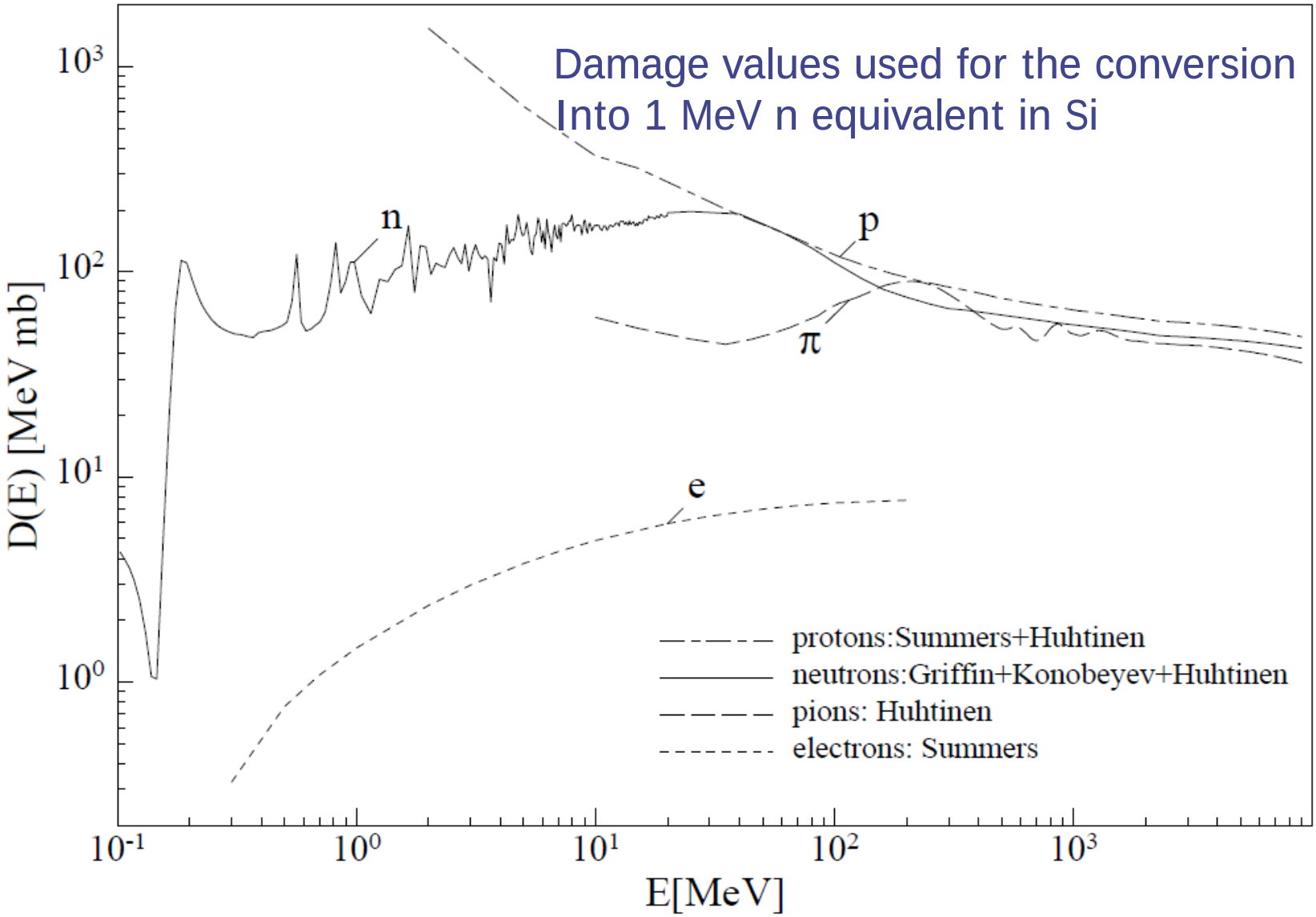
Corresponding FLUKA Estimators

Category		Scales with simulated/measured quantity
Single Event effects (Random in time)	***Single Event Upset (SEU)***	HADGT20M [cm^{-2}] (+/or HEHAD-EQ, THNEU-EQ)
	Single Event Latchup (SEL)	HADGT20M [cm^{-2}] (+/or HEHAD-EQ)
Cumulative effects (Long term)	***Total Ionizing Dose (TID)***	DOSE [GeV/g] -> stricly IONIZING only!
	Displacement damage	SI1MEVNE [cm^{-2}] {NIEL}

* Reality is more complicated (*e.g.*, contribution of thermal neutrons)

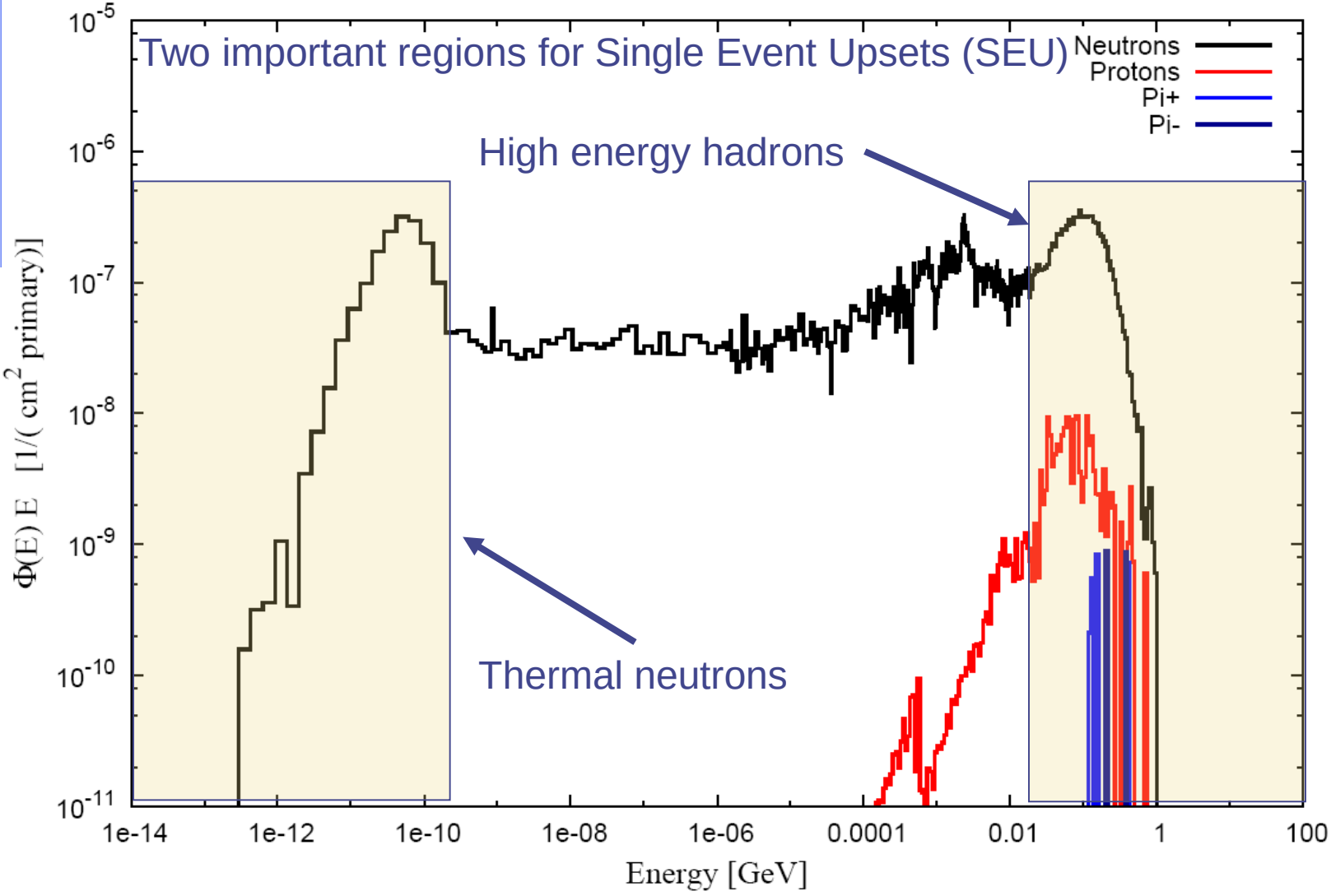
** Energy threshold for inducing SEL is often higher than 20 MeV (*e.g.*, 5-20MeV, see scoring lecture and discussion on future scoring possibility)

1MeV n Si Neutron Equivalent



SEUs in mixed radiation field

$$\#SEU = \sigma_{Th\ n} \cdot \Phi_{Th\ n} + \sigma_{HEH} \cdot \Phi_{HEH}$$

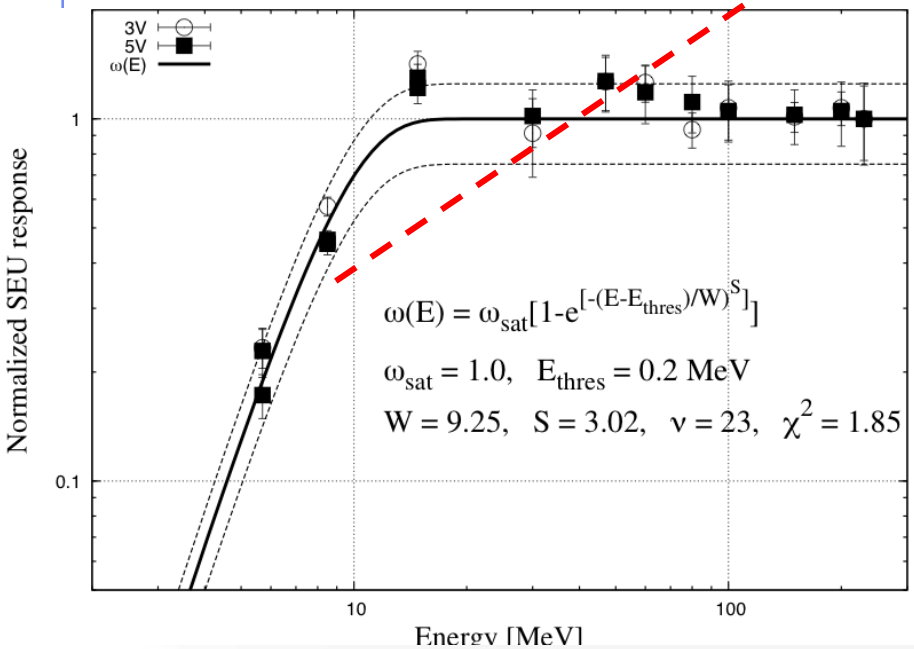


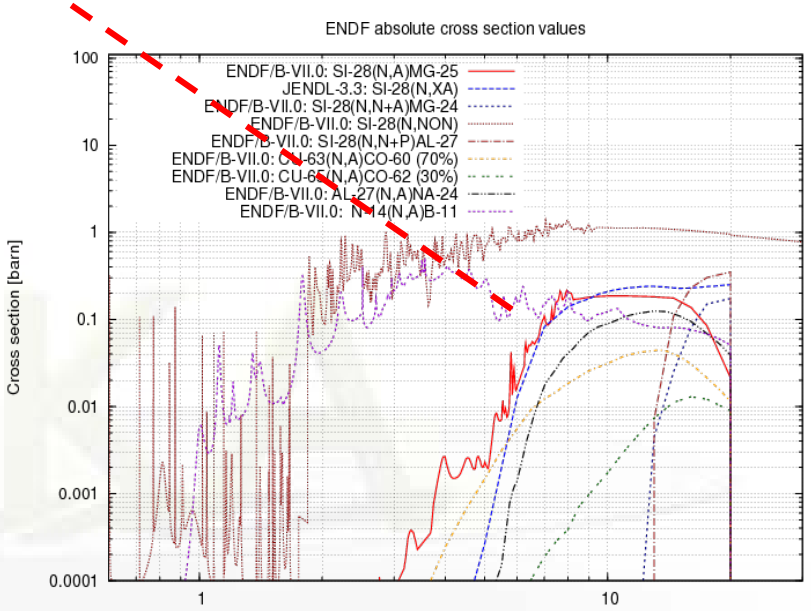
Device response

e.g. LHC RadMon

HEHAD-EQ

The behavior below 20 MeV is ≈ driven by the $^{28}Si(n,\alpha)$ cross section

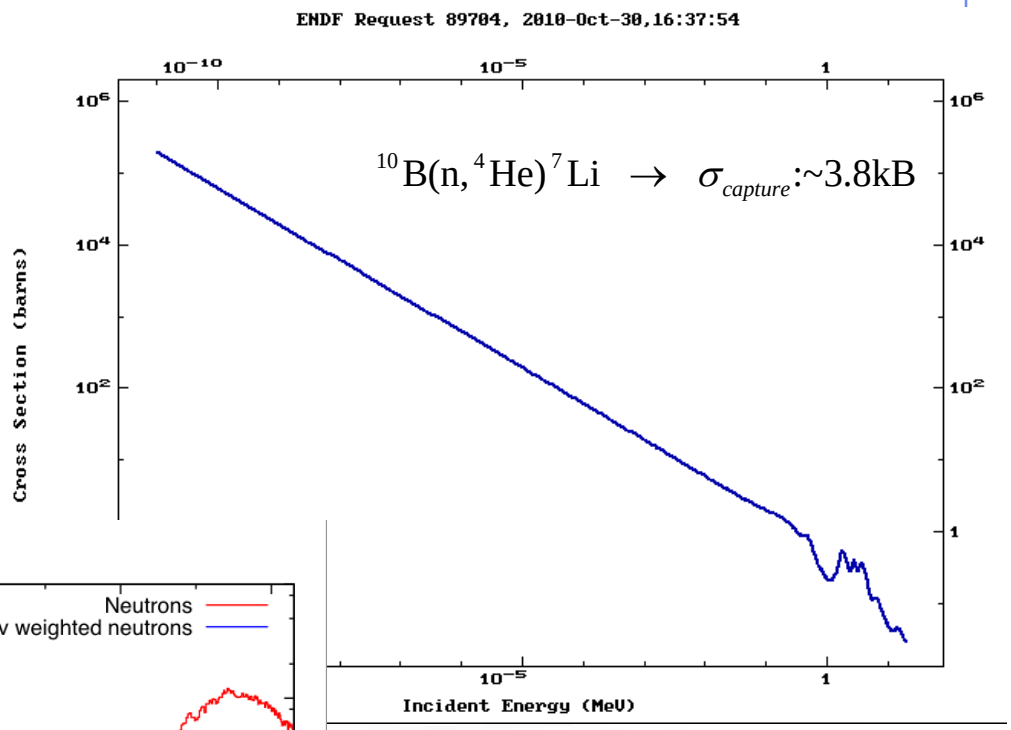


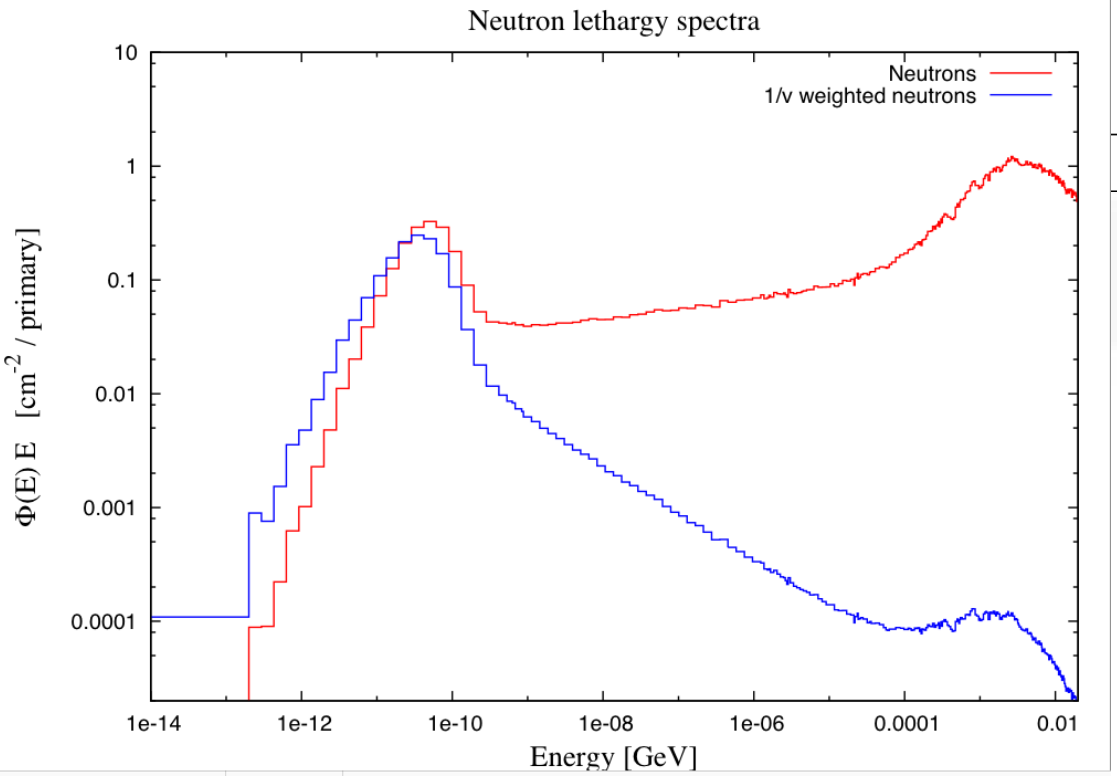


$$\Phi_{HEH} = \int_{0.2\mathrm{MeV}}^{20\mathrm{MeV}} \omega(E)\,\phi_n(E)\,dE + \int_{20\mathrm{MeV}}^{\infty} \phi_{Had}(E)\,dE$$

"Method for Measuring Mixed Field Radiation Levels Relevant for SEEs at the LHC", RADEC 2011, TNS 2012, 10.1109/TNS.2012.2183677

THNEU-EQ


ENDF Request 89704, 2010-Oct-30,16:37:54
Cross Section (barns)
Incident Energy (MeV)
$^{10}B(n,^{4}He)^{7}Li \rightarrow \sigma_{capture}$:~3.8kB


Neutron lethargy spectra
Neutrons
1/v weighted neutrons
Φ(E) E [cm^{-2} / primary]
Energy [GeV]

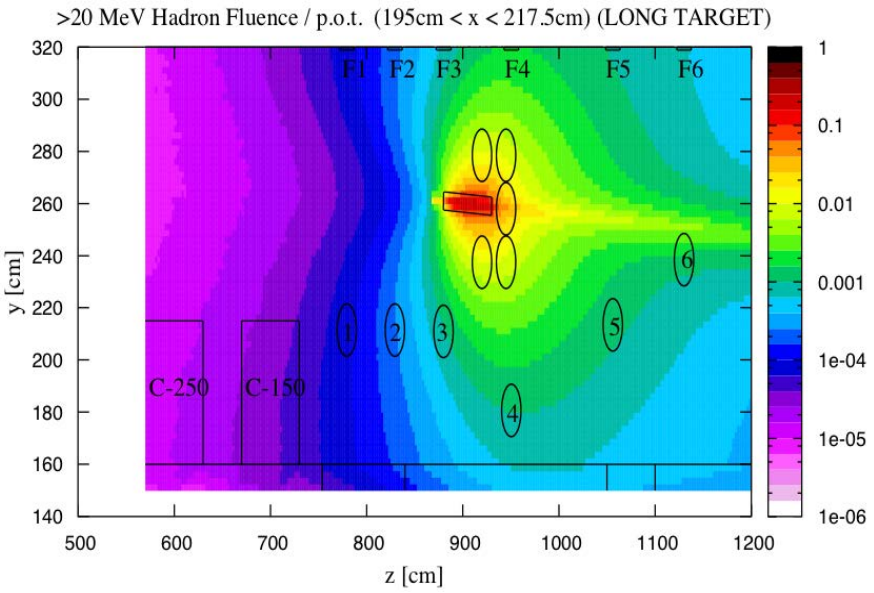
Related Scoring CARDS & Quantities

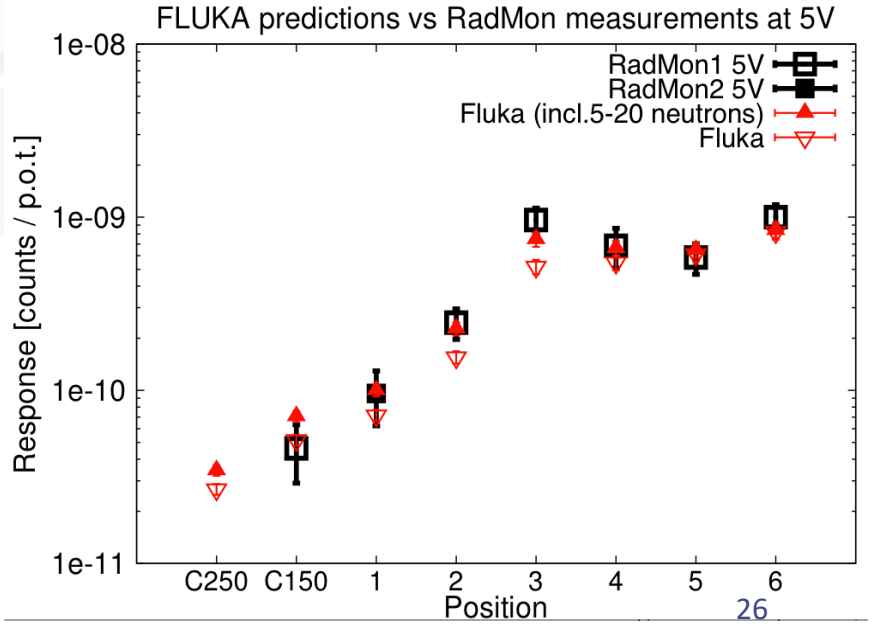
DOSE	total ionizing dose (TID) in (obviously…) GeV/g!
SI1MEVNE	Silicon 1 MeV-neutron equivalent fluence
HADGT20M	Hadrons fluence with energy > 20 MeV
HEHAD-EQ	as above, but weighted for n < 20 MeV
THNEU-EQ	1/v weighted neutrons

Application benchmark @ CERF

- Response of monitor measured in a mixed field facility and compared to predictions by Monte Carlo simulations

$$\#SEU = \sigma_{Th\_n} \cdot \Phi_{Th\_n} + \sigma_{HEH} \cdot \Phi_{HEH}$$





Neutrons

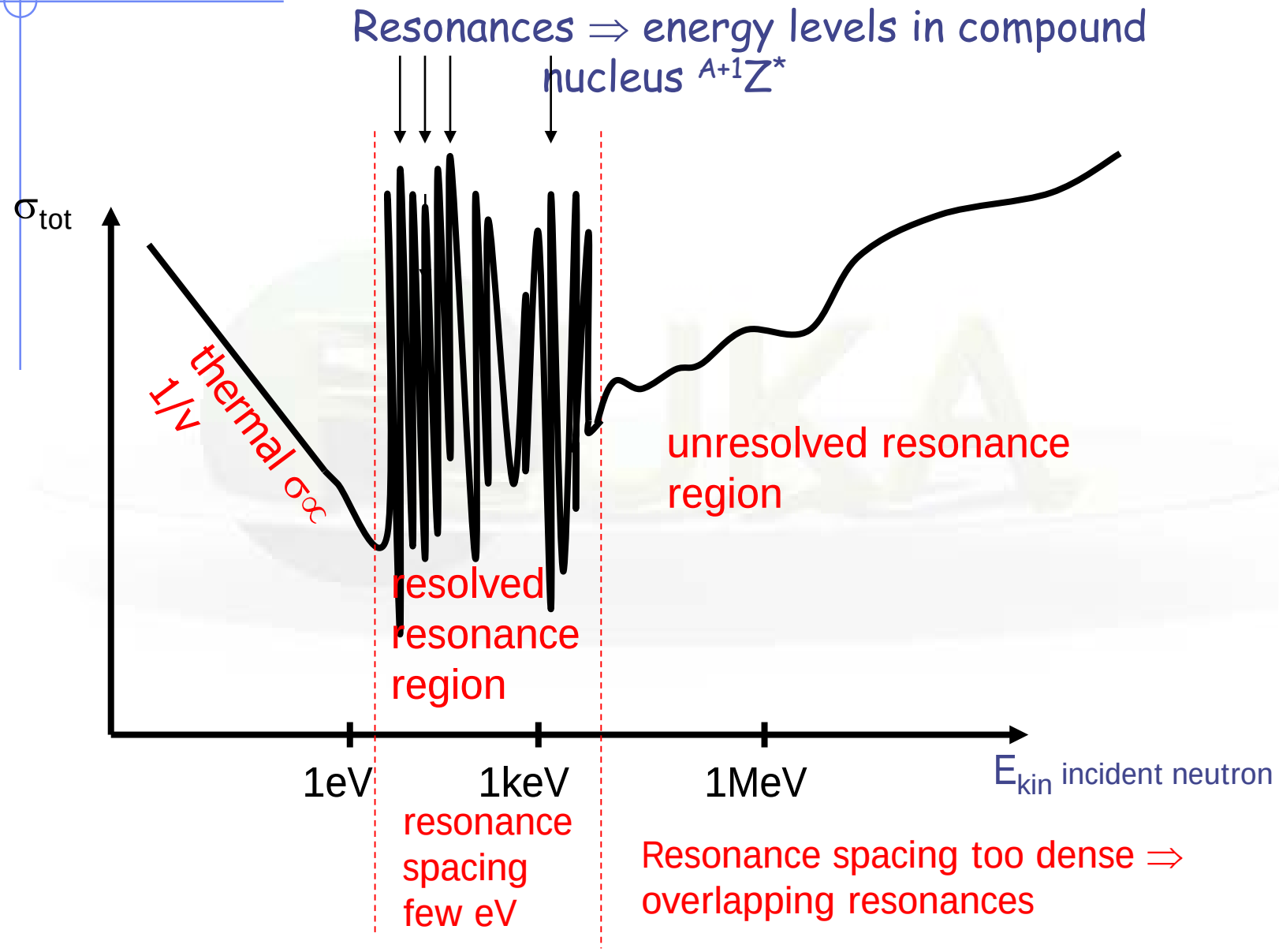
Reminder Neutrons

- 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



Material Correspondence: LOW-MAT

- The LOW-MAT card sets the correspondence between FLUKA materials and the low energy neutron cross sections
- If a material has the same name as a name given in the list of low neutron materials, the correspondence between material and low energy neutron transport is set automatically, and 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 that 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

Basis: 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

Point-wise and Group-wise cross sections

- In neutron transport codes in general two approaches are used: point-wise ("continuous" cross sections) and group-wise transport
- Point-wise follows cross section precisely but it 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 application

Complex programs (NJOY, PREPRO...) convert ENDF files to point-wise or group-wise cross sections, including Doppler broadening etc.

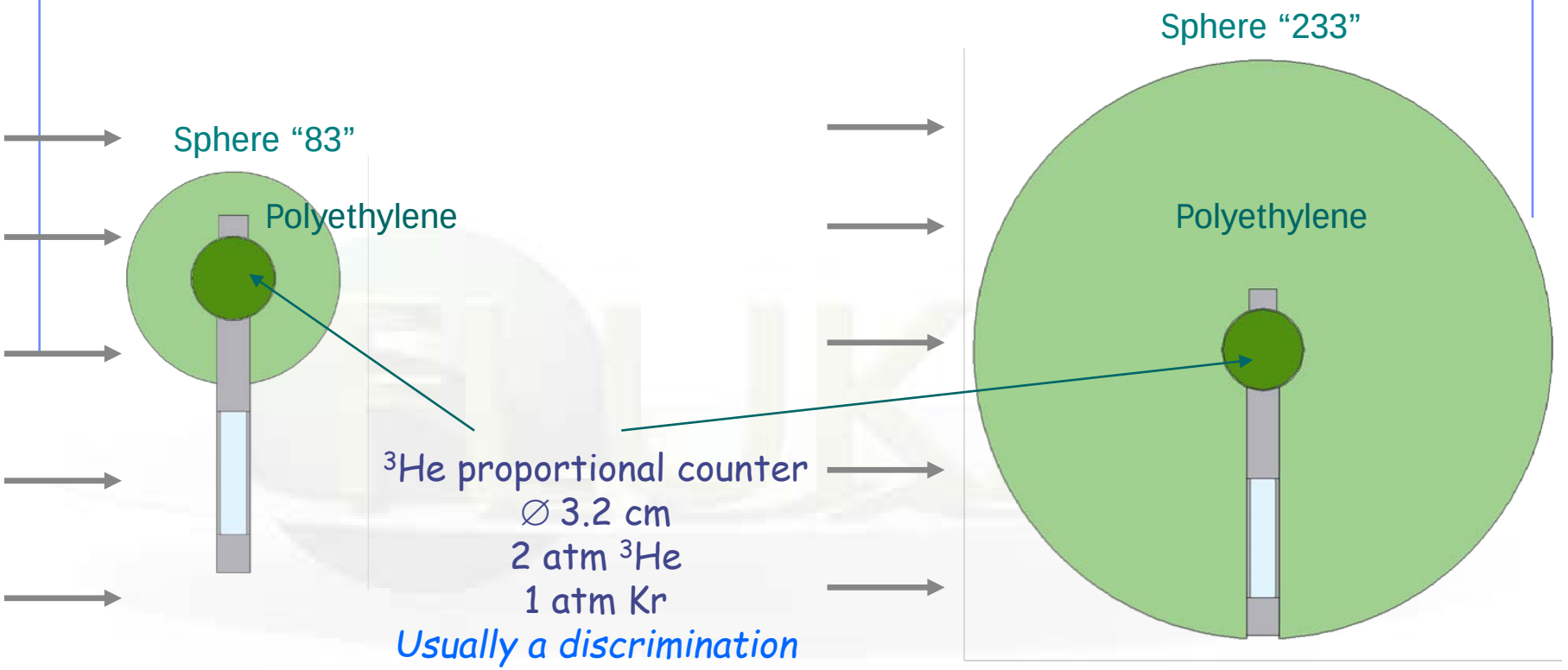
FLUKA: Point-Wise Neutron Cross Sections

- ***Point-wise neutron transport*** is available for ^{1}H (above 10 eV if bound H requested, down to 10^{-5} eV otherwise) and ^{6}Li
- ***Detailed correlated reaction products*** are available for ^{1}H, ^{6}Li, ^{10}B (only for the reaction $^{10}B(n,\alpha)^{7}Li$), and the $^{14}N(n,p)$ reaction. All reaction products are then transported explicitly according to transport setting (**PHYSICS**).
- Recoil proton production is ON by default for H and $^{14}N(n,p)$
- while for the others and for point-wise treatment it depends on the **DEFAULT** set chosen
- Both are important for precision studies, detector response (exp. scintillators) , borated materials…
- To require ***point-wise neutron transport and reaction products*** (where available), use the **LOW-NEUT** card with WHAT(6)=1.

Materials with molecular binding S(α,β)

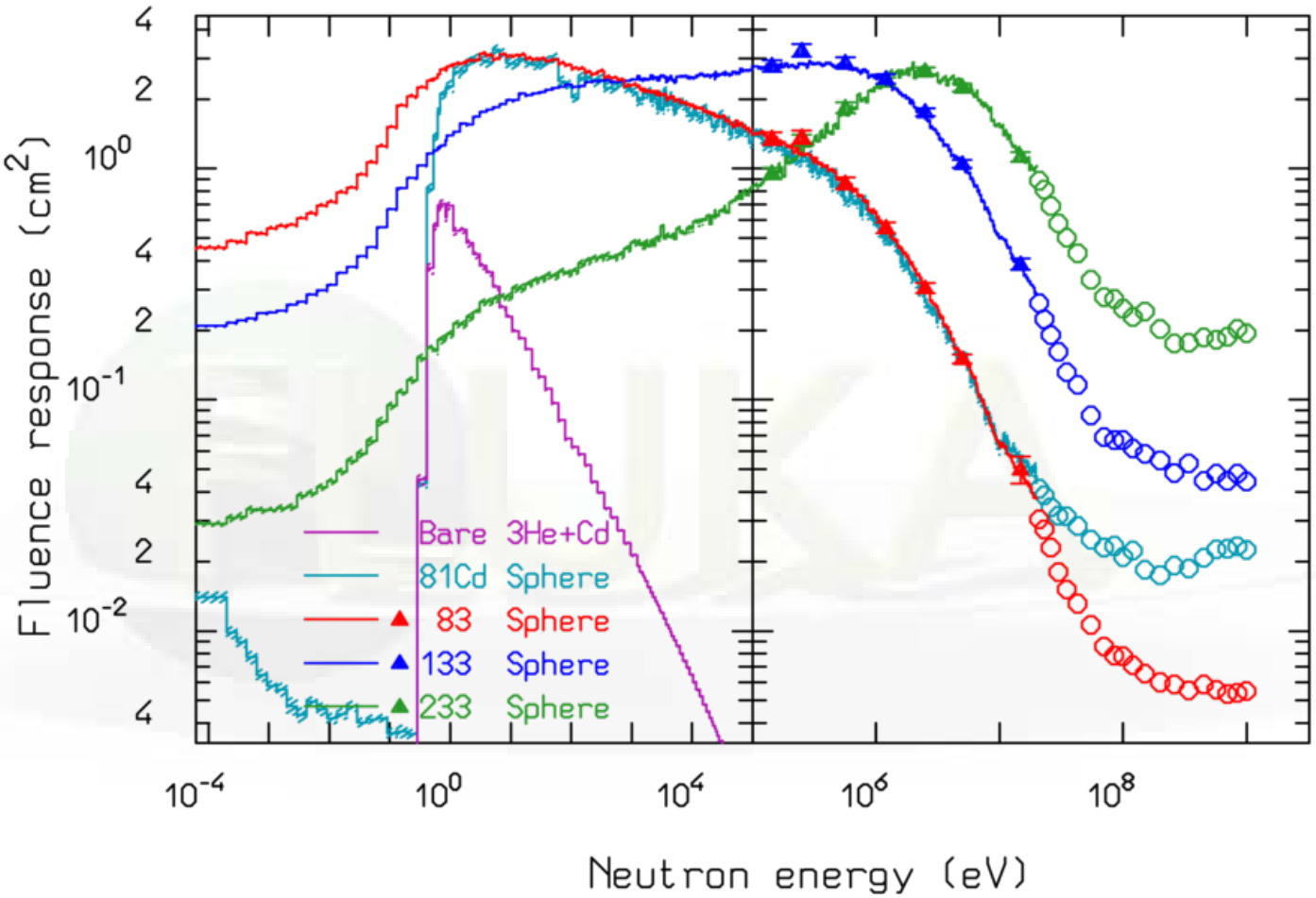
- Available materials with molecular bindings at 296K:
  - H (natural isotopic amount) in H_2O, CH_2
  - ^1H in H_2O, CH_2
  - ^2D in D_2O
  - C in graphite
- Use of these materials makes the thermal neutron calculation more realistic and can affect the energy and spatial distributions
- Example: CH_2 (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
- Reminder: for hydrogen, H bound in water is the default, because it is the first in the list of low energy neutron materials

Bonner spheres: lateral irradiation geometry:



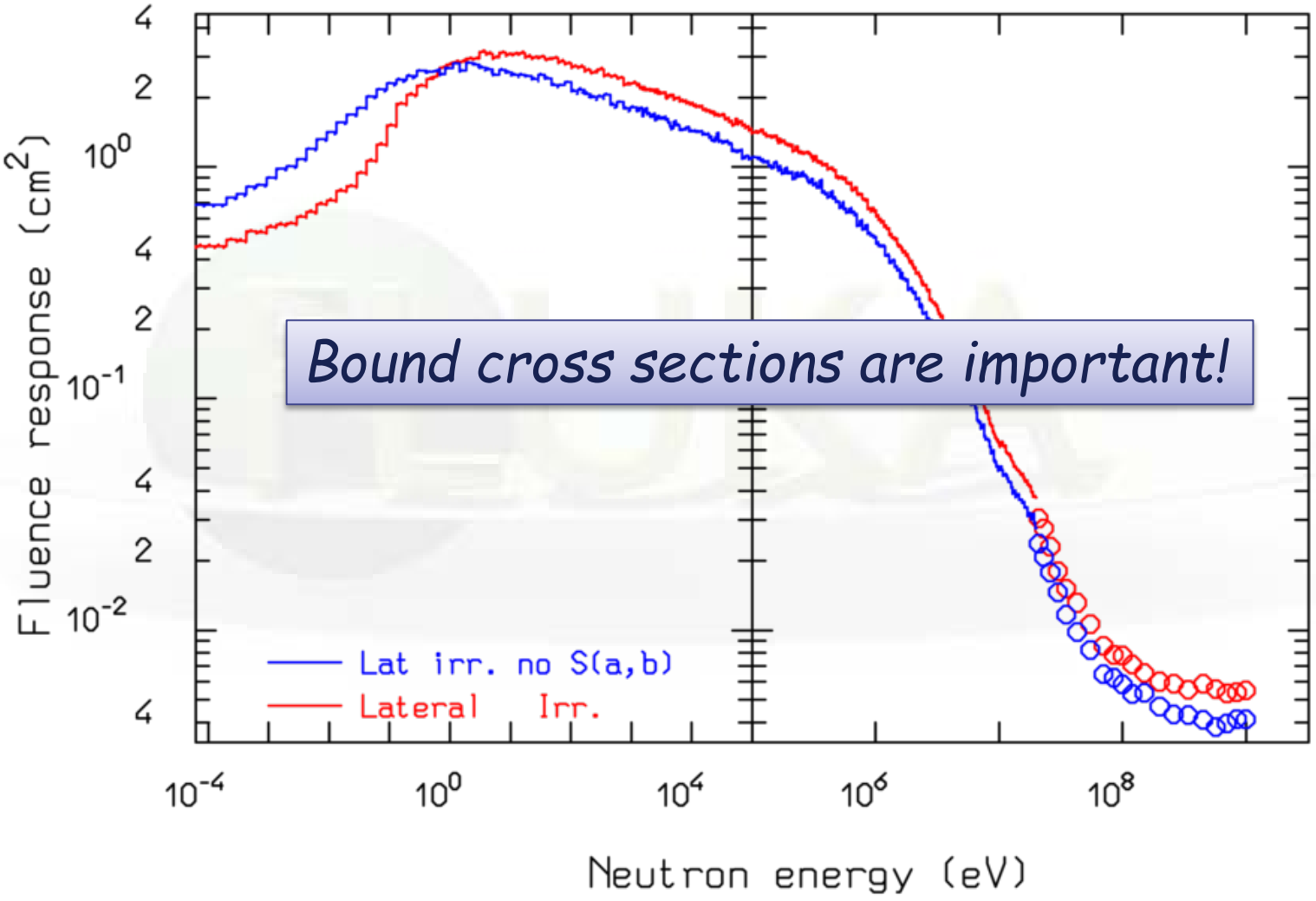
Usually a discrimination threshold is set around 100-300 keV to reject photons or other backgrounds

Bonner spheres: response functions



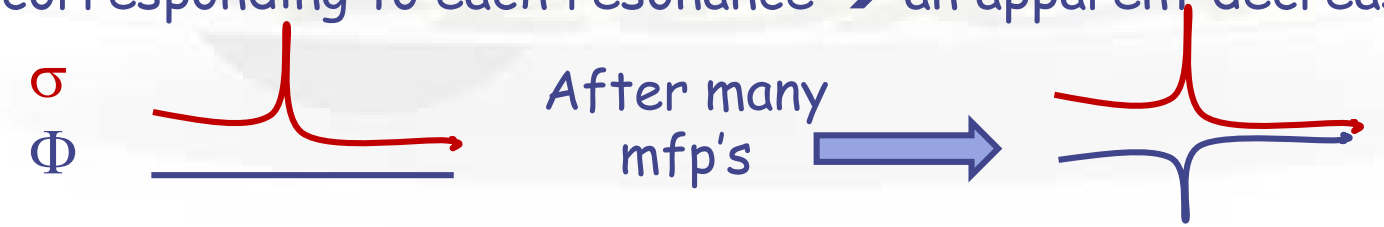
Computed response functions by folding the neutron fluence inside the counter with σ(n,p), using 200 keV as discrimination threshold for the (n,el), (n,d) reactions. The symbols are exp. data obtained with mono-energetic neutron beams at PTB

S(α,β) vs free gas for H: Sphere 83



Self-shielding [1/4]

- 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, $\langle\sigma\rangle_g = \int_{Group} \sigma(E)\Phi(E)dE \,/\, \int_{Group} \Phi(E)dE$ over the width of each energy group, unless a special correction is made

Self-shielding [2/4]

Self-shielded materials in FLUKA:

- ^{27}Al at 296K, 87K, 4K, 430K
- ^{nat}Ar, ^{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 (^{nat}Fe +2-4%C) at 296K, 87K, 4K, 430K (see slide further on)

Self-shielding [3/4]

- 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 them self- shielded

Self-shielding [4/4]

- 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 2-4% carbon. The amount of carbon doesn't need to be exactly that one.
- How to create self-shielded cast iron?
  - Define a material iron called FeCarbSS (or any other name you like) with a MATERIAL card (parameters as for natural iron)
  - Insert a LOW-MAT card for FeCarbSS with the proper identifiers for cast iron in WHAT(2)-WHAT(4) and SDUM
  - Insert a MATERIAL card to declare a compound material called CastFe (or any other name you like)
  - Insert a COMPOUND card for defining CastFe as a compound of FeCarbSS and CARBON (predefined)