FLUKA

蘭州大學
LANZHOU UNIVERSITY

Low energy neutrons

23rd FLUKA Beginner's Course
Lanzhou University
Lanzhou, China

June 2–7, 2024

Outline

Outline

Motivation

- Low energy neutrons are essential in our modern life
- Practically, no advanced technological progress is possible without low energy neutrons
- They are used to study and development of advanced materials which make our life so convenient
  - Nuclear power plants
  - Solar cells
  - Electric cars
  - All advanced electronic devices (CPUs, mobile phones, etc)
  - Flat screens
  - Medicine, Biology, Archeology
  - …and much more

FLUKA $\geq$2024.1 can do very accurate treatment of low energy neutron transport

Neutron simulations

Evaluated nuclear data files
(10 µeV up to 20–50/200 MeV)
depends on specific isotope

(Monte Carlo) Models
(from 10–20 MeV up to few TeV)

Neutron energy

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Neutron energy

- Based on expert "evaluations" of available experimental data
  - often complemented by models
- High energy (>20 MeV) evaluations based on complex (non Monte Carlo) nuclear models
  - GNASH, Talys, Empire
  - become less reliable with increasing energy

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- Monte Carlo nuclear models aimed at the description of particle production spectra by whichever projectile
- A large variety available
  - not necessarily all good

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Neutron energy

Pros (=benefits):

- $<$20 MeV: as good as our knowledge
- Standard file formats
- Processing tools available
- Fast (but memory-hungry)
- No real alternatives below 20 MeV
  - due to complex nature of low energy neutron interactions

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Pros:

- Work for all projectiles, energies, targets
- (At least the good models) produce fully correlated physical effects
  - i.e. conservation laws fulfilled event-by-event
- Easy go update
  - just update the code and run again

Neutron simulations

Evaluated nuclear data files
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depends on specific isotope

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Neutron energy

Cons (=drawbacks):

- No correlations!
- Slow and complex to update with new data and improved models
- Sometimes incomplete or inconsistent

Neutron simulations

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Neutron energy

Cons (=drawbacks):

- No correlations!
- Slow and complex to update with new data and improved models
- Sometimes incomplete or inconsistent

Cons:

- As good as physics inside
  - sometimes good for most applications
  - but horrible for a few
- Not really usable below 10–20 MeV
  - or even higher for many models

Neutron simulations

Evaluated nuclear data files
(10 μeV up to 20–50/200 MeV)

depends on specific isotope

(Monte Carlo) Models
(from 10–20 MeV up to few TeV)

Neutron energy

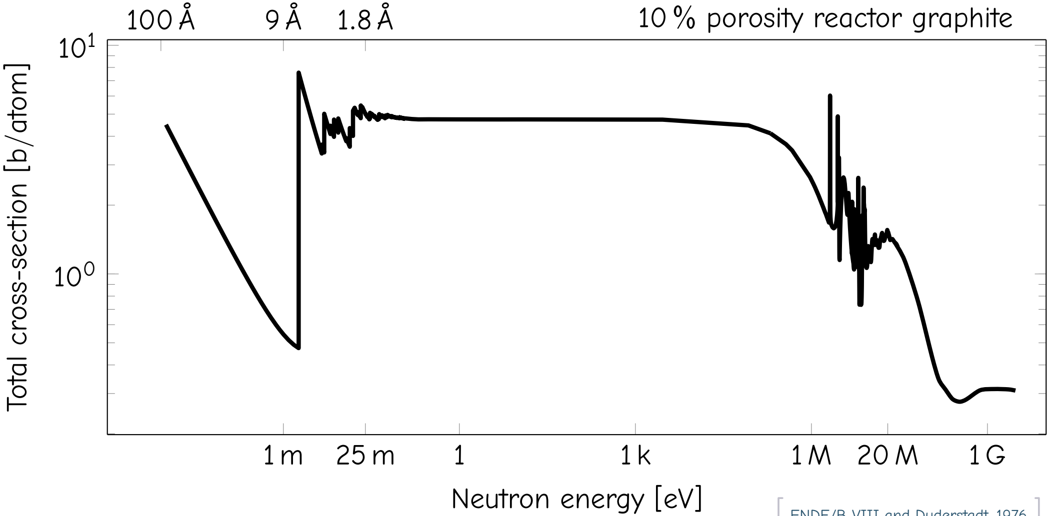
- In FLUKA, we refer to neutrons below 20 MeV as low energy neutrons
  - transport and interactions of low energy neutrons are handled by dedicated data files
- Neutron interactions at higher energies are handled by nuclear models

Why are low energy neutrons special?

- The neutron has no charge and long lifetime
  - ⇒ can (only) undergo nuclear interactions even at very low energies ($\sim$ meV)
- Even very slow (few meV) neutrons can still generate energetic photons (several MeV) and/or charged particles through capture
  - ⇒ important to transport low energy neutrons in shielding-related calculations
- Neutron cross sections are complex and structure-rich
  - cannot be calculated by models
    - ⇒ we (like all other codes) rely on evaluated data files (measurements)

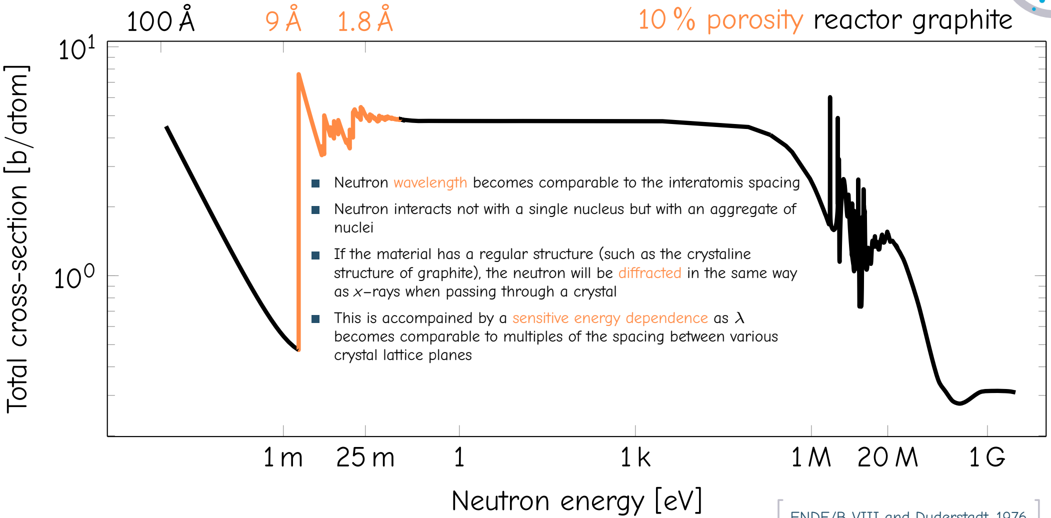
Outline

Typical neutron cross section



[ENDF/B-VIII and Duderstadt, 1976]

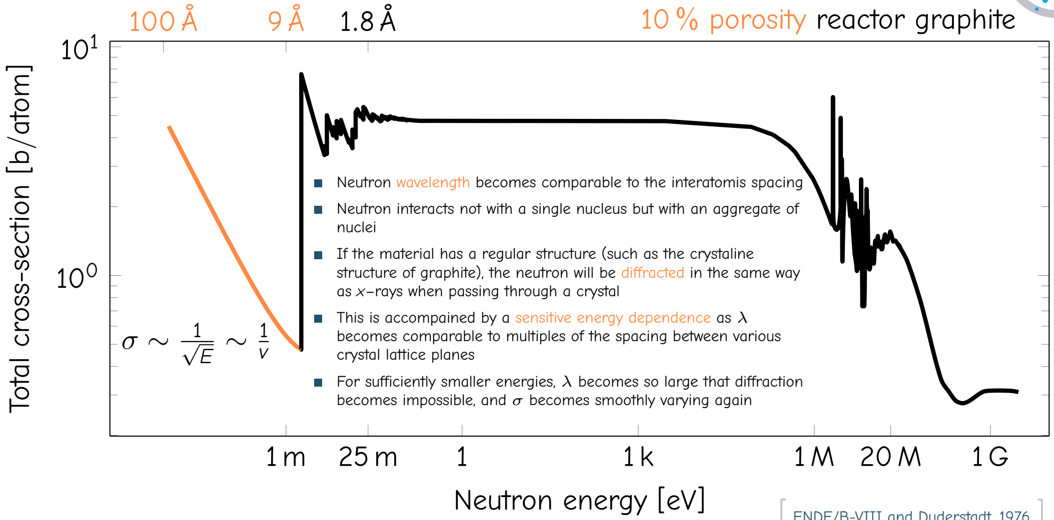
Typical neutron cross section
Diffraction



- Neutron wavelength becomes comparable to the interatomis spacing
- Neutron interacts not with a single nucleus but with an aggregate of nuclei
- If the material has a regular structure (such as the crystaline structure of graphite), the neutron will be diffracted in the same way as x−rays when passing through a crystal
- This is accompanied by a sensitive energy dependence as λ becomes comparable to multiples of the spacing between various crystal lattice planes

[ENDF/B-VIII and Duderstadt, 1976]

Typical neutron cross section
Large wavelengths



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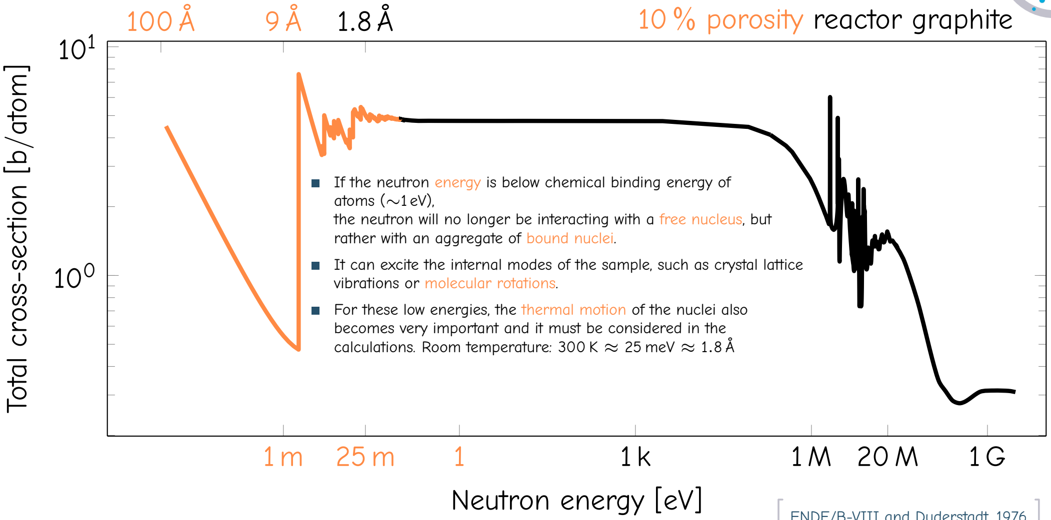
- This is accompanied by a sensitive energy dependence as λ becomes comparable to multiples of the spacing between various crystal lattice planes
- For sufficiently smaller energies, λ becomes so large that diffraction becomes impossible, and σ becomes smoothly varying again

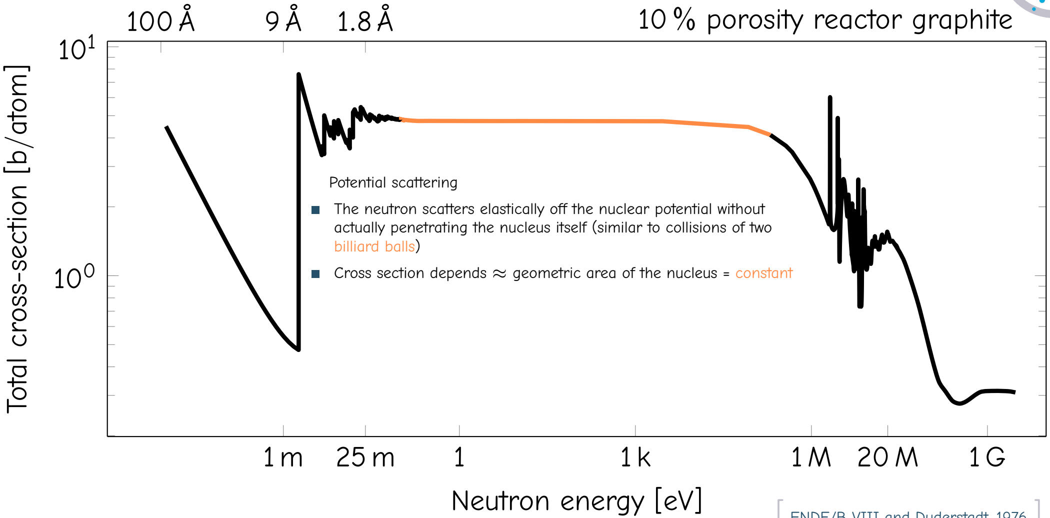
[ENDF/B-VIII and Duderstadt, 1976]

Typical neutron cross section
Very low energies



- If the neutron energy is below chemical binding energy of atoms (~1 eV), the neutron will no longer be interacting with a free nucleus, but rather with an aggregate of bound nuclei.
- It can excite the internal modes of the sample, such as crystal lattice vibrations or molecular rotations.
- For these low energies, the thermal motion of the nuclei also becomes very important and it must be considered in the calculations. Room temperature: 300 K ≈ 25 meV ≈ 1.8 Å

[ENDF/B-VIII and Duderstadt, 1976]



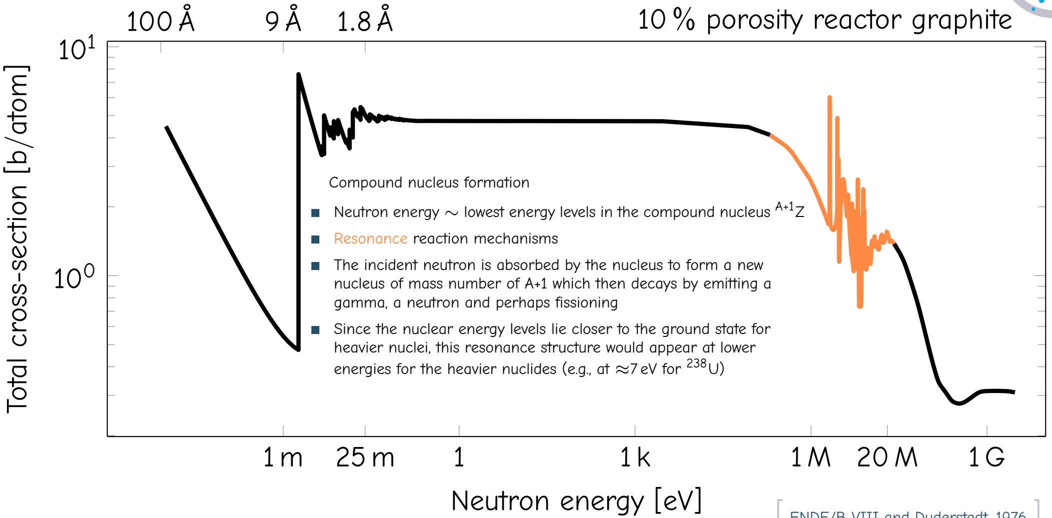
Potential scattering

- The neutron scatters elastically off the nuclear potential without actually penetrating the nucleus itself (similar to collisions of two billiard balls)
- Cross section depends ≈ geometric area of the nucleus = constant

[ENDF/B-VIII and Duderstadt, 1976]

Typical neutron cross section

Resonances

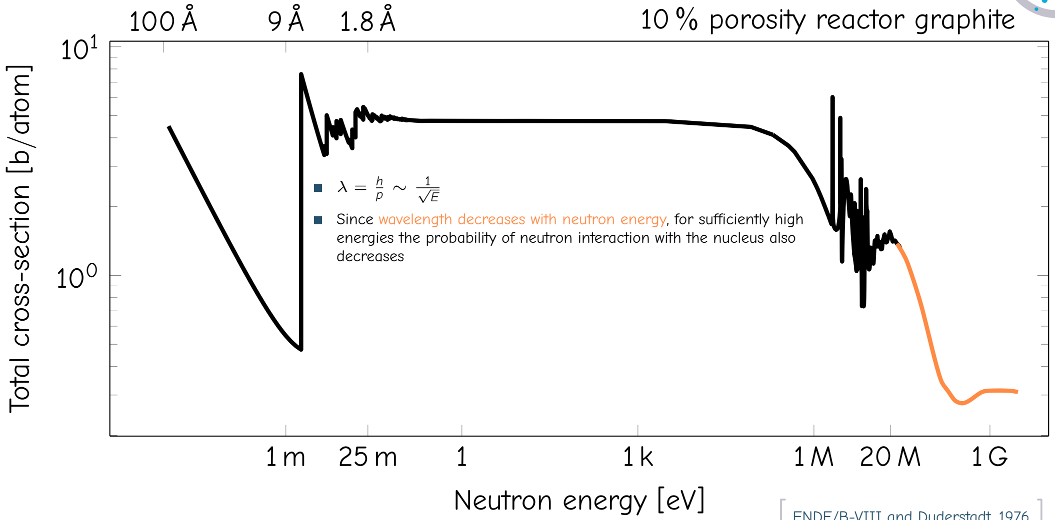


Compound nucleus formation

- Neutron energy ~ lowest energy levels in the compound nucleus ^{A+1}Z
- Resonance reaction mechanisms
- The incident neutron is absorbed by the nucleus to form a new nucleus of mass number of A+1 which then decays by emitting a gamma, a neutron and perhaps fissioning
- Since the nuclear energy levels lie closer to the ground state for heavier nuclei, this resonance structure would appear at lower energies for the heavier nuclides (e.g., at ≈7 eV for ^{238}U)

[ENDF/B-VIII and Duderstadt, 1976]

Typical neutron cross section
Falloff



- $\lambda = \frac{h}{p} \sim \frac{1}{\sqrt{E}}$
- Since wavelength decreases with neutron energy, for sufficiently high energies the probability of neutron interaction with the nucleus also decreases

[ENDF/B-VIII and Duderstadt, 1976]

Evaluated Nuclear Data Files (ENDF)

- Cross section data have been accumulated over the past few decades by different institutions
- In order to consolidate and standardise it into one data set, the ENDF was established
- ENDF contains both photon and neutron cross sections
  - …and software to convert data in the user-desired format
- Several evaluation sets are available: CENDL, ENDF, JENDL, ROSFOND, TENDL, …
- The standard source of nuclear data

`https://www-nds.iaea.org/exfor/endf.htm`

Point-wise and Group-wise cross sections

Two approaches are used in neutron transport codes:

Point-wise

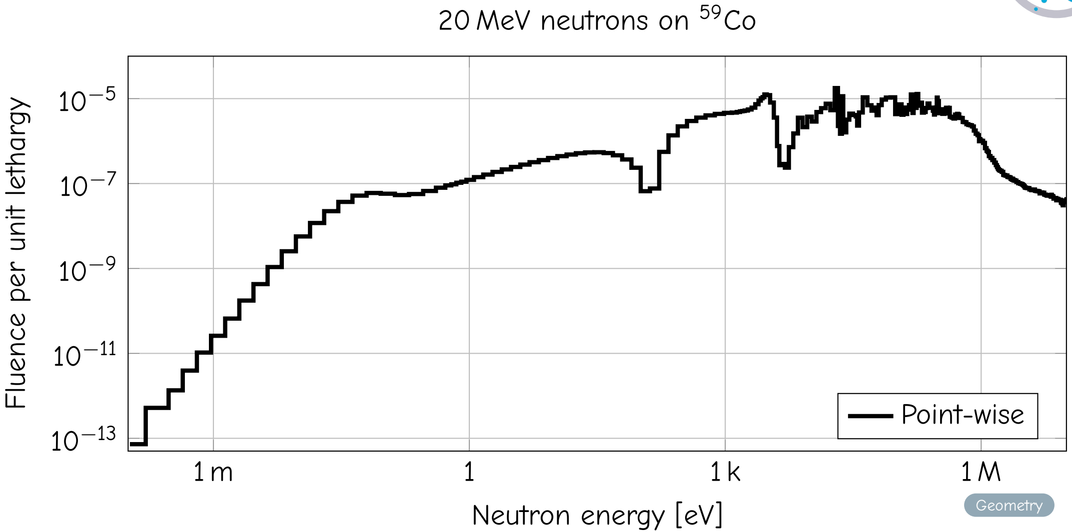
- Continuous energy cross sections
- Follows σ precisely but it can be CPU time and memory consuming

Group-wise

- Energy group averaged cross sections
- Widely used in neutron transport codes because it is fast and gives good results for most applications

- To keep the size of ENDF files reasonable, they contain a combination of actual data tables and resonance parameters that can be reconstructed into point-wise or group-wise data with specialised tools:
  - NJOY, PREPRO, ACEMAKER, GRUCON
  - all available open-source
- FLUKA can use both point- and group-wise cross sections

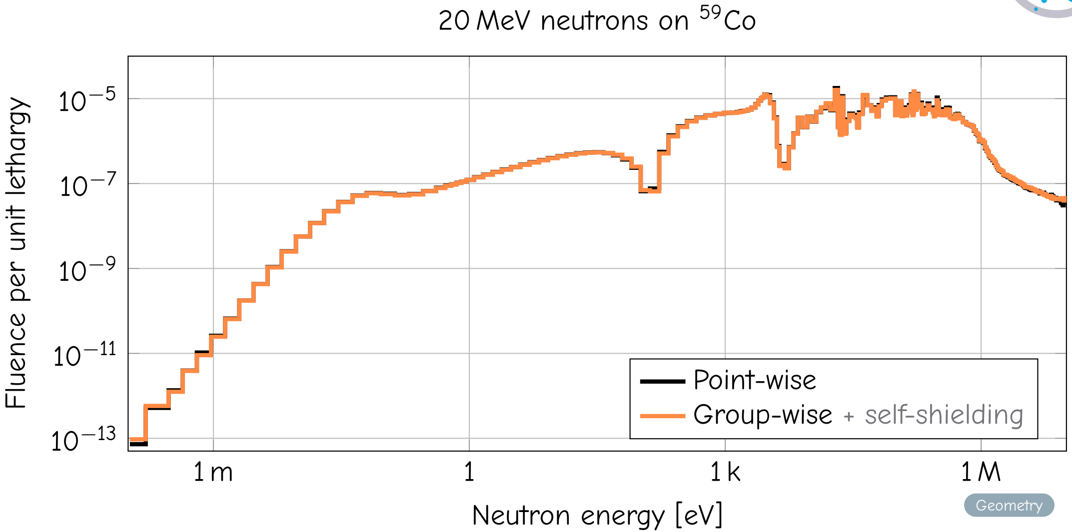
Point-wise and Group-wise cross sections
Example: Neutron spectrum



Geometry

Point-wise and Group-wise cross sections

Example: Neutron spectrum



Geometry

Outline

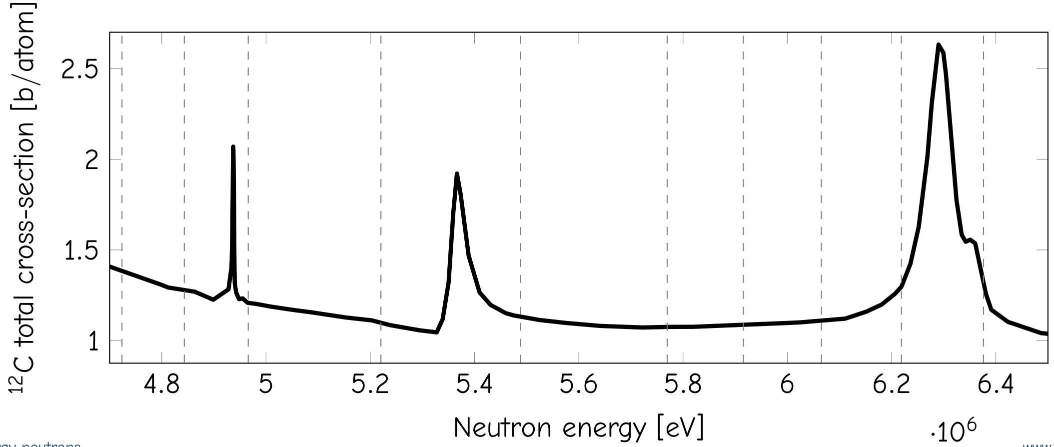
Multigroup neutron transport (group-wise)

- Neutron interactions are not simulated as exclusive processes, but by downscattering and upscattering matrices which define group-to-group transfer probabilities
- The energy range of interest is divided in a given number of discrete intervals (energy groups)
  - In FLUKA: 260 energy bins between 0.01 meV and 20 MeV
  - approx. equal logarithmic width
- The angular range is divided by 3 discrete polar angle cosines (and corresponding probabilities)

  ⇒ for a given group-to-group transition, only 3 polar angle values are possible
    - but many more for a given scattering considering all possible outcomes Example
- Advantage: fast
- Major limitations:
  - self-shielding effect needs specific treatment (see later)
  - most of charged secondary particles are not transported (their energy is deposited at the interaction point)

- 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 with probability given by the matrix elements
- If the neutron does not lose enough energy to be in another group, it will stay in the same group (in-scattering)
- Upscattering matrix
  - In the thermal energy region ($\lesssim 25\,\mathrm{meV}$) neutrons can gain energy. This is taken into account by upscattering matrix, containing the transfer probability to a group of higher energy

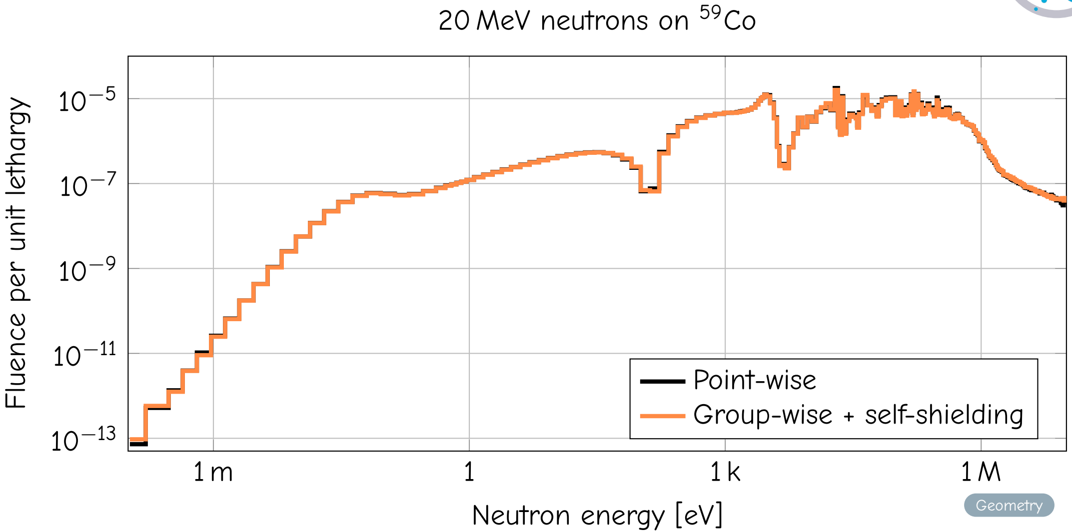
The group structure is necessarily coarse with respect to the resonance structure in many materials:



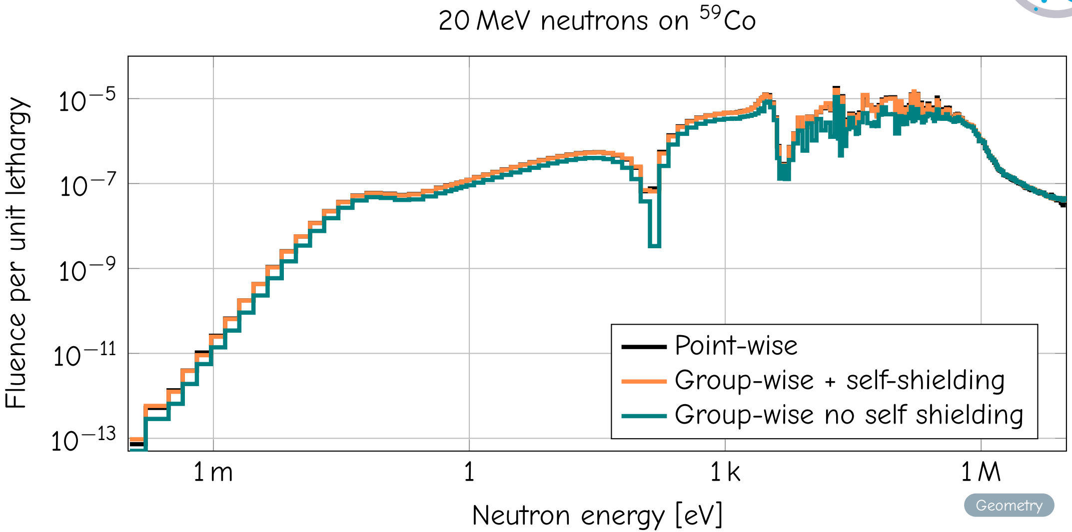
- A large resonance will cause a depression in the neutron population around that energy
  - this may not be reflected in simulations where this feedback is not fully taken into account
- It is particularly problematic with group-wise neutron transport where these resonances are not resolved
- This effect results in a lower reaction rate $(\sigma\Phi)$, which is called self-shielding
  - it must be accounted in the process of cross section averaging
- FLUKA group-wise cross sections are typically provided with- and without self-shielding correction
  - see table 10.3 of the Manual
  - can be printed with LOW-NEUT card
- Self-shielding correction depends on the presence of other isotopes and the region dimension

Point-wise and Group-wise cross sections

Example: Neutron spectrum



Geometry



20 MeV neutrons on ^{59}Co
Fluence per unit lethargy
10^{-5}
10^{-7}
10^{-9}
10^{-11}
10^{-13}
1 m
1
1 k
1 M
Neutron energy [eV]
Point-wise
Group-wise + self-shielding
Group-wise no self shielding

Geometry

- 260 energy groups between 0.01 meV and 20 MeV
  - approximately equal logarithmic widths
  - 31 groups in the thermal region
  - 30 upscattering groups
- 3 angular groups
- Based on recent versions of ENDF data files (mostly ENDF/B-VIII.0)
- About 300 isotopes/materials available
- Almost all materials available at two temperatures: 87 K and 296 K
  - some also at 4 K, 120 K and 430 K
  - Doppler broadening at the relevant temperatures is taken into account
- Gamma generation ← grouped as well
- For some isotopes/materials:
  - self-shielding
  - molecular binding

Outline

Point-wise neutron transport

- Fully correlated
  - with exact energy/momentum conservation event-by-event
- for all stable isotopes
- a few important unstable isotopes
- the most important transuranic elements
- at different temperatures: 4 K, 87 K, 296 K, 430 K and 686 K
- Self-shielding is automatically accounted for by point-wise cross sections

Group- vs point-wise

Group-wise

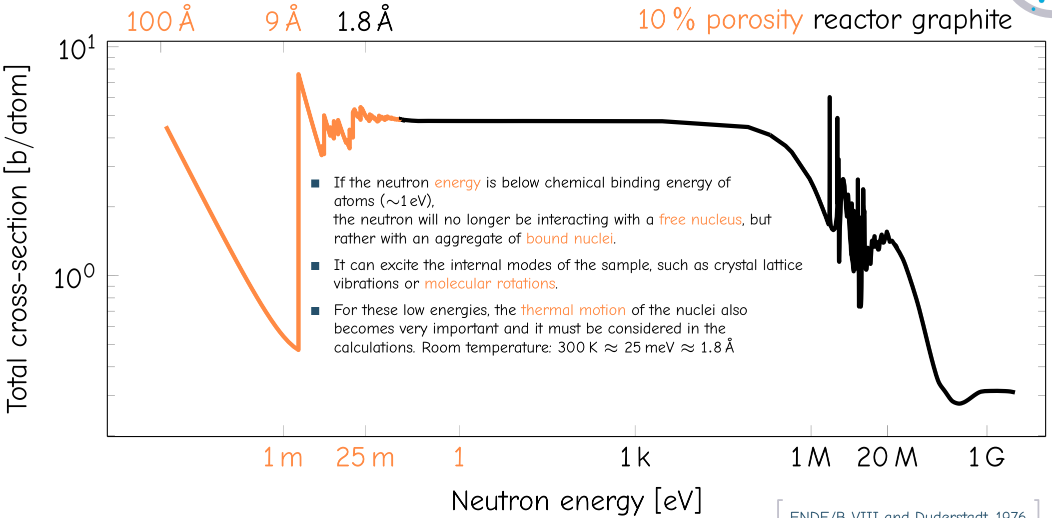
- Faster than point-wise
- Safe to use for many applications (shielding, high energy cosmic ray showers)
- Major limitation: self-shielding effect needs specific treatment
  - user should use a given set of cross sections for every self-shielding situation

Point-wise

- Precise
- Event-by-event correlations are possible
- …but do not use it if you don't really need it because it is slower than group-wise
  - from $\sim 20\,\%$ with general runs
  - to a factor of few with pure neutronic calculations

Outline

Typical neutron cross section
Very low energies



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[ENDF/B-VIII and Duderstadt, 1976]

Thermal scattering kernels

The nature of the physics of nuclear reactions is fundamentally different between MeV and sub-eV energies:

- Above a few eV ($\lambda \ll 1\,\text{Å}$), neutron transport is insensitive to chemical structures and materials are treated as regions without any atomic-level order (since neutron wavelength is much smaller than chemical structures).
- At lower energies ($\lambda > 1\,\text{Å}$), molecular excitations (e.g. rotations or vibrations) and collective excitations (known as phonons), are crucial to the understanding of how neutrons interact with the material.

Example: Water

As a result, H_2O cannot be treated as simply a mixture of hydrogen and oxygen atoms, but must be seen as hydrogen and oxygen specifically bound within water molecules.

Thermal scattering kernels

The nature of the physics of nuclear reactions is fundamentally different between MeV and sub-eV energies:

- The phase of the material must also be known.
  - e.g. whether it be liquid, gas or any one of potentially numerous possible solid phases
- If there are defects, the density of these defects must be considered as well
  - e.g. graphite with a given porosity
- Even the spin isomeric states must be considered for elemental hydrogen
  - i.e. para-hydrogen $\neq$ ortho-hydrogen

    This is absolutely essential for production of cold neutrons which are the key tool for solid state physics research!

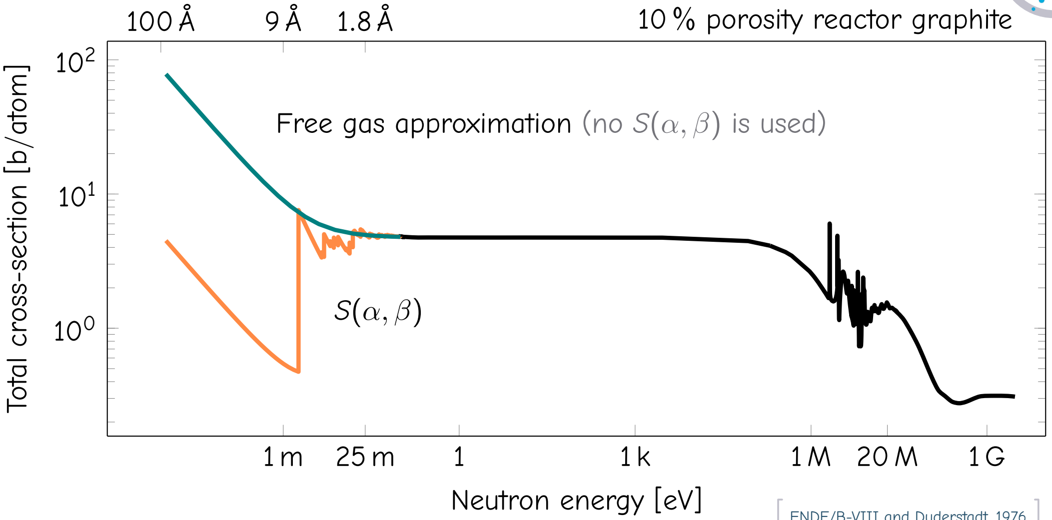
Thermal scattering kernels

The nature of the physics of nuclear reactions is fundamentally different between MeV and sub-eV energies:

- All of these factors contribute to how low energy neutrons scatter within the material
- If you need to take them into account, you have to specify them in your input by assigning special cross-sections to your materials to be used with neutrons in the thermal region. These cross sections are called
  - thermal scattering law (TSL) data libraries which contain information about
  - $S(\alpha, \beta)$ scattering kernels
- TSL are used to describe how scattering changes the energy and the angle of incident neutrons below few eV
- In FLUKA, they can be used both with group-and point-wise cross-sections

Typical neutron cross section

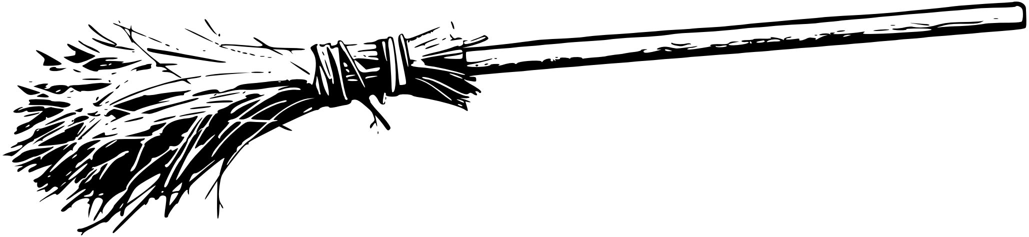
Free gas approximation



[ENDF/B-VIII and Duderstadt, 1976]

Outline

Broomstick



[Adobe Stock]

Broomstick test
Geometry

Incident

25 meV neutrons

"Broomstick" R $\sim$ atom size

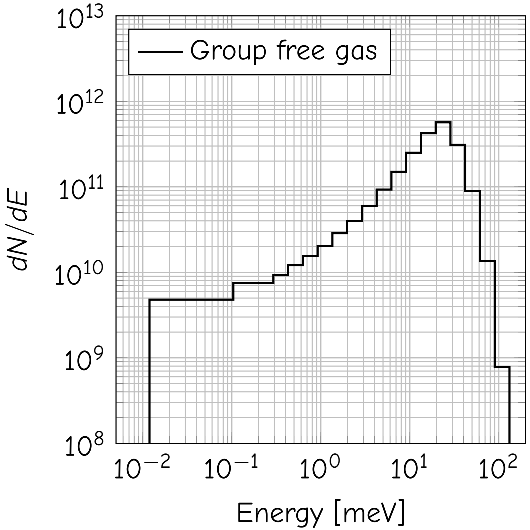
very long

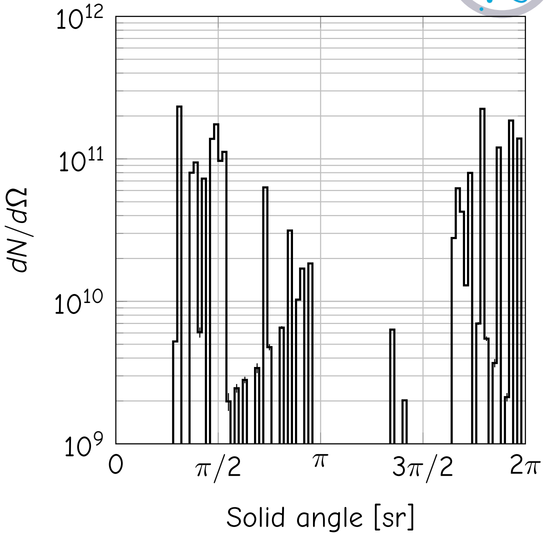
- Extremely long and narrow cylinder
  - so long that essentially all neutrons will collide there
  - so narrow that every scatter causes the neutron to scatter out of the cylinder without undergoing any more collisions
- By measuring the leakage from the cylinder we are directly measuring the single collision distribution
  - Energy: kinetic energy of scattered neutrons
  - Solid angle: $\Omega = 2\pi(1 - \cos\theta)$, where θ is the angle between the scattered neutron trajectory and the normal to the boundary at the point of crossing
- Material: 10 % porosity reactor graphite at room temperature

[Cullen, 2003]

Broomstick test

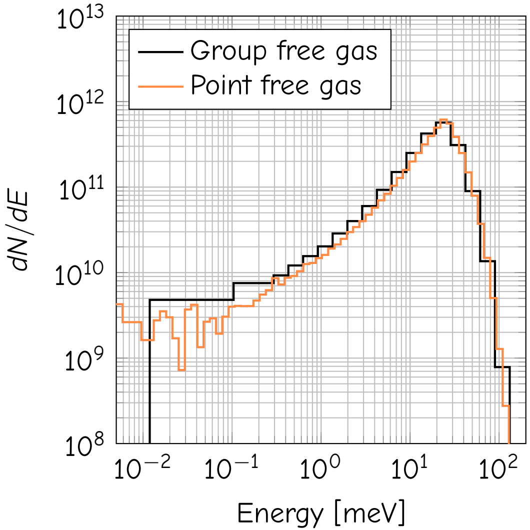
10 % porosity reactor graphite

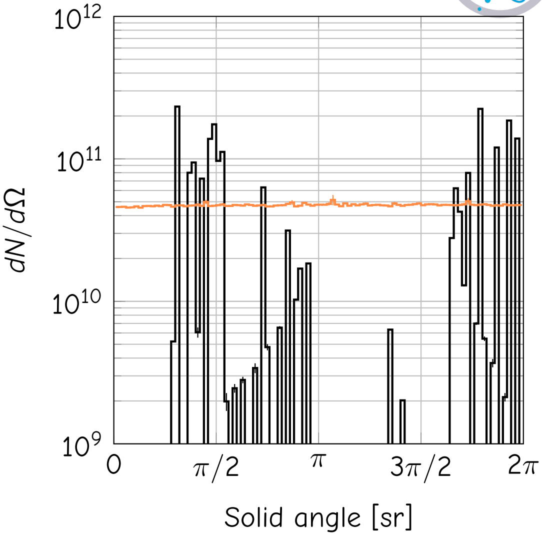




Broomstick test

10 % porosity reactor graphite





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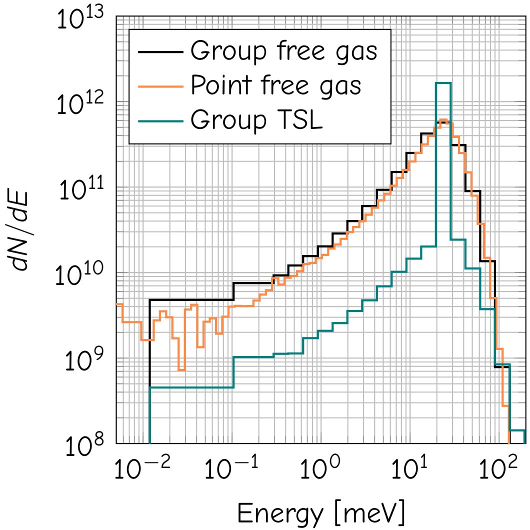

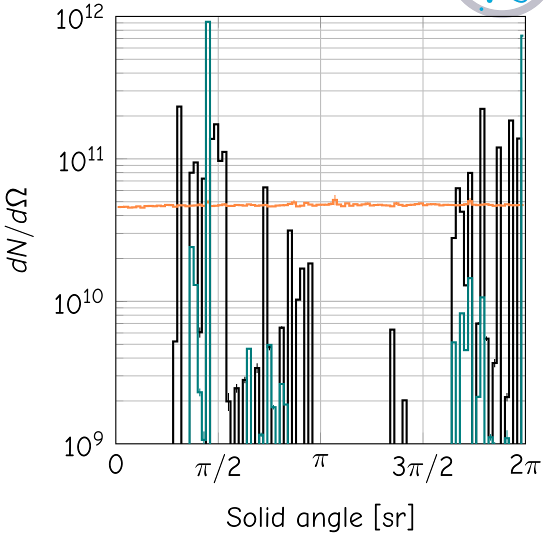

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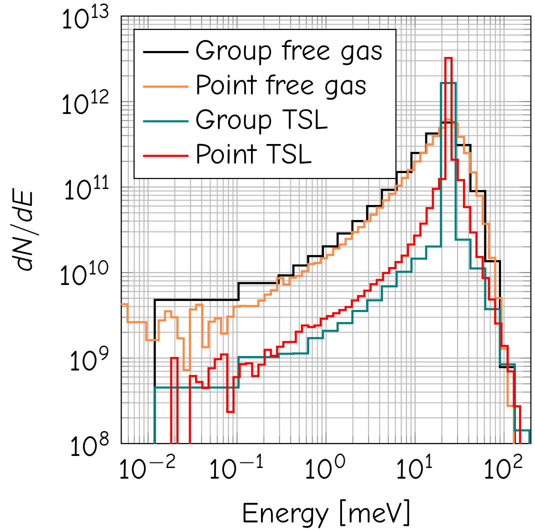

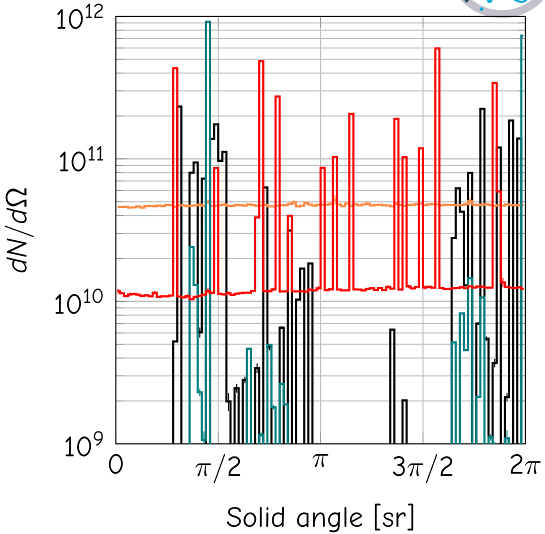

Outline

Usage

- cards
  - DEFAULTS
    - PAR-THR
  - LOW-MAT
  - LOW-NEUT
  - LOW-PWXS
    - TSL-PWXS

Usage
Very rough decision tree

Note: just setting the appropriate DEFAULTS is enough in most problems

Do I need to transport low energy neutrons?
normally: yes

no
- Either set DEFAULTS to EM-CASCAde
- or increase the neutron transport cut-off to 20 MeV with PAR-THR to speed-up calculations

yes or unsure
- Do I use non-standard material names? → Map materials and neutron cross sections LOW-MAT
- Am I interested in the neutron spectra $\leq$ thermal energies or event-by-event correlations?
  - yes
    - Use point-wise LOW-PWXS ~~LOW-MAT~~
    - Do I request special features? (molecular binding, temperature) → $S(\alpha,\beta)$ TSL-PWXS
  - no
    - Use group-wise ~~LOW-PWXS~~ ~~TSL-PWXS~~ → Mind self-shielding, temperature, molecular binding → Map materials and neutron cross sections LOW-MAT

www.fluka.org

Bibliography

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FLUKA: a multi-particle transport code (FLUKA Manual)
2024

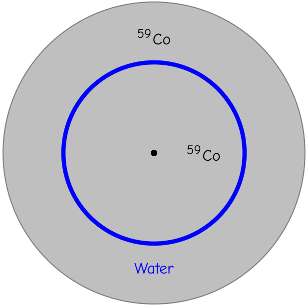
James J. Duderstadt, Louis J. Hammilton
Nuclear reactor analysis
1976

NEA report 7511
Thermal Scattering Law $S(\alpha, \beta)$: Measurement, Evaluation and Application
2020

Backup slides

Test geometry

for group- and point-wise transport validation



- Source: isotropic 20 MeV neutrons injected at the centre
- Neutron spectra are scored at all boundaries

Back

Multigroup neutron transport
Gamma generation

- Gamma generation from neutron capture reactions (n,γ) is possible only for those elements for which data are available in the ENDF
- Performed by a multigroup scheme as well
  - 42 energy bins between 1 keV and 50 MeV
- The energy of the generated photon is sampled randomly in the energy interval corresponding to its gamma group
  - Exceptions for important isotopes where a single monoenergetic photon is emitted
- Both capture gammas and gammas from inelastic reactions like (n, n') are included
- The transport is done by the ElectroMagnetic FLUKA (EMF) module
  - in the same way as all other gammas in FLUKA

Multigroup neutron transport

Energy deposition

- Energy deposited through charged particles is deposited on spot as a single value (using kerma approximation)
  - i.e., the charged particles are not generated explicitly
- Consequence:
  - no event-by-event energy deposition scoring is possible
  - = the energy deposited locally by a neutron of a given energy interacting in a given material is always the same
  - The number and energy of outgoing neutrons and photons can instead vary from interaction to interaction

- Neutrons from (n,xn) reactions are taken into account implicitly by a group-dependent probability
  - the average multiplicity of the outgoing neutrons

Multigroup neutron transport
Fission neutrons

- Fission neutrons are treated by a group-dependent fission probability
- Emitted isotropically with an energy sampled from a fission spectrum
  - appropriate for the target isotope and incoming neutron energy
- The fission neutron multiplicity is obtained separately from ENDF
- The fission fragments are not transported
  - their energy is deposited at the spot (by means of kerma factors)

- Residual nuclei are nuclei that result from a reaction and are at rest.
  - e.g., ^{28}Al after a neutron capture reaction $^{27}\mathrm{Al}(n,\gamma)^{28}\mathrm{Al}$
- Data for estimating residual nuclei production are available for all materials
  - for each energy group, there is a vector with the relative probabilities for the residual nuclei that can be produced in that group
- card: RESNUCLEi