Aalto University
School of Science
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Monte Carlo method in particle transport simulations
Lecture 3 – Interaction physics

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Topics of this lecture

Lecture topics:

- Reaction probabilities, microscopic and macroscopic cross sections
- Sampling the reaction mode: capture, fission, scattering
- Production of secondary fission neutrons
- Collision kinematics for elastic scattering

3rd programming exercise

Good background material:

https://www.reactor-physics.com/what-is-nuclear-reaction-definition/

and other pages under pull-down menu “Nuclear fission”.

Simulated random walk

The simulated random walk in Monte Carlo particle transport calculation proceeds from one interaction to the next, following a very simple procedure:

1) Sample path length (distance to next collision)
2) Transport neutron to the collision point
3) Sample interaction

If the sampled interaction is scattering, the procedure restarts from beginning by sampling the distance to the next collision. The direction and energy are changed in the scattering event.

If the sampled interaction is fission, a number of new neutrons are produced with energy and direction sampled from the associated distributions.

This lecture is focused on interaction physics, without considering the actual transport of neutrons through space. This essentially corresponds to Monte Carlo simulation in an infinite homogeneous medium.

The next lecture combines the physics routines with the geometry model discussed in Lecture 2, which allows performing transport simulations in heterogeneous geometries.

The "laws of physics" are represented by isotopic continuous-energy cross sections and probability distributions describing the emission of secondary particles.

Reaction probabilities: microscopic cross section

Interaction probability between the neutron and a single target nucleus is characterized by the microscopic cross section, σ. The total microscopic cross section can be interpreted as the effective cross-sectional area of the nucleus. The standard unit is barn: 1b = 10^{-24} cm^2.

Total cross section is the sum over partial cross sections (capture, fission, elastic, etc.):

$$\sigma_{\mathrm{tot}}(E) = \sigma_{\mathrm{capt}}(E) + \sigma_{\mathrm{fiss}}(E) + \sigma_{\mathrm{ela}}(E) + \ldots \tag{1}$$

and it represents the total collision probability between the neutron and the target.

The conditional probability of reaction mode x is simply:

$$P_x = \frac{\sigma_x(E)}{\sigma_{\mathrm{tot}}(E)} \tag{2}$$

Similar definitions are often used for total absorption, total fission, total scattering, total inelastic scattering, total non-elastic, etc. reaction modes.

Microscopic cross sections are essentially natural constants, which depend on the target nuclide, reaction type and neutron energy.[1] Scattering cross sections can also be associated with energy transfer and scattering angle, in which case the parameter is referred to as the differential scattering cross section.

[1] To be precise, the relative kinetic energy between neutron and the target.

Reaction probabilities: macroscopic cross section

Macroscopic cross section, Σ, describes the neutron interaction probability in a medium, and it is defined using the microscopic cross section σ and the nuclide density N:

$$\Sigma(\mathbf{r}, E) = N(\mathbf{r})\sigma(E) \tag{3}$$

The physical interpretation is that the total macroscopic cross section Σ_{tot} gives the total interaction probability <u>per path length</u> traveled by the neutron. The average neutron mean-free-path (mfp) in a homogeneous medium is given by $1/\Sigma_{\mathrm{tot}}$.

Similar to microscopic cross sections, total macroscopic cross section can be defined as the sum over partial reaction modes:

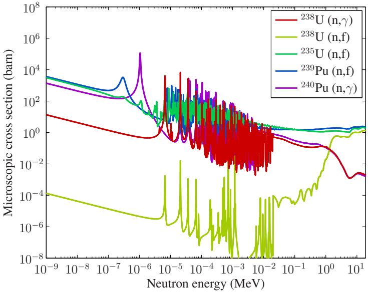
$$\begin{aligned} \Sigma_{\mathrm{tot}}(\mathbf{r}, E) &= \Sigma_{\mathrm{capt}}(\mathbf{r}, E) + \Sigma_{\mathrm{fiss}}(\mathbf{r}, E) + \Sigma_{\mathrm{ela}}(\mathbf{r}, E) + \ldots \\ &= N(\mathbf{r})\left[\sigma_{\mathrm{capt}}(E) + \sigma_{\mathrm{fiss}}(E) + \sigma_{\mathrm{ela}}(E) + \ldots\right] \end{aligned} \tag{4}$$

And if the medium consists of multiple nuclides:

$$\Sigma(\mathbf{r}, E) = \sum_i \Sigma_i(\mathbf{r}, E) = \sum_i N_i(\mathbf{r})\sigma_i(E) \tag{5}$$

where index i refers to the nuclide species and cross sections Σ and σ to any partial or total reaction mode.

Reaction probabilities: examples



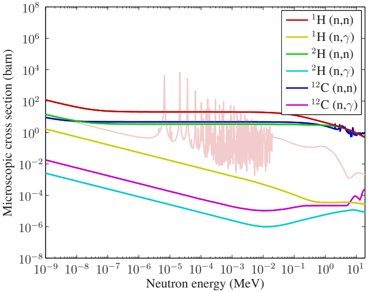


Figure 1: Microscopic cross sections of fuel and moderator isotopes. Left: fission and radiative capture cross sections of actinides. Right: elastic scattering and radiative capture cross sections of hydrogen, deuterium and ^{12}C. Capture cross section of ^{238}U is plotted in the background for comparison. Molecular and lattice bonding has a significant effect for light elements at low energy. This is not reflected in the free-atom scattering cross sections.

Reaction probabilities: examples

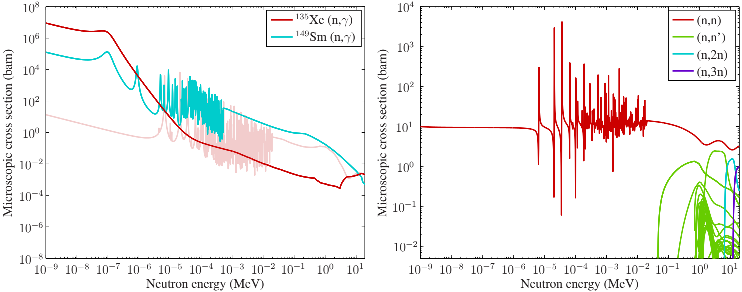


Figure 2: Left: absorption cross sections of fission product poisons. Right: elastic and inelastic scattering cross sections of ^{238}U.

Reaction probabilities: continuous-energy cross section format

One of the advantages of the Monte Carlo method is its capability to utilize cross sections in a continuous-energy format. The data is provided as energy-cross section pairs, and the resolution can be arbitrarily refined by adding more points in the energy grid.

Cross section σ at energy E is obtained from the point-wise data by linear interpolation:

$$\sigma(E) = \frac{\sigma_{j+1} - \sigma_j}{E_{j+1} - E_j}\,(E - E_j) + \sigma_j \tag{6}$$

Energy grid index j for which $E_j \leq E < E_{j+1}$ is obtained by a search algorithm (e.g. binary search).

For threshold reactions (inelastic scattering, etc.) there is a minimum energy E_{min} below which the reaction probabilities and cross sections are zero.

The current standard for storing cross sections and other nuclear and reaction data is the ENDF data format, in which each reaction mode is identified with a specific MT number (see Table 1).

Reaction probabilities: continuous-energy cross section format

Table 1: ENDF MT numbers for the most common reaction modes.

MT	Reaction
1	total
2	elastic scattering
16	(n,2n)
18	total fission (sum over partial fission channels)
51-90	inelastic scattering to discrete excited states
91	inelastic scattering to continuum
102	(n,γ)
103	(n,p)
104	(n,d)
105	(n,t)
106	(n,^{3}He)
107	(n,α)

Sampling the reaction mode

The physics routine in a Monte Carlo simulation is called after the particle has reached the collision site. The simulation proceeds to sampling the target nuclide. The probability of selecting nuclide n is given by:

$$P_n = \frac{\Sigma_n}{\Sigma} = \frac{N_n \sigma_{\mathrm{tot},n}}{\sum_i N_i \sigma_{\mathrm{tot},i}} \tag{7}$$

where Σ is the total macroscopic cross section of the medium where the collision occurs, and N and σ are the atomic densities and microscopic total cross sections of the constituent nuclides, respectively.

The selection is carried out by sampling a uniformly distributed random variable ξ on the unit interval and searching index n such that:

$$\sum_{i=1}^{n-1} \Sigma_i < \xi \Sigma \leq \sum_{i=1}^{n} \Sigma_i \tag{8}$$

Once the target nuclide is sampled, the reaction mode is selected in a similar way, using the microscopic cross sections. The probability of reaction mode x is given by:

$$P_x = \frac{\sigma_x}{\sigma_{\mathrm{tot}}} \tag{9}$$

In practice, the procedure is similar to (8).

Neutron interactions: capture

Neutron interactions can be roughly divided into three categories:

1) Capture
2) Fission
3) Scattering

Capture covers all reactions, in which the incident neutron is lost, and no secondary neutrons are emitted, for example:

- Radiative capture (MT 102):

$$ {}^{238}_{92}\mathrm{U} + {}^{1}_{0}\mathrm{n} \longrightarrow {}^{239}_{92}\mathrm{U} + \gamma \tag{10} $$

- Alpha emission (MT 107):

$$ {}^{10}_{5}\mathrm{B} + {}^{1}_{0}\mathrm{n} \longrightarrow {}^{7}_{3}\mathrm{Li} + {}^{4}_{2}\mathrm{He} \tag{11} $$

- Proton emission (MT 103):

$$ {}^{3}_{2}\mathrm{He} + {}^{1}_{0}\mathrm{n} \longrightarrow {}^{3}_{1}\mathrm{H} + {}^{1}_{1}\mathrm{H} \tag{12} $$

In analog Monte Carlo, capture terminates the neutron history. Capture can also be handled implicitly, by reducing the statistical weight of the neutron according to the capture probability.[2]

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[2] See Lux & Koblinger, Chapter 3/II.B.

Neutron interactions: fission

Fission (MT 18) terminates the history and a number of new neutrons are emitted. The typical method for sampling the number of fission neutrons is to take the average fission neutron yield $\overline{\nu}$, truncate the value to the nearest integer n, and include one extra neutron if:

$$\xi < \overline{\nu} - n \tag{13}$$

where ξ is a uniformly distributed random number on the unit interval.

The direction of emitted neutrons is sampled isotropically,[3] and the energy distribution follows the Maxwell:

$$f(E) = C_0 \sqrt{E} e^{-E/T} \tag{14}$$

or Watt:

$$f(E) = C_0 e^{-E/a} \sinh \sqrt{bE} \tag{15}$$

fission spectrum, where C_0 is a normalization constant and T, a and b depend on the fissioned nuclide and the incident neutron energy. In most recent evaluated nuclear data files the fission spectra are given as tabular distributions.

Secondary fission neutrons are stored in a "bank", which is a data structure that holds the position, direction, energy and time of each new particle. The transport routine retrieves particles from the bank, and moves on to the next source particle when the bank is empty.

[3] For an algorithm for sampling the direction vector from an isotropic distribution see Lux & Koblinger, Chapter 2/I.J.

Neutron interactions: fission

Algorithm 1 Sampling from a Maxwellian energy distribution

input: T ▷ Distribution parameter (nuclear temperature)
do
    Sample ξ_1 and ξ_2 ▷ Sample two random numbers on the unit interval
    $R \leftarrow \xi_1^2 + \xi_2^2$
while $R > 1$
Sample ξ_3 and ξ_4 ▷ Sample two random numbers on the unit interval
$E \leftarrow -T(\xi_1^2 \log(\xi_3)/R + \log(\xi_4))$ ▷ Calculate final energy
output: E ▷ Energy sampled from Maxwellian distribution

Notes:

- The algorithm is from MCNP4C manual, page 2-44.
- Nuclear temperature T can be set to 1.2895 MeV for ^{235}U fission.
- The same algorithm can be used to sample target energies for the free-gas model, in which case T is the material temperature in MeV (Temperature in Kelvin multiplied by Boltzmann constant k = 8.6167$\cdot 10^{-11}$ MeV/K).

Neutron interactions: fission

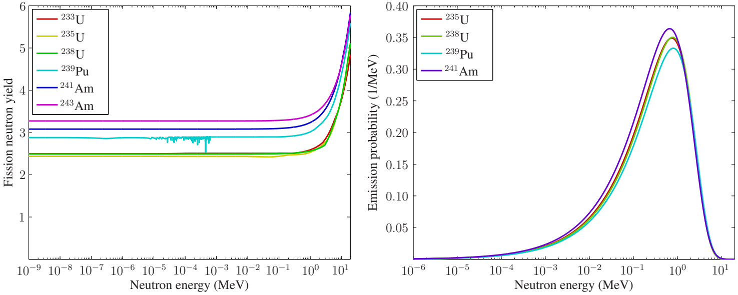

Figure 3: Left: Fission neutron yields of various actinides as function of neutron energy. The yield is actually a linear function of energy, which only appears to increase sharply in the MeV-range because of the logarithmic scale. The number of emitted neutrons increases along with actinide mass.
Right: The Maxwellian energy distributions of ^{235}U, ^{238}U, ^{239}Pu and ^{241}Am fission neutrons. The peak position varies slightly for different actinides, but is practically independent of neutron energy. The average energy for ^{235}U fission neutrons is around 2 MeV.

Neutron interactions: scattering

Scattering includes all elastic and inelastic reaction modes in which the incident neutron is not lost. Additional neutrons may be produced in multiplying (n,2n), (n,3n), etc. reactions. In Monte Carlo simulation, scattering is handled by sampling a new direction and energy for the collided neutron and continuing the random walk.[4]

In two-particle collisions the scattering angle is coupled to energy transfer by conservation of energy and momentum. In such case, it is sufficient to sample the scattering angle and calculate the corresponding value for energy on-the-fly.

This is not the case for:

- Neutron-multiplying reactions: (n,2n), (n,3n), etc.
- Reactions where additional particles are emitted: (n,np), (n,nα)
- Continuum inelastic scattering (no discrete Q-value)

and the solution is to sample energy and angle from their own distributions, which preserve the conservation laws on the average.

[4] The additional neutrons emitted in multiplying scattering reactions are banked and their random walk is simulated once the original history is completed. In implicit Monte Carlo simulation the multiplication can be accounted for by increasing the neutron weight.

Neutron interactions: scattering

The most common interaction in reactor applications is elastic scattering (MT 2), which in LWR's constitutes over 90% of all interactions. Accurate modeling of collision kinematics is therefore absolutely essential for neutron slowing-down and thermalization.

Handling of elastic scattering can be divided into three different approximations:

1) Scattering from stationary nuclides
2) Scattering with free-gas model
3) Thermal scattering from bound moderator nuclides

The collision kinematics is best understood by defining three coordinate systems:

1) Laboratory frame-of-reference (L-frame), where the coordinates are fixed to the geometry
2) Target-at-rest frame-of-reference (T-frame), where the coordinates are fixed on the target
3) Center-of-mass frame-of-reference (C-frame), where the coordinates are fixed on the center-of-mass of the neutron-target system

The center-of-mass frame of reference is a coordinate system where the total momentum of the neutron-target system is zero, and <u>neutron kinetic energy is preserved in elastic scattering</u>.

In the execises it is assumed that all scattering is isotropic in the C-frame.

Neutron interactions: scattering

Handling of elastic scattering is greatly simplified by the fact that the reaction is in most cases isotropic in the C-frame.[5]

The relation between neutron L-frame and C-frame velocities can be written as:

$$\mathbf{v}_\mathrm{C} = \mathbf{v}_\mathrm{L} - \mathbf{V}_\mathrm{CM} \tag{16}$$

where the center-of-mass velocity is given by:

$$\mathbf{V}_\mathrm{CM} = \frac{\mathbf{v}_\mathrm{L} + A\mathbf{V}_\mathrm{L}}{1 + A} \tag{17}$$

where $\mathbf{V}_\mathrm{L}$ is the target velocity in L-frame and A is the atomic weight ratio, i.e. the ratio of the target mass M to neutron mass m:

$$A = \frac{M}{m} \tag{18}$$

When elastic scattering is assumed isotropic in C-frame:

- Neutron speed $|\mathbf{v}_\mathrm{C}|$ is not changed (kinetic energy is preserved)
- New direction can be sampled isotropically

In the case of anisotropic scattering, the scattering angle μ is sampled and the new direction vector is randomly rotated over the azimuthal angle.

[5] This is a good approximation for hydrogen, but it also applies to heavier nuclides away from resonances.

Neutron interactions: scattering

The procedure for C-frame isotropic inelastic level-scattering is very similar, but some fraction of the initial kinetic energy is lost to the excited state of the target nucleus.[6]

From the conservation of energy and momentum it follows that the neutron speeds before and after the collision are related by:

$$|\mathbf{v}_{\mathrm{C}}'| = \sqrt{\mathbf{v}_{\mathrm{C}}^2 + \frac{2AQ}{(A+1)m}} \tag{19}$$

where Q is the energy of the excited state. Similar to the elastic case, the C-frame direction can be sampled randomly when the reaction is isotropic.

After the procedure for elastic or inelastic level scattering is completed, a coordinate transformation is made back to L-frame:

$$\mathbf{v}_{\mathrm{L}}' = \mathbf{v}_{\mathrm{C}}' + \mathbf{V}_{\mathrm{CM}} \tag{20}$$

and the tracking continues.

NOTE: It is important to note that scattering isotropy in C- and L-frame are two completely different concepts. Scattering from hydrogen is an anisotropic reaction in the L-frame, which is easy to see by considering the collision between two billiard balls (the ball hitting a stationary target ball cannot bounce backwards).

[6] Level-scattering refers to an inelastic reaction in which the target is left at an excited state. Cross sections for each excited level are provided separately, and unresolved levels summed into a single "continuum" channel.

Neutron interactions: scattering

When the neutron collides at high energy, the velocity of the target can be approximated as zero.

The probability of up-scattering increases as the neutron is slowed down, and the stationary target approximation becomes poor when the neutron velocity is comparable to thermal motion.

A better approximation is then the free-gas model, which essentially means that the target velocity is sampled from a Maxwellian-based distribution before the collision: [7]

$$f(V, \mu) = C_0 v_{\mathrm{T}} V^2 e^{-\gamma^2 V^2} \tag{21}$$

where C_0 is a normalization constant,

$$\gamma = \sqrt{\frac{M}{2kT}} \tag{22}$$

and M is the target mass, k is the Boltzmann-constant and T is the temperature of the medium.

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[7] The difference between Eq. (21) and the Maxwell-Boltzmann distribution for speed is term v_{T}, which is the neutron speed in T-frame, i.e. the relative speed between the neutron and the target:

$$v_{\mathrm{T}} = \|\mathbf{v}_{\mathrm{L}} - \mathbf{V}\| = \sqrt{v_{\mathrm{L}}^2 + V^2 - 2v_{\mathrm{L}} V \mu} \tag{23}$$

where $\mu = \cos\theta$ is the cosine of the angle between the two velocity vectors.

Neutron interactions: scattering

NOTE: In the exercises it is assumed for simplicity that the kinetic energy of the target follows the Maxwell-Boltzmann distribution, i.e. (21) without multiplier (23).

Algorithm 2 Elastic scattering with free-gas model

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if $E < E_{\mathrm{fg}}$ **then** ▷ Check if free-gas model should be used
    $E \leftarrow f_{\mathrm{MB}}(T)$ ▷ Sample target energy from Maxwellian distribution at temperature T
    $V \leftarrow \sqrt{2E/M}$ ▷ Calculate target speed and sample direction randomly
else
    $V \leftarrow 0$ ▷ Ignore target motion
end if
$\mathbf{V}_{\mathrm{CM}} \leftarrow (\mathbf{v}_{\mathrm{L}} + A\mathbf{V}_{\mathrm{L}})/(1 + A)$ ▷ Calculate center-of-mass velocity
$\mathbf{v}_{\mathrm{C}} \leftarrow \mathbf{v}_{\mathrm{L}} - \mathbf{V}_{\mathrm{CM}}$ ▷ Coordinate transformation from L- to C-frame
$\hat{\mathbf{\Omega}}_{\mathrm{C}} \leftarrow$ [isotropic] ▷ Sample direction isotropically
$\mathbf{v}'_{\mathrm{L}} \leftarrow \mathbf{v}'_{\mathrm{C}} + \mathbf{V}_{\mathrm{CM}}$ ▷ Coordinate transformation from C- to L-frame

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The free-gas model can be omitted when the target is heavier than hydrogen and neutron energy is above $\sim$200 eV.

Inelastic scattering is a threshold reaction that (typically) occurs well above 200 eV, and can be handled without the free-gas model.

Neutron interactions: scattering

The free-gas approximation is capable of modeling up-scattering and the collection of neutrons in the thermal region, but the model has two limitations:

1) Approximating scattering as a collision between two free particles fails when the neutron energy is comparable to the molecular and lattice binding energies of the target
2) The distribution of target velocity given by (21) assumes that the cross section is constant within the range of relative energy between the neutron and the target, which is a poor approximation near low-energy resonances

Molecular and lattice binding effects become important in moderator materials, such as light and heavy water and graphite, and they can be accounted for by using scattering laws with explicit cross sections and energy and angular distributions in the thermal region.

The second problem can be taken into account using the so-called Doppler-broadening rejection correction (DBRC) method, which is beyond the scope of this course.

Neutron interactions: scattering

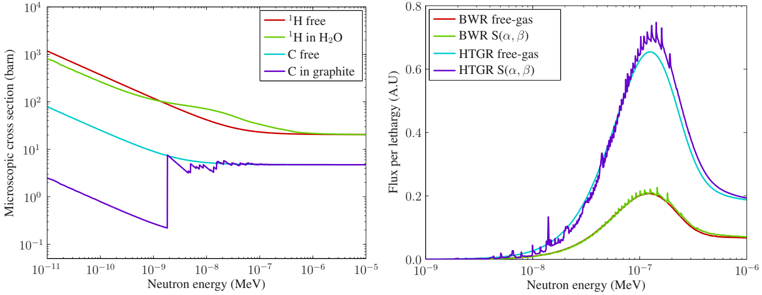

Figure 4: Left: Free-atom elastic scattering cross sections of ^{1}H and carbon compared to corresponding bound-atom cross sections in light water and graphite (all cross sections at 300 K). The secondary angular and energy distributions are given using so-called S(α, β) scattering laws. Right: thermal peak formed in water (BWR) and graphite (HTGR) in a Monte Carlo neutron transport simulation using the free-gas model and explicit thermal scattering laws (600 K temperature). The peaks in the distributions are not physical, but rather the result of sampling from discrete energy-angle distributions.

3rd programming exercise

The main goal in the 3rd programming exercise is to implement the physics routine for neutron interactions. The tasks involve simulation of neutron histories starting from a given distribution until all neutrons are absorbed. The geometry is assumed infinite and homogeneous (no coupling to geometry routine).

Cross sections are provided in ASCII files with simple format:[8]

```
SYM Z A AW T
NNU
E1 NU1
E2 NU2
...
MT1 Q1 NE1
E1 XS1
E2 XS2
...
MT2 Q2 NE2
...
```

The first line gives the nuclide symbol, proton number, mass number, atomic weight and temperature in Kelvin. This is followed by fission nubar data (number of energy-nubar pairs and values) and the reactions (MT number, Q-value, number of energy-cross section pairs and values).

Energy distribution of fission neutrons is assumed to follow the maxwellian ^{235}U fission spectrum and the directional distribution is isotropic.

[8] http://virtual.vtt.fi/virtual/montecarlo/misc/PHYS-E0565/

3rd programming exercise

Mandatory tasks:

- Implement an input routine that reads cross section data in the previously described format. Extract the following cross sections and plot the data using Matlab (or similar):
  1) Microscopic total cross sections of ^{1}H and ^{16}O
  2) Microscopic fission and radiative capture cross sections of ^{235}U and ^{238}U
  3) Microscopic inelastic scattering cross sections of ^{238}U
  4) Macroscopic total cross sections of water and natural uranium (0.72% ^{235}U, 99.28% ^{238}U)

  The data should be plotted in 4 figures, using log-log scale and 500 energy points log-uniformly distributed between 1E-11 and 20.0 MeV.
- Implement the simplified random walk procedure (no geomery) described on Slide 3 and the physics routines to handle capture, fission and elastic scattering, including the production of secondary fission neutrons and free-gas model for elastic scattering.
- Simulate the slowing-down of 14 MeV neutrons in pure hydrogen (^{1}H) and deuterium (^{2}H). Calculate the average neutron energy as function of collisions. Plot and explain the results (use log-scale for energy).
- Simulate the multiplication of 1 MeV neutrons in uranium oxide (UO_2) comprised of pure ^{238}U and natural uranium. Calculate the average total number of fission neutrons produced per each source neutron. Repeat the calculation for a 50/50 molar mixture of natural uranium and water. Explain the results.

3rd programming exercise

Bonus tasks:

1. Calculate the average number of sampled reactions (per nuclide and reaction mode) in the previous cases and the associated relative statistical errors. (+1 point)
2. Include inelastic level scattering in the physics routine and repeat the calculation involving neutron multiplication. Report the differences. (+1 point)
3. Find a rough estimate for the critical enrichment of ^{235}U in homogeneous uranium and 50/50 molar mixture of uranium and water. The system is critical when multiplication becomes infinite (plot results on a curve and extrapolate). (+2 points)
4. Add time-dependence in the simulation by sampling the distance between collisions from:

$$l = -\log(\xi)/\Sigma_{\mathrm{tot}} \tag{24}$$

   where Σ_{tot} is the macroscopic total cross section and ξ is a uniformly distributed random variable on the unit interval. Plot the number of emitted fission neutrons as function of time in a homogeneous medium consisting of natural uranium and uranium enriched to 50% ^{235}U. (+3 points)
5. Evaluate k_{eff} and the terms in the four-factor formula (google) for a 50/50 molar mixture of natural uranium and water. (+3 points)

3rd programming exercise

Milestones:

- Implementation of physics routines needed later for neutron transport simulation.
- Expanding input routine to read cross section data.

Tips:

- The average relative energy loss in C-frame isotropic elastic scattering from a stationary target is:
$$\frac{\Delta E}{E_0} = \frac{1-\alpha}{2} \tag{25}$$
where
$$\alpha = \left(\frac{1-A}{1+A}\right)^2 \tag{26}$$
and A is defined in (18). This result is useful for checking that the elastic scattering routine works as expected. The expected shapes of the slowing-down curves are plotted in Figure 5.
- Simulating super-critical systems (infinite multiplication) requires applying a time or generation cut-off to terminate expanding fission chains.

3rd programming exercise

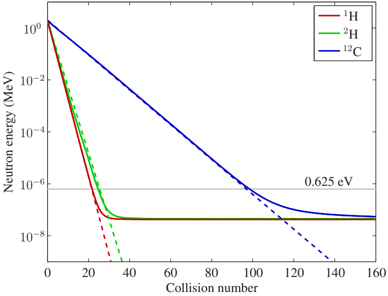

Figure 5: Average energy of fission neutrons slowed down by collisions from different light nuclides. Slowing-down curves predicted by Eq. (25) are plotted with dashed lines. The moderator is at 300K temperature, and the slowing-down process is terminated by up-scattering when the neutron energy is comparable to thermal motion of the collision targets. NOTE: The curves were calculated using the Serpent code, applying a model that slightly differs from the one used in the exercises.