22.211 Lecture 2

Neutron Slowing Down

Benoit Forget

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Outline

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Objectives

- Elastic scattering
- Definition of lethargy
- Elastic scattering kernel by generation
- Basic Monte Carlo for slowing down

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1. Objectives
2. Elastic scattering
3. Basic Monte Carlo
4. Slowing down

Relating energy and angle between Lab and CM

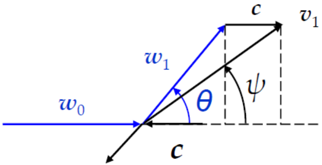
From energy and momentum conservation principles, we can relate the change in angle in the CM to the change of angle in the LAB and the change in energy (under the assumption of stationary target). We find

$$\mu = \frac{1 + A\eta}{\sqrt{1 + A^2 + 2A\eta}}$$

and

$$\frac{E_1}{E_0} = \frac{A^2 + 1 + 2A\eta}{(A+1)^2}$$

What are the energy loss limits?



Isotropic scattering in CM

$$p(\theta)d\theta = \frac{A_{ring}}{A_{sphere}} = \frac{2\pi(rsin\theta)(rd\theta)}{4\pi r^2}$$

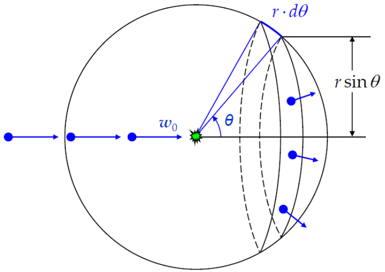
$$p(\theta)d\theta = \frac{1}{2}sin\theta d\theta$$

change of variable

$$\eta = cos(\theta) \quad p(\eta)d\eta = -p(\theta)d\theta$$

which yields

$$p(\eta)d\eta = -\frac{1}{2}sin\theta d\theta = \frac{1}{2}d(cos\theta) = \frac{1}{2}d\eta$$



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Energy distribution

There is a one-to-one relation between post collision energy and the cosine of the scattering angle. Our goal is to relate the isotropic distribution function in the CM to a relation in energy in the lab.

$$p(E)dE = p(\eta)d\eta$$

Isotropic in CM means

$$p(\eta)d\eta = \frac{1}{2}d\eta \Rightarrow \frac{d\eta}{dE} = \frac{(A+1)^2}{2AE_0}$$

which implies

$$p(E) = \frac{(A+1)^2}{4AE_0} = \frac{1}{(1-\alpha)E_0}$$

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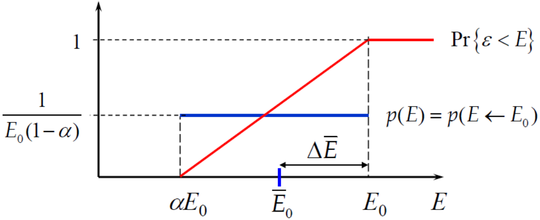
Scattering kernel



We can also calculate the average energy post-collision and average energy loss.

$$\bar{E} = \frac{1+\alpha}{2}E_0 \quad \overline{\Delta E} = \frac{1-\alpha}{2}E_0$$

Lethargy space

Lethargy is defined as

$$u = ln\left(\frac{E_{ref}}{E}\right)$$

E_{ref} is commonly set to the maximum energy of a library (i.e. 10-20 MeV), this ways u is always positive and increases as E decreases.

$$u_1 - u_0 = -ln\left(\frac{A^2 + 1 + 2A\eta}{(A+1)^2}\right) \qquad p(u \rightarrow u') = \frac{e^{-u}}{1-\alpha}$$

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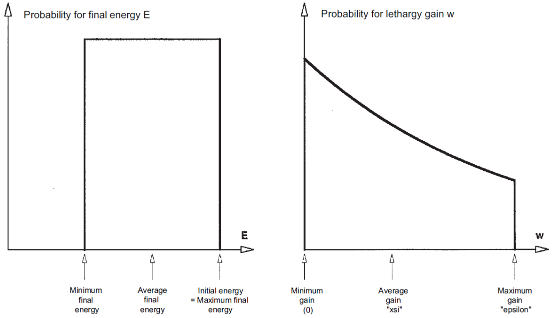
Scattering kernel - lethargy



Maximum Lethargy gain

Maximum energy loss or lethargy gain happens for $\eta = -1$

$$u_1 - u_0 = -ln\left(\frac{A^2 + 1 + 2A\eta}{(A+1)^2}\right)$$

thus the maximum lethargy gain becomes

$$\Delta u_{max} = -ln\left(\frac{A^2 + 1 - 2A}{(A+1)^2}\right) = -ln\left(\frac{(A-1)^2}{(A+1)^2}\right) = -ln\alpha$$

Average Logarithmic Energy Loss

A useful quantity that we can calculate is

$$\xi = \overline{ln\frac{E_0}{E}} = \frac{\int_{E_0}^{\alpha E_0} ln\frac{E_0}{E} p(E)dE}{\int_{E_0}^{\alpha E_0} p(E)dE} = 1 + \frac{\alpha}{1-\alpha} ln\alpha$$

where

$$\alpha = \left(\frac{A-1}{A+1}\right)^2$$

This expression does not depend on the initial energy, and thus applied to any scattering collision during the slowing down. It thus allows us to approximate the average number of collisions needed to scatter down from E_0 to an energy E_n

$$n \approx \frac{1}{\xi} ln\frac{E_0}{E_n}$$

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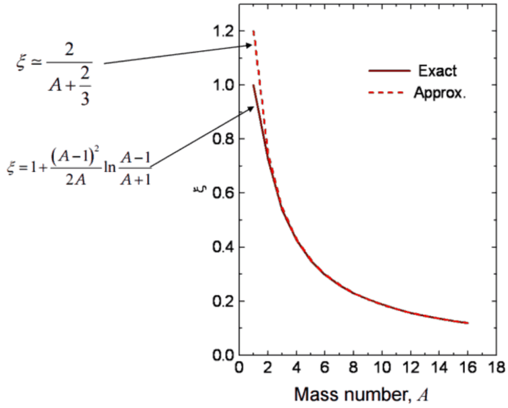
Approximating ξ

$$\xi \simeq \frac{2}{A+2/3} \quad \text{for } A>10$$



Courtesy of www.nuclear-power.net

Collisions to thermal

Element	A	ξ	Collisions 2 MeV→1eV
H	1	1	15
D	2	0.750	20
H_2O	-	0.920	16
D_2O	-	0.509	29
He	4	0.425	34
Be	9	0.207	70
C	12	0.158	92
O	16	0.120	121
Na	23	0.084	172
Fe	56	0.035	414
^{238}U	238	0.008	1812

Courtesy of www.nuclear-power.net

Moderator Selection

Computing ξ for a molecule

$$\bar{\xi} = \frac{1}{\Sigma_s} \sum \xi_i \Sigma_{si}$$

Element	A	ξ	Collisions 2 MeV→1eV	MSDP	MR
H_2O	-	0.920	16	1.35	71
D_2O	-	0.509	29	0.176	5670
Be	9	0.207	70	0.158	143
C	12	0.158	92	0.060	192

Courtesy of www.nuclear-power.net

Average Collision Angle - CM

$$\eta = cos(\theta)$$

$$\bar{\eta} = \int_{-1}^{1} \eta p(\eta) d\eta$$

$$\bar{\eta} = \int_{-1}^{1} \eta \frac{1}{2} d\eta = 0$$

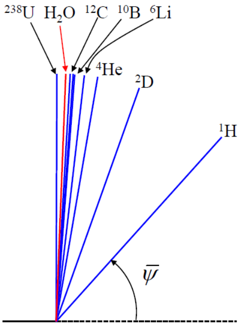
$$\mu = cos(\psi) \quad \bar{\mu} = \int_{-1}^{1} \mu p(\mu) d\mu$$

we know that

$$p(\mu)d\mu = p(\eta)d\eta \qquad \mu = \frac{1 + A\eta}{\sqrt{1 + A^2 + 2A\eta}}$$

thus

$$\bar{\mu} = \int_{-1}^{1} \frac{1 + A\eta}{\sqrt{1 + A^2 + 2A\eta}} \frac{1}{2} d\eta = \frac{2}{3A}$$



When can we assume target at rest?

$$E = \frac{1}{2}mv^2 \qquad v = \sqrt{\frac{2E}{m}}$$

- mass of a neutron is 1.675×10^{-27} kg
- mass of a proton is 1.673×10^{-27} kg
- energy of most probable velocity of a Maxwellian is kT, which is 0.0253 eV at 293K
- coolant temperature of 565K in PWR, roughly 0.05 eV
- In a PWR, the velocity of an hydrogen atom is about 3000 m/s (O-16 is a factor of 4 slower).
- A 10 eV neutron has a velocity of about 43000 m/s (14 times faster)

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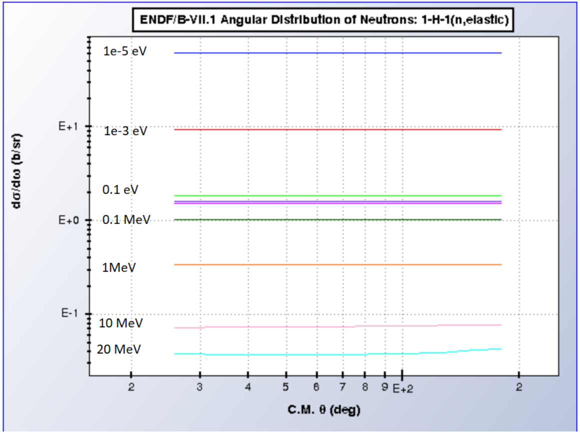
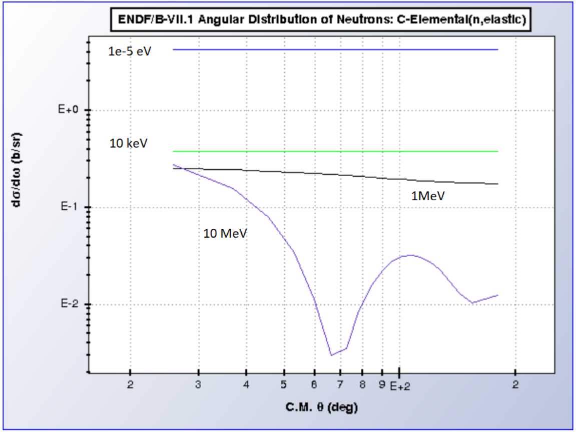
When can we assume isotropic in CM? For H-1

Elastic scattering is nearly isotropic at all energies of interest for H-1



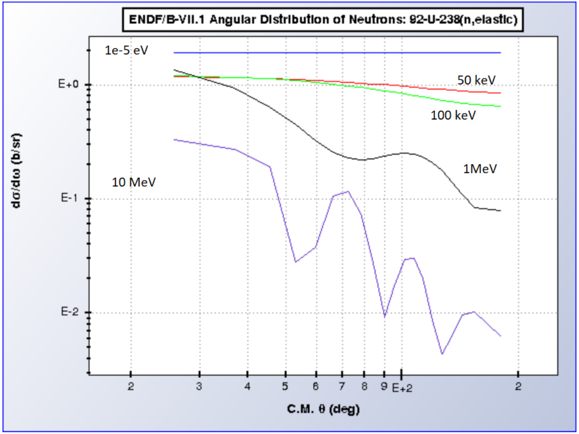
Angular Distribution C-12

Elastic scattering is nearly isotropic at all energies of interest for C-12



Angular Distribution U-238

Elastic scattering is isotropic for U238 in the thermal range



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Random Number Generators

- Numbers are not random; a sequence of numbers can be.
- Truly random sequences are not always desirable
  - Physical generators can create truly random sequences
    - Counting decays of a radioactive source
    - Tapping into electrical noise
  - Lack of reproducibility creates problems when debugging and when making (anti-) correlated computations.
- Pseudo-random sequences are most often used
  - Deterministic process that imitates random sequence
  - Must pass a series of randomness tests

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Linear Congruential Generator

Most common pseudo-random number generators used in particle are LCGs.

- Well-understood and robust
- Simple and fast

$$S_{i+1} = (S_i \cdot g + c) \bmod p$$

- S_0 is the seed
- g is the multiplier
- c is the adder
- p is the modulus (usually a basis of 2)

How it works

- Select an initial seed (S_0) - integer
  - Calculate random number $r_k = S_k/p$
    - r_k will always be a real between 0 and 1
  - Calculate S_{k+1}

$$S_{k+1} = (S_k \cdot g + c) \bmod p$$

  - Iterate

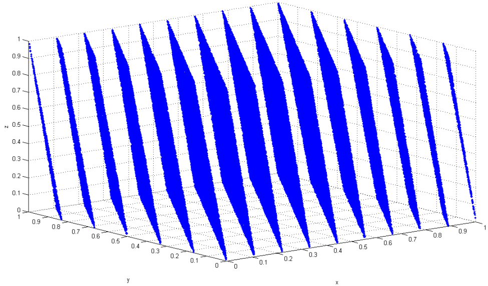
Example 1

Using parameters $g = 47, c = 1, S_0 = 1, p = 100$

$$
\begin{aligned}
s_0 &= 1 \\
s_1 &= (47 \cdot 1 + 1) \bmod 100 && = 48 \bmod 100 && = 48 && r_0 = 0.48 \\
s_2 &= (47 \cdot 48 + 1) \bmod 100 && = 2257 \bmod 100 && = 57 && r_0 = 0.57 \\
s_3 &= (47 \cdot 57 + 1) \bmod 100 && = 2680 \bmod 100 && = 80 && r_0 = 0.80 \\
s_4 &= (47 \cdot 80 + 1) \bmod 100 && = 3761 \bmod 100 && = 61 && r_0 = 0.61 \\
s_5 &= (47 \cdot 61 + 1) \bmod 100 && = 2868 \bmod 100 && = 68 && r_0 = 0.68 \\
s_6 &= (47 \cdot 68 + 1) \bmod 100 && = 3197 \bmod 100 && = 97 && r_0 = 0.97 \\
s_7 &= (47 \cdot 97 + 1) \bmod 100 && = 4560 \bmod 100 && = 60 && r_0 = 0.60
\end{aligned}
$$

RANDU

Not all LCGs are created equal!



Monte Carlo Sampling

Elastic Scattering is a uniform distribution between $[\alpha E_0, E_0]$. You can sample an energy using a random number ξ that is uniform between $[0, 1]$ using the following relation

$$E = (E_0 - \alpha E_0) \times \xi_1 + \alpha E_0$$

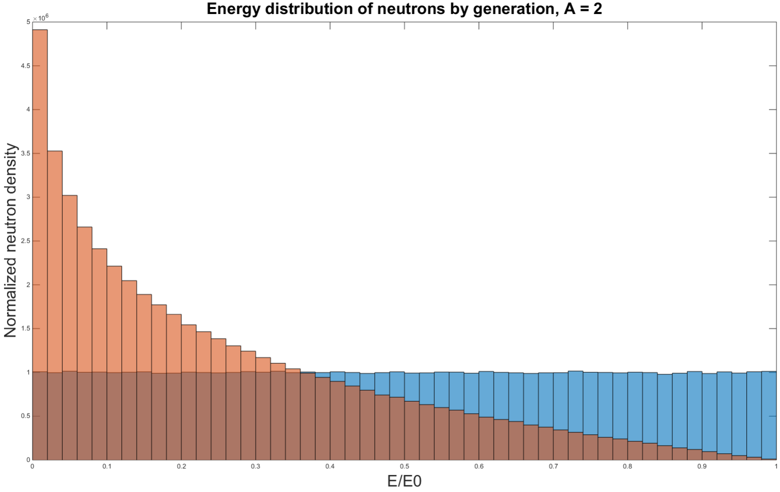
If an isotropic angle is desired, this corresponds to sampling from two uniform distributions, one between $[0, 2\pi]$ for the azimuthal angle, and another between $[-1, 1]$ for the cosine of the polar angle.

$$\phi = 2\pi \times \xi_2$$

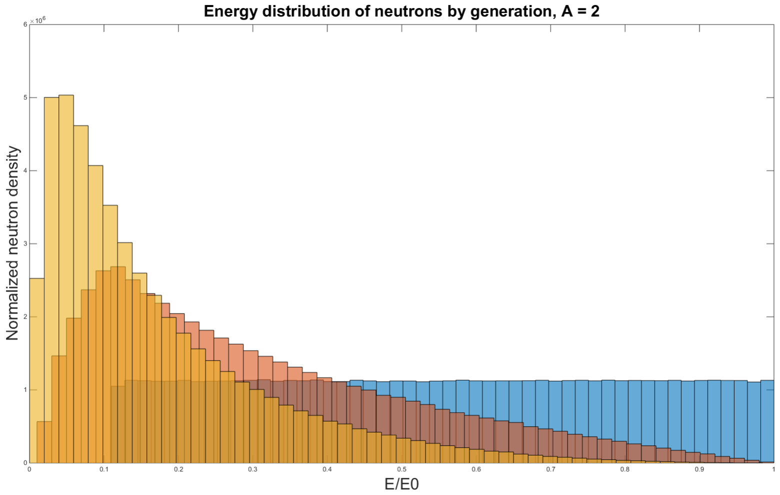
$$\mu = 2 \times \xi_3 - 1$$

Outline

Slowing by generation - H1



Slowing by generation - H2



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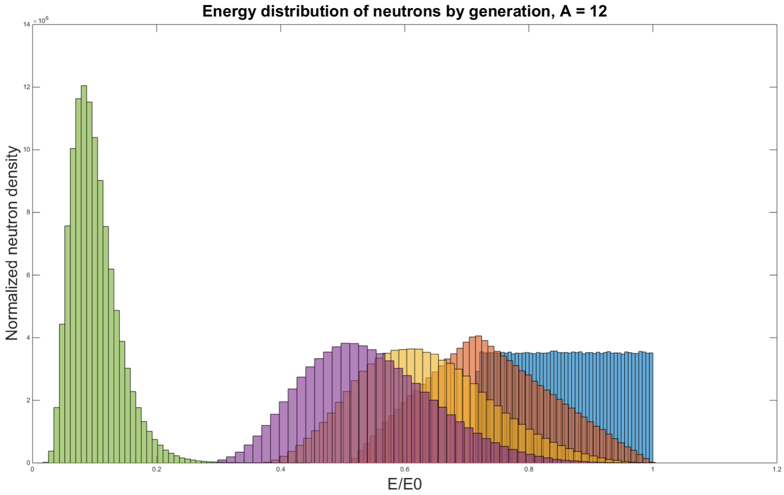
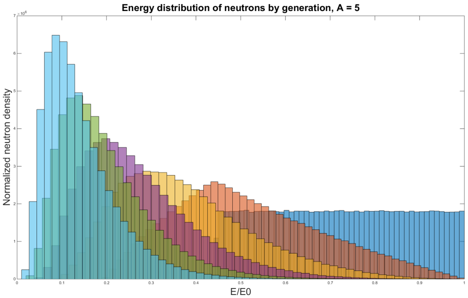
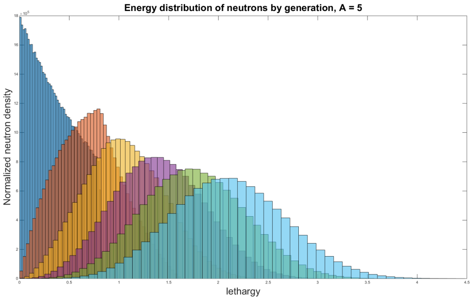
Slowing by generation - C12



Why use lethargy?

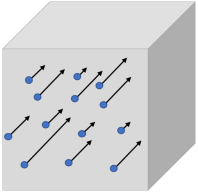




Neutron Flux

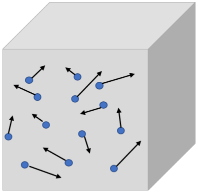
Mathematically, it is defined as the neutron density multiplied by the velocity (units of neutrons/cm^2.s).

The angular flux only keeps track of neutrons going in the solid angle.



$$\psi(\vec{r}, \vec{\Omega}, E)$$

The scalar flux keeps track of all neutrons regardless of direction.



$$\phi(\vec{r}, E) = \int \psi(\vec{r}, \vec{\Omega}, E) d\vec{\Omega}$$

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What are Tallies?

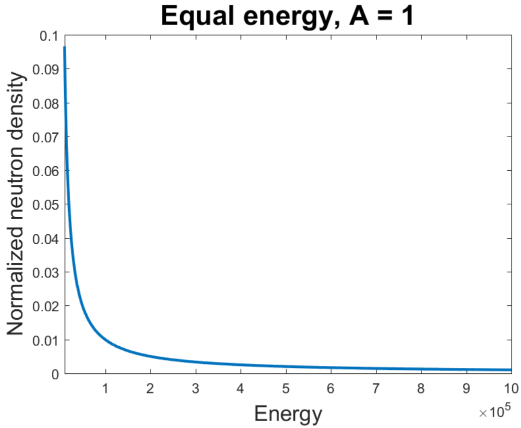
- Tally: A current score or amount.
- A Monte Carlo simulation tracks particles through a random walk. This random walk includes travel through many cells, materials and boundaries.
- During a history (i.e. 1 random walk), we will tally events of interest (e.g. reaction rates, energy deposition, flux, ...)
- After the history is complete, compute total score and its square.
- After all histories are complete, compute sample mean and sample variance

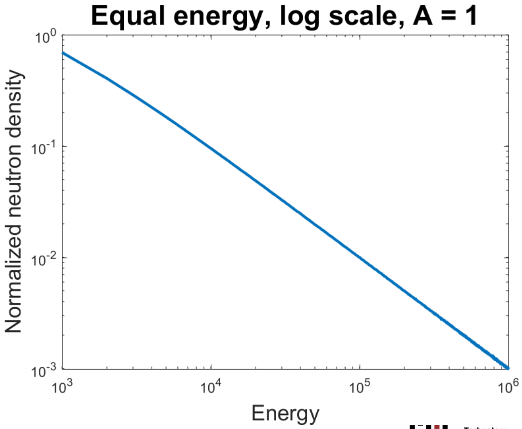
Flux Tally - Collision

- Using the collision approach to evaluate reaction rates, we can also define an alternate flux estimator
- For each collision in the volume of interest, sum the neutron weight divided by the total macroscopic cross-section
- Divide by the cell volume and the total starting weight.

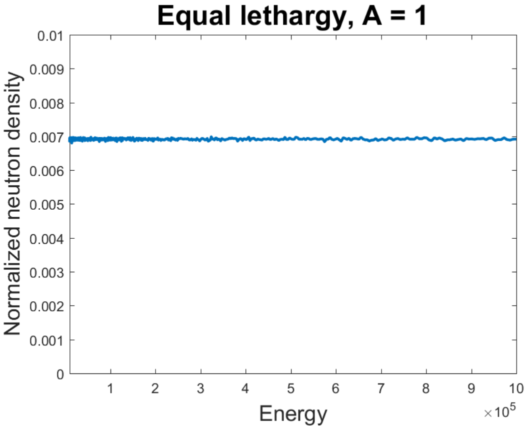
$$\phi = \frac{1}{V}\frac{1}{W}\sum_{\text{all n collisions in cell}} \frac{wgt_j}{\Sigma_t}$$

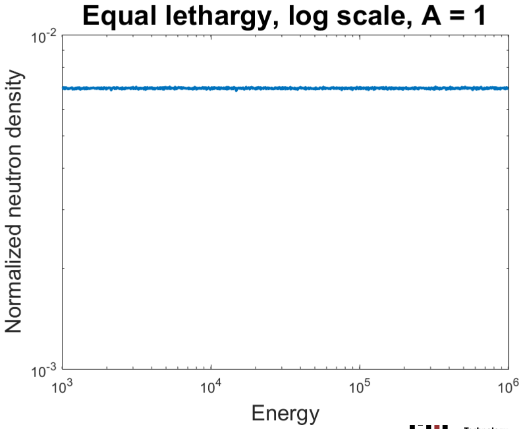
1/E flux - Energy Spacing - H1





1/E flux - Lethargy Spacing - H1





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