Reconstruction of Neutron Cross-sections and Sampling

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Outline

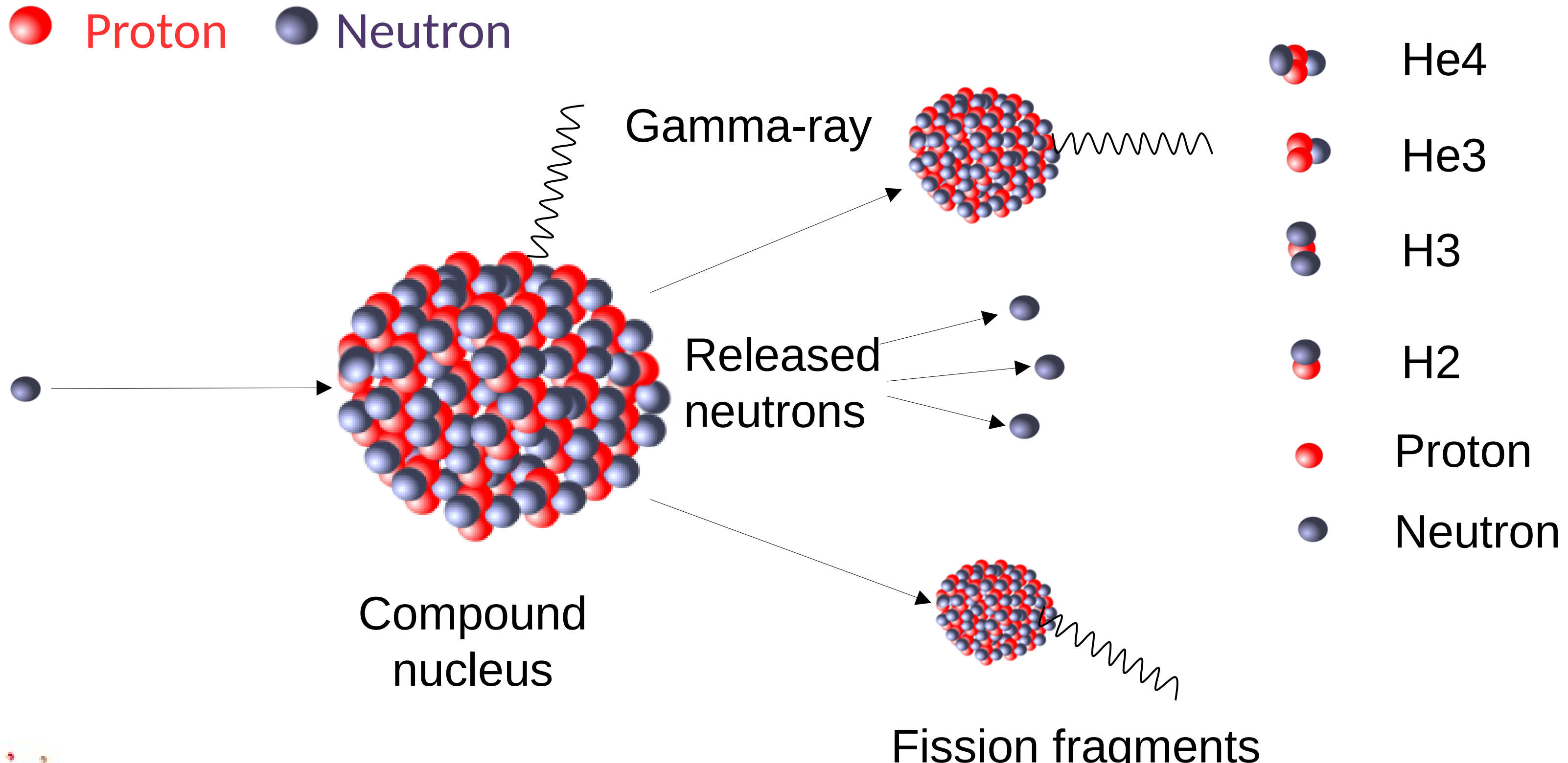
- Introduction
- Reconstruction of resonance cross-section
- Linearization of cross-section
- Unionization
- Doppler broadening at higher temperature
- Sampling
- Independent angular distribution
- Independent energy distribution
- Energy-angle correlated distribution
- Fission fragments and fission neutrons
- Summary

Introduction: Importance of low energy neutrons

- Most of the neutron applications are in low energy region (<20MeV) i.e. material studies/diffraction, fusion and fission reactors, Nuclear medicine, Radiation dosimetry in accelerator and nuclear devices etc.
- Low energy neutron transport takes significant time in hadron transport because of charge neutrality.
- Radiation dosimetry and shielding calculations in GEANT4 is not comparable with experimental data.

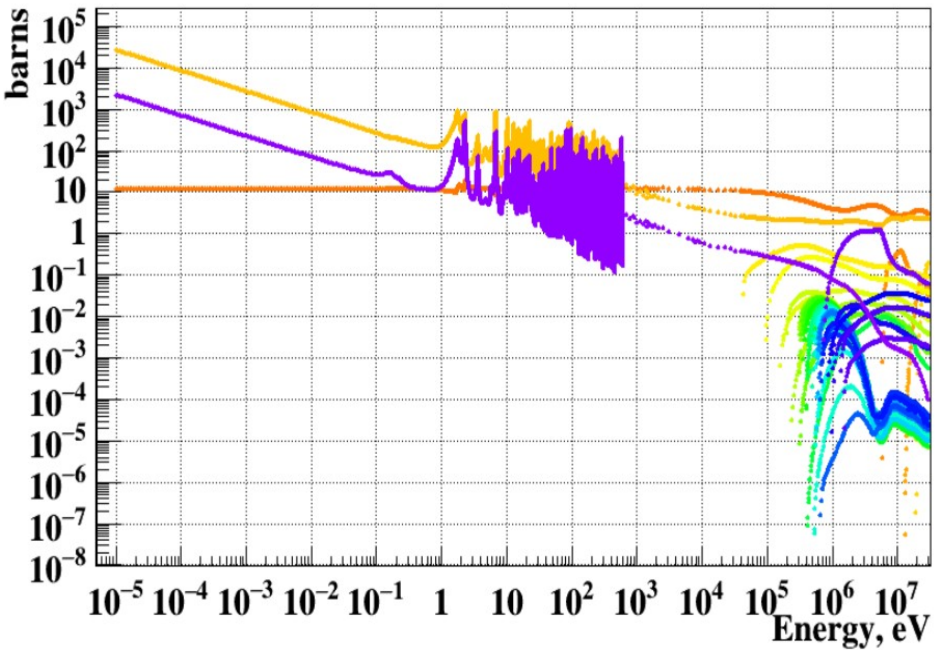
Introduction: Compound nucleus reactions

- The absence of coulomb barrier between neutron and nucleus as compared to charge particles makes neutron interactions special.
- It can penetrate deep inside the nucleus even at meV energies.

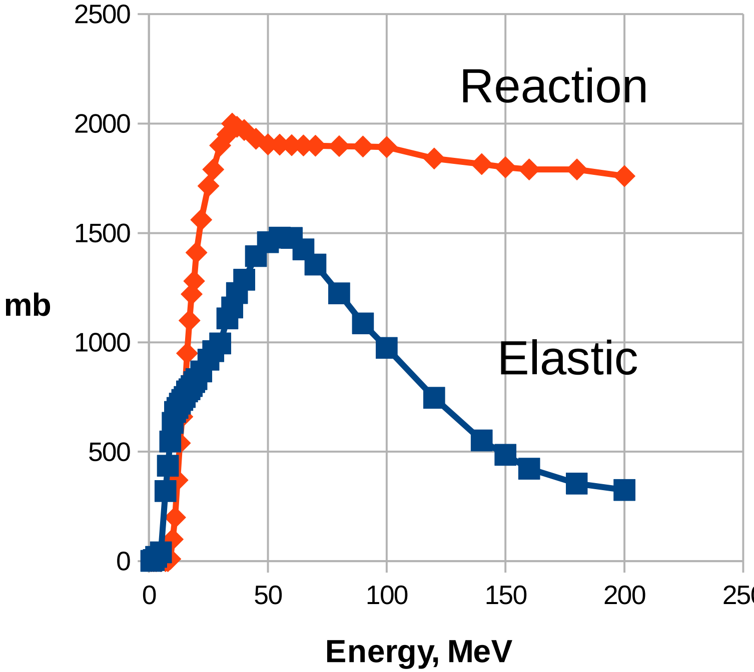


Introduction: neutron and proton cross-sections

Neutron interactions below 20MeV or 200MeV in some cases.

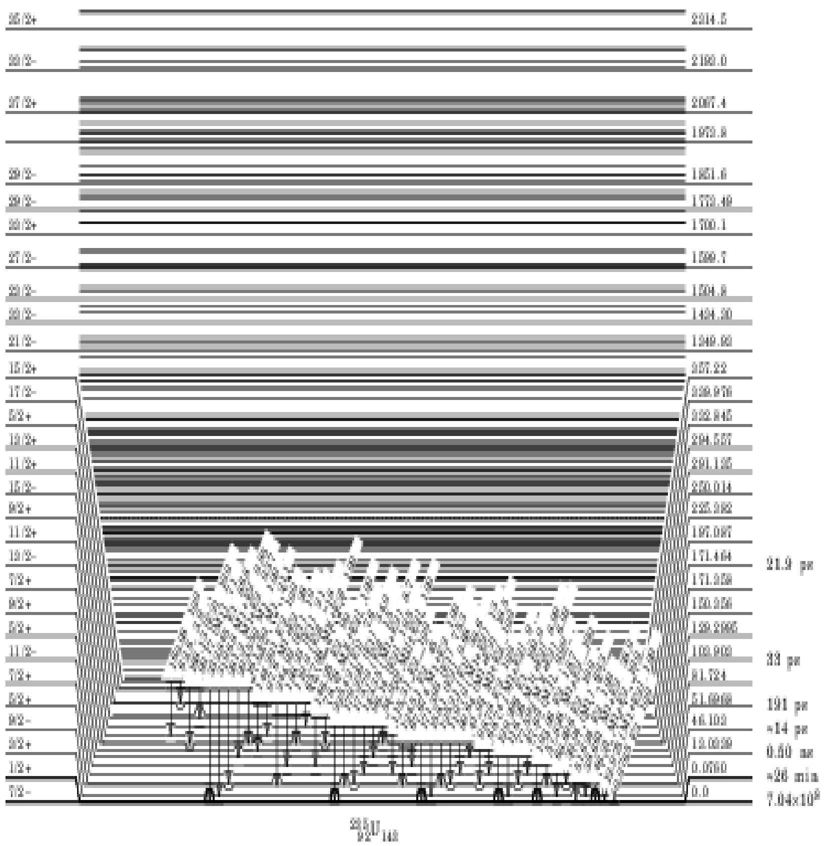


Neutron cross-sections



Proton cross-sections

Introduction: Evaluated Nuclear Data File



- Whether model can predict the cross-sections? No
- Nuclear structure contribute to the final states.
- No single model for all the Isotopes that can work reasonably well

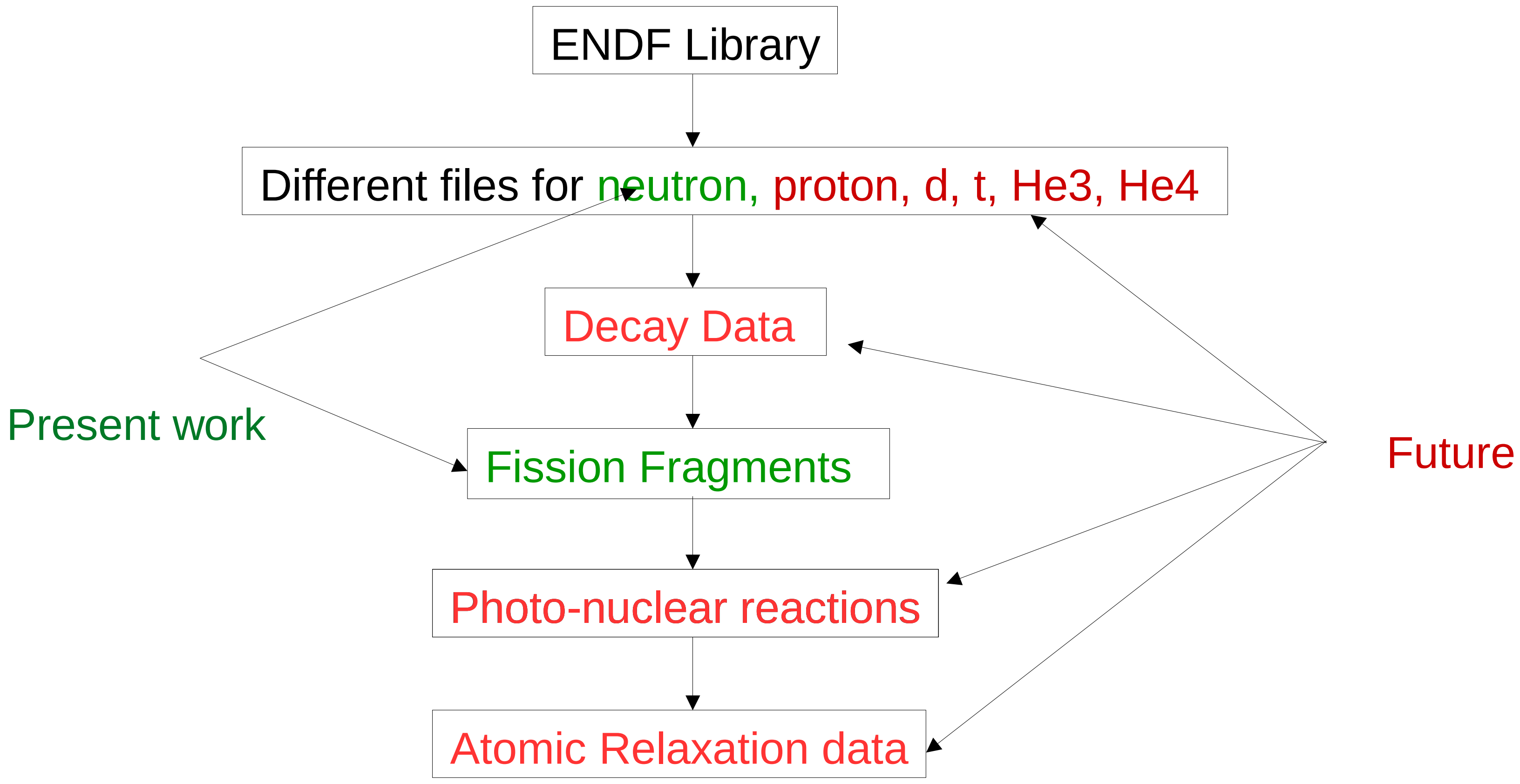
  What is the alternative solution?

- Evaluated Nuclear Data

  Disadvantage

- Too many data points due to resonance structure

Introduction: Evaluated Nuclear Data Library



Introduction: Evaluated Nuclear Data File

ENDF File

↓

Different sections

↓

1 → General description, Fission neutron multiplicity, partial photon data
2 → Resonance parameters for cross-section
3 → Cross-sections for all reactions
4 → Independent angular distributions
5 → Independent energy distributions
6 → Correlated angle-energy distributions
7 → Thermal neutron scattering data
8 → Decay data and fission products
9 → Multiplicities for radio-active nuclide production
10 → Production cross-section for radio-active nuclide
11 → General comments for Photon production
12 → Photon production multiplicities
13 → Photon production cross-section
14 → Photon angular distributions
15 → Continuous photon energy distribution

12 More sections about atomic reactions, errors, photon, election interaction

Introduction: Evaluated Nuclear Data File

How the data file look like ?

```
[MAT, 2,151/  ZA, AWR,   0,   0, NIS,    0]HEAD (NIS=1)
[MAT, 2,151/ ZAI, ABN,   0,LFW, NER,    0]CONT (ZAI=ZA,ABN=1,LFW=0,NER=1)
[MAT, 2,151/  EL,  EH,LRU,LRF, NRO,NAPS]CONT (LRU=0,LRF=0,NRO=0,NAPS=0)
[MAT, 2,151/ SPI,  AP,   0,   0, NLS,    0]CONT (NLS=0)}
[MAT, 2,   0/ 0.0, 0.0,   0,   0,    0,    0]SEND
[MAT, 0,   0/ 0.0, 0.0,   0,   0,    0,    0]FEND
```

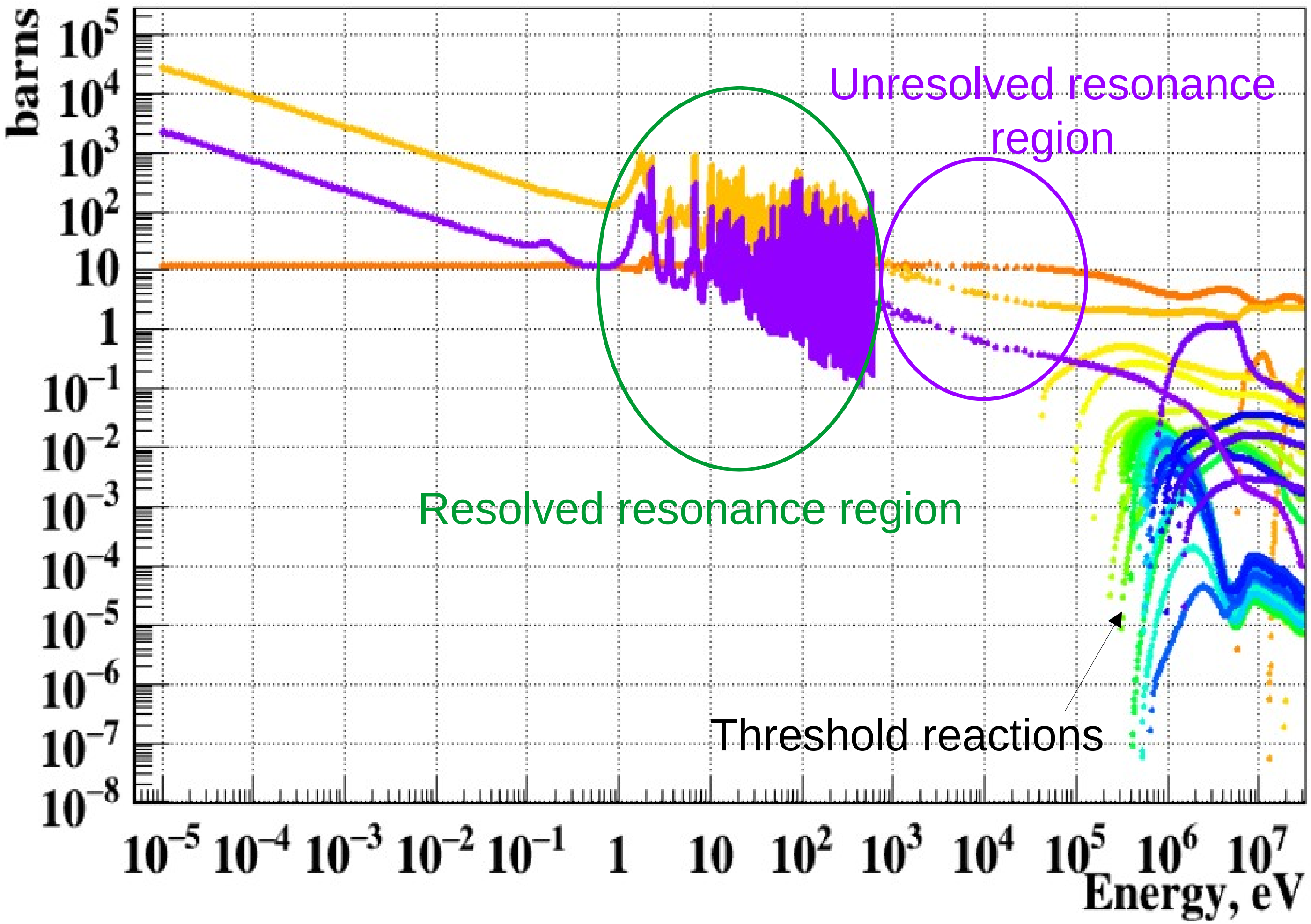
```
 9.223500+4 2.330248+2          0          0          1          09228 2151    1
 9.223500+4 1.000000+0          0          1          2          09228 2151    2
 1.000000-5 2.250000+3          1          3          0          19228 2151    3
 3.500000+0 9.602000-1          0          0          1          39228 2151    4
 2.330200+2 9.602000-1          0          0      19158        31939228 2151    5
-2.038300+3 3.000000+0 1.970300-2 3.379200-2-4.665200-2-1.008800-19228 2151    6
```

There are many different sub-sections with different set of parameters and different structures

Introduction: Why point data are not given but parameters

- Too many data point
- We don't understand from collection of points (lack of information about physics)
- Data should be interpreted by nuclear theory so that one can understand the physics
- We should be able to extrapolate and interpolate in the missing energy range
- Experimental information is utmost important to derive useful data.
- Further up-gradation of data is possible

Introduction: Typical cross-section



Reconstruction: Convert ASCII file to ROOT file

Read all sections from neutron data file

Read data from sub-libraries

a) fission fragment yield
b) decay data
c)
d)
.
.
.
.
Convert **9.223500+4** data structure into **Doubles/Float**

Store into ROOT file → file size reduces 2-3 times

This is done before simulation into offline mode but one can do during simulation and go for a Coffee break

Reconstruction: Linearization and Unionization

Read ROOT file

No Resonance Parameters

Linearization

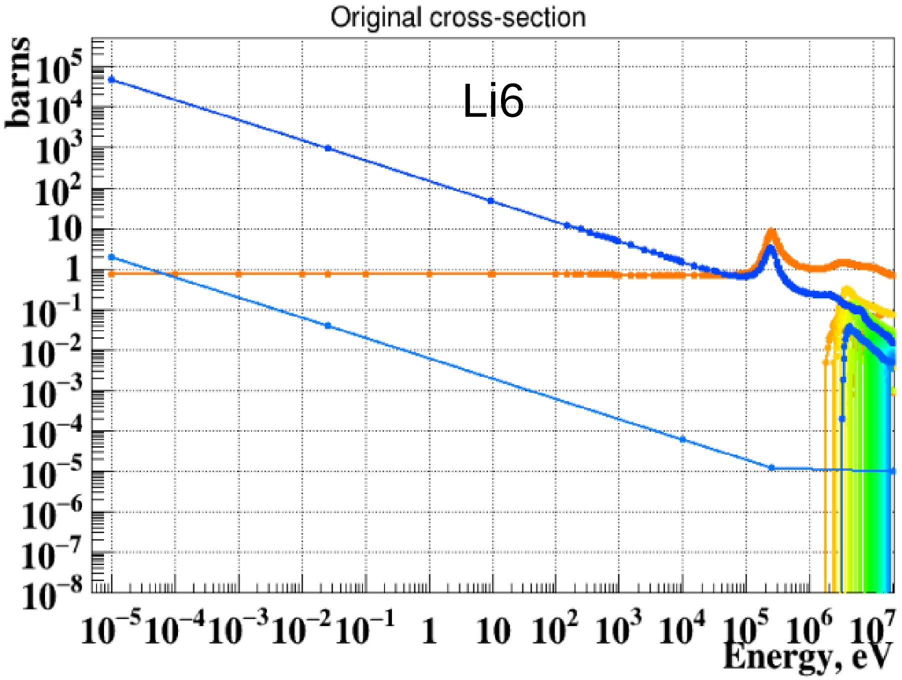
0.1% precision

1 → Log-Log

2 → Log-Linear

3 → Linear-Log

4 → Linear-Linear



Unionization

1 → Make union of all energy points from different reactions

2 → Delete duplicate points

3 → Calculate all cross-sections for these energy points

Reconstruction: Total cross-section

Read ROOT file

↓

No Resonance Parameters

↓

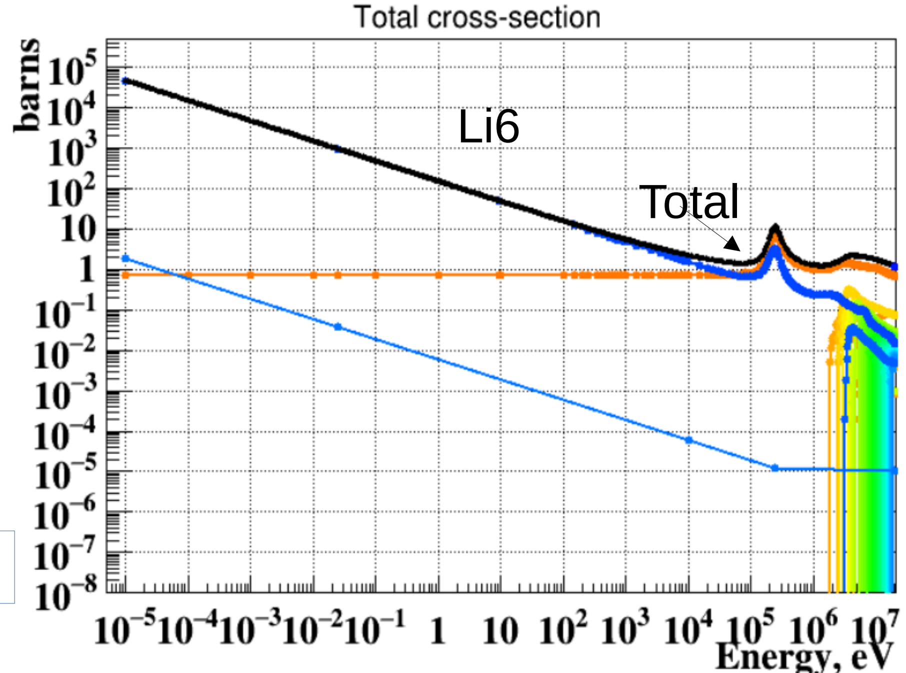
Linearization

↓

Unionization

↓

Doppler broadening at higher temperature



1 → Add all cross-sections and generate total cross-section

2 → Store only non zero data points

↓

Construct Total cross-section

↓

Modify ROOT file to replace old cross-sections with new linearized point cross-sections

This is done before simulation into offline mode but one can do during simulation and go for a Lunch break

Reconstruction: Hydrogen cross-section

- Linear in log scale

  96 data points

- Linear data points

  487 data points

- Doppler broadning

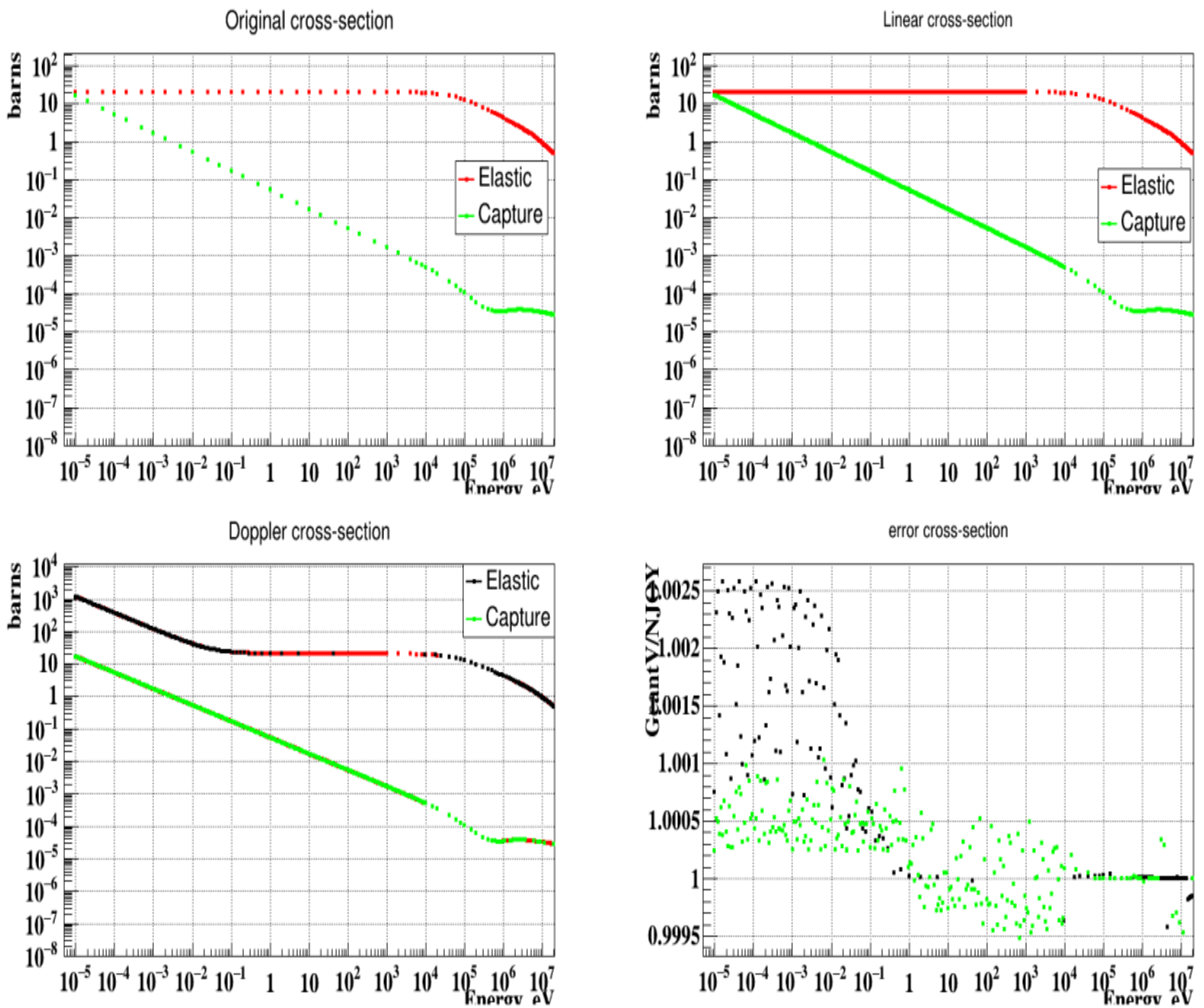
  at 293.6Kelvin

- Linearization is

  to be done to

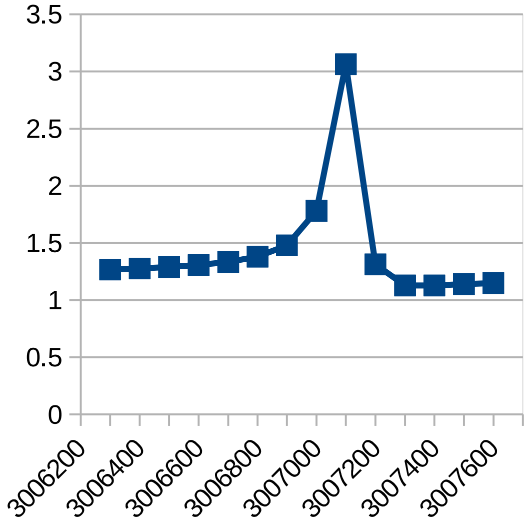
  gain some memory

  sometimes

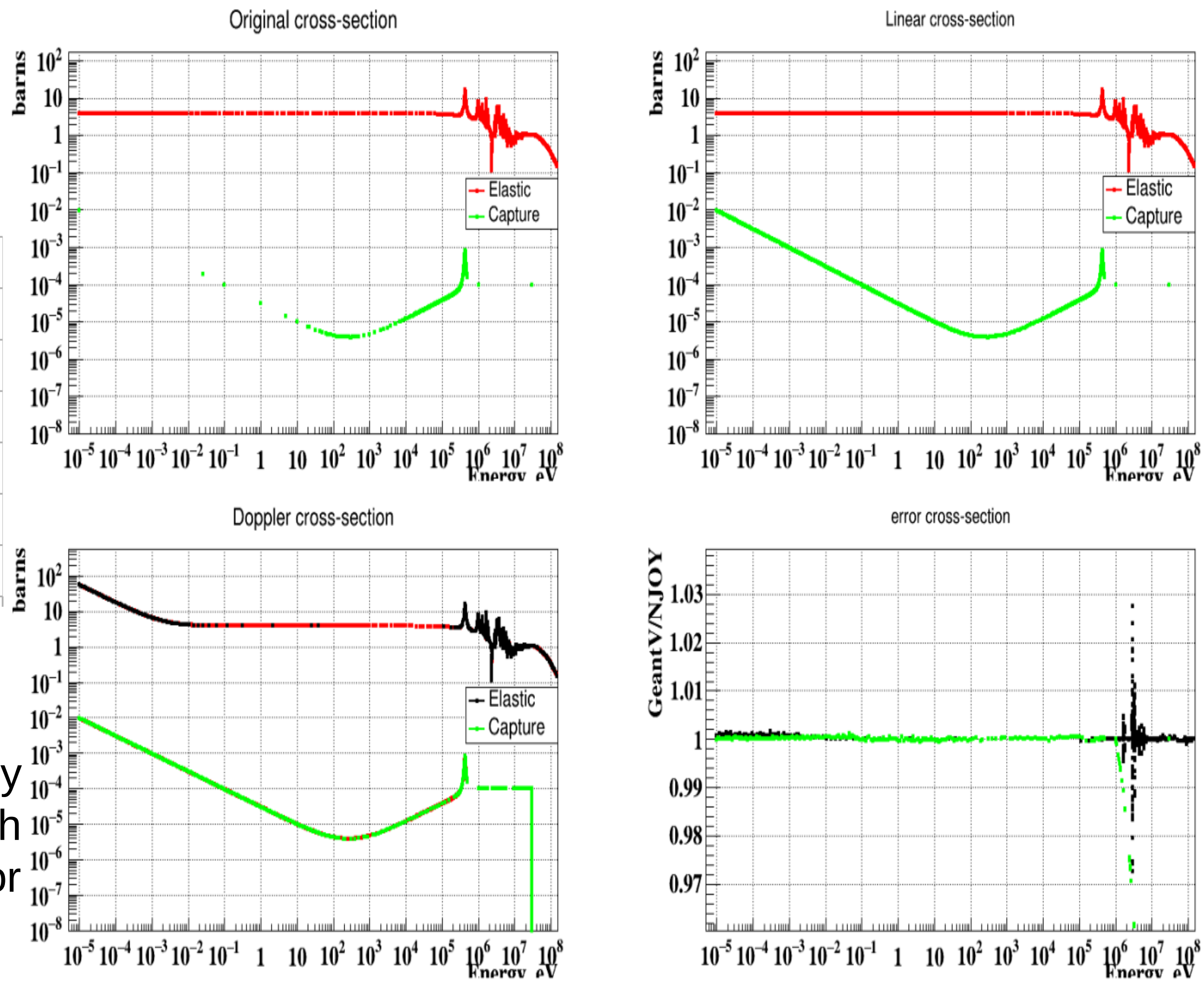


Reconstruction: O16 cross-section

Data are given up to 200 MeV



Peak like cross-section
But linearly interpolatable Which gives some Error compared to NJOY



Reconstruction: Resonance cross-section

Read Resonance Parameters →

1 → Resonance energy points

2 → Resonance widths

3 → Resonance types

(Single level Breit-Wigner,

Multi- level Breit-Wigner,

Reich-Moore, Adler-Adler,

R-Matrix)

1 → Calculate phase shifts, shift factors, penetration factors for higher angular momenta

Single level Breit-Wigner → 8 isotopes

Multi- level Breit-Wigner → 268 isotopes

Reice-Moore → 54 isotopes (best results)

Adler-Adler → None

R-Matrix → None (Very hard to implement)

Reconstruction: Single Level Breit Wigner

$$\sigma_{n,n}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma^l_{n,n}(E),$$

Elastic cross-section

$$\begin{aligned}\sigma^l_{n,n}(E) &= (2l+1)\frac{4\pi}{k^2}\sin^2\phi_l \\ &+ \frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{\mathrm{NR}_J} \frac{\Gamma_{nr}^2 - 2\Gamma_{nr}\Gamma_r \sin^2\phi_l + 2(E-E'_r)\,\Gamma_{nr}\sin(2\phi_l)}{(E-E'_r)^2 + \frac{1}{4}\Gamma_r^2}\end{aligned}$$

Capture cross-section

$$\sigma_{n,\gamma}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma^l_{n,\gamma}(E)$$

$$\sigma^l_{n,\gamma}(E) = \frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\,\Gamma_{\gamma r}}{(E-E'_r)^2 + \frac{1}{4}\Gamma_r^2}$$

Fission cross-section

$$\sigma_{n,f}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma^l_{n,f}(E)\ ,$$

$$\sigma^l_{n,f}(E) = \frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\Gamma_{fr}}{(E-E'_r)^2 + \frac{1}{4}\Gamma_r^2}$$

Reconstruction: Multi-Level Breit Wigner

Elastic cross-section

$$\sigma_{n,n}^{l(R)}(E) = \frac{\pi}{k^2} \sum_J g_J \sum_{r=1}^{NR_J} \frac{G_r \Gamma_r + 2H_r(E - E_r)}{(E - E_r')^2 + (\Gamma_r/2)^2}$$

$$G_r = \frac{1}{2} \sum_{r'=1, r' \neq r}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\Gamma_{nr'}(\Gamma_r + \Gamma_{r'})}{(E_r' - E_{r'}')^2 + \frac{1}{4}(\Gamma_r + \Gamma_{r'})^2},$$

$$H_r = \sum_{r'=1, r' \neq r}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\Gamma_{nr'}(E_r - E_{r'})}{(E_r' - E_{r'}')^2 + \frac{1}{4}(\Gamma_r + \Gamma_{r'})^2}$$

Capture cross-section

$$\sigma_{n,\gamma}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma_{n,\gamma}^l(E)$$

$$\sigma_{n,\gamma}^l(E) = \frac{\pi}{k^2} \sum_J g_J \sum_{r=1}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\,\Gamma_{\gamma r}}{(E - E_r')^2 + \frac{1}{4}\Gamma_r^2}$$

Fission cross-section

$$\sigma_{n,f}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma_{n,f}^l(E)\ ,$$

$$\sigma_{n,f}^l(E) = \frac{\pi}{k^2} \sum_J g_J \sum_{r=1}^{\mathrm{NR}_J} \frac{\Gamma_{nr}\Gamma_{fr}}{(E - E_r')^2 + \frac{1}{4}\Gamma_r^2}$$

Reconstruction: Reich-Moore

$$\sigma_T(E) = \frac{2\pi}{k^2} \sum_{l=0}^{\mathrm{NLS}-1} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J \mathrm{Re}\left[1 - U_{lsJ,lsJ}\right]$$

Elastic cross-section

$$\sigma_{nn}(E) = \frac{2\pi}{k^2} \sum_{l=0}^{\mathrm{NLS}-1} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J \left|1 - U_{lsJ,lsJ}\right|^2$$

Fission cross-section

Capture cross-section
= Absorption - fission

$$\sigma_f(E) = \frac{2\pi}{k^2} \sum_{l=0}^{\mathrm{NLS}-1} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J \left[\left|U_{nf1}^{lsJ}\right|^2 + \left|U_{nf2}^{lsJ}\right|^2\right]$$

$$\sigma_{abs}(E) = \sigma_T(E) - \sigma_{nn}(E)$$

$$U_{nb}^J = e^{-i(\phi_n+\phi_b)} \left\{2\left[(I-K)^{-1}\right]_{nb} - \delta_{nb}\right\},$$

$$(I-K)_{nb} = \delta_{nb} - \frac{i}{2}\sum_r \frac{\Gamma_{nr}^{1/2}\Gamma_{br}^{1/2}}{E_r - E - i\,\Gamma_{\gamma r}/2}$$

Reconstruction: Unresolved resonance

Elastic cross-section

$$\sigma_{n,n}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma^l_{n,n}(E),$$

$$\sigma^l_{n,n}(E) = \frac{4\pi}{k^2}(2l+1)\sin^2\phi_l + \frac{2\pi^2}{k^2}\sum_J^{\mathrm{NJS}}\left[\frac{g_J}{\overline{D}_{l,J}}\left\langle\frac{\Gamma_n\Gamma_n}{\Gamma}\right\rangle_{l,J} - 2\overline{\Gamma}_{nl,J}\sin^2\phi_l\right]$$

Average widths are used along with fluctuation $\left\langle\frac{\Gamma_n\Gamma_n}{\Gamma}\right\rangle_{l,J} = \left(\frac{\overline{\Gamma}_{nl,J}\overline{\Gamma}_{nl,J}}{\overline{\Gamma}_{l,J}}\right) R_{n,l,J}$

Width fluctuation parameter R is calculated using MC^2-II method.

Capture cross-section

$$\sigma_{n,\gamma}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma^l_{n,\gamma}(E),$$

$$\sigma^l_{n,\gamma}(E) = \frac{2\pi^2}{k^2}\sum_J^{\mathrm{NJS}}\frac{g_J}{\overline{D}_{l,J}}\left\langle\frac{\Gamma_n\Gamma_\gamma}{\Gamma}\right\rangle_{l,J}$$

Fission cross-section

$$\sigma_{n,f}(E) = \sum_{l=0}^{\mathrm{NLS}-1} \sigma^l_{n,f}(E),$$

$$\sigma^l_{n,f}(E) = \frac{2\pi^2}{k^2}\sum_J^{\mathrm{NJS}}\frac{g_J}{\overline{D}_{l,J}}\left\langle\frac{\Gamma_n\Gamma_f}{\Gamma}\right\rangle_{l,J}$$

Reconstruction: Resonance cross-section

Read ROOT file

↓

Reconstruct resonance cross-sections → Linearization of resonance data is done during reconstruction

↓

Add Linearized data if given in cross-section files
And insert additional data at higher energy range

↓

Unionization

↓

Doppler broadening at higher temperature

↓

1 → Add all cross-sections and generate total cross-section

2 → Store only non zero data points

↓

Construct Total cross-section

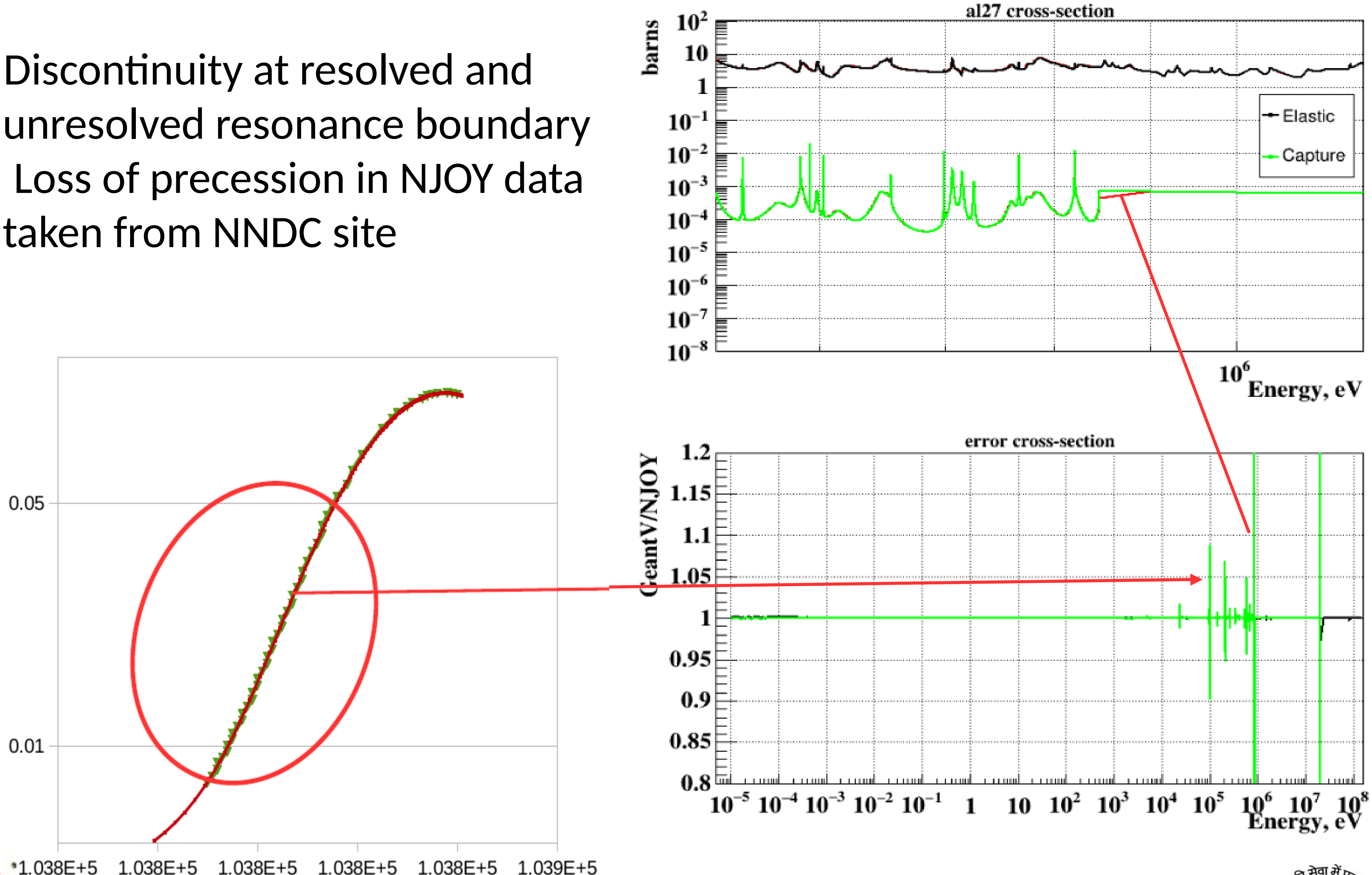
↓

Modify ROOT file to replace old cross-sections with new linearized point cross-sections

This is done before simulation into offline mode but one can do during simulation and go for a Lunch break

Reconstruction: Al27 cross-section

- ➢ Discontinuity at resolved and unresolved resonance boundary
- ➢ Loss of precession in NJOY data taken from NNDC site

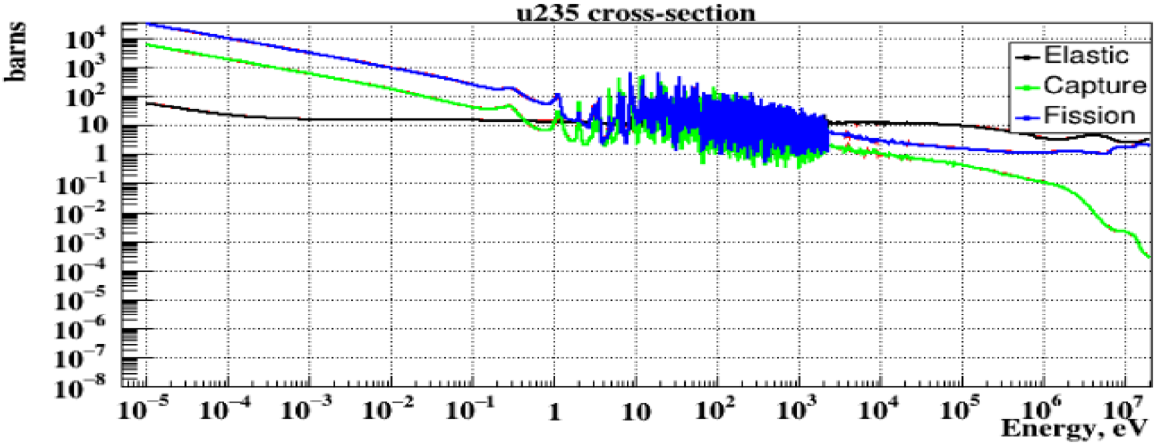


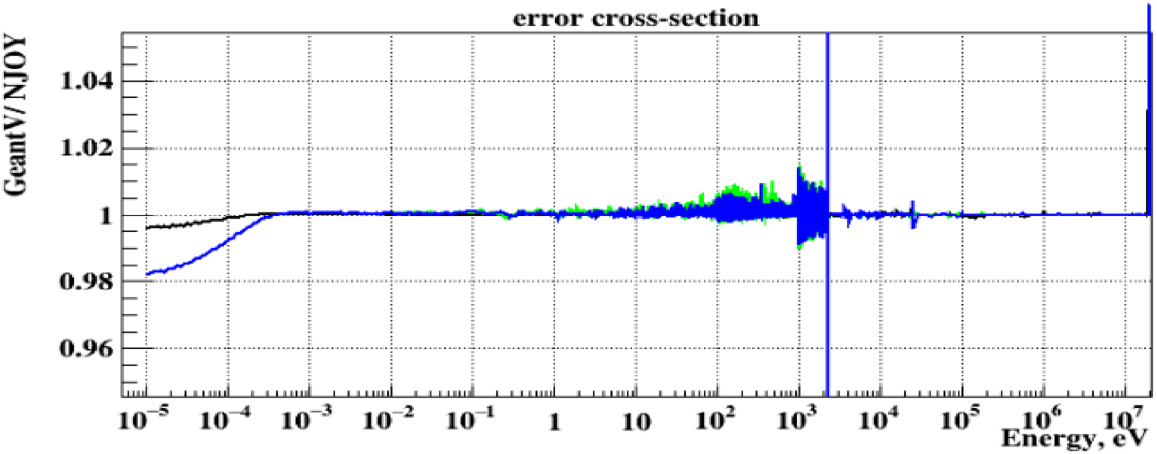
Reconstruction: U235 cross-sections

Data are given up to 30 MeV

Resolved and un-resolved resonance boundary shows discrepancy due to discontinuity

RR data are agreeing within 0.5%

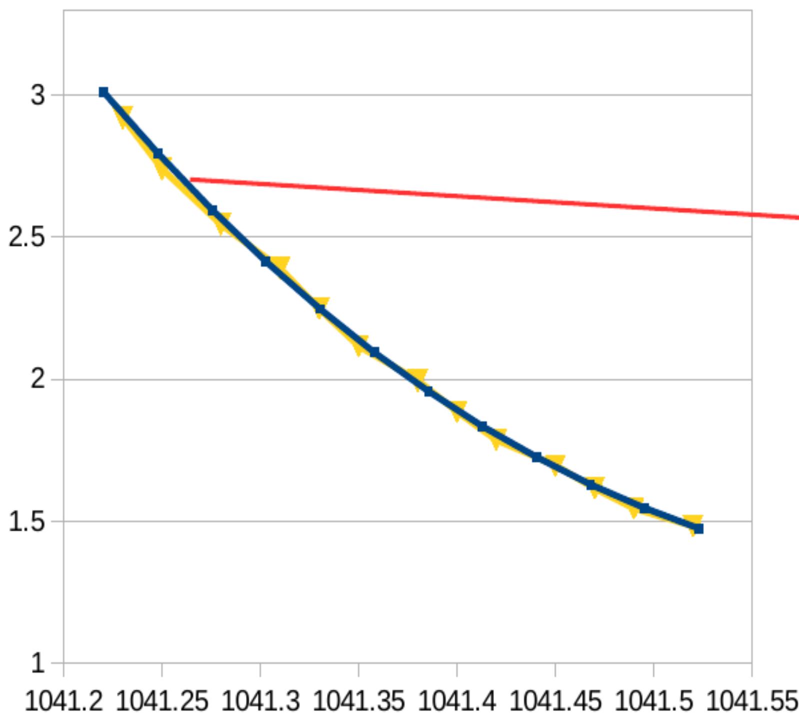


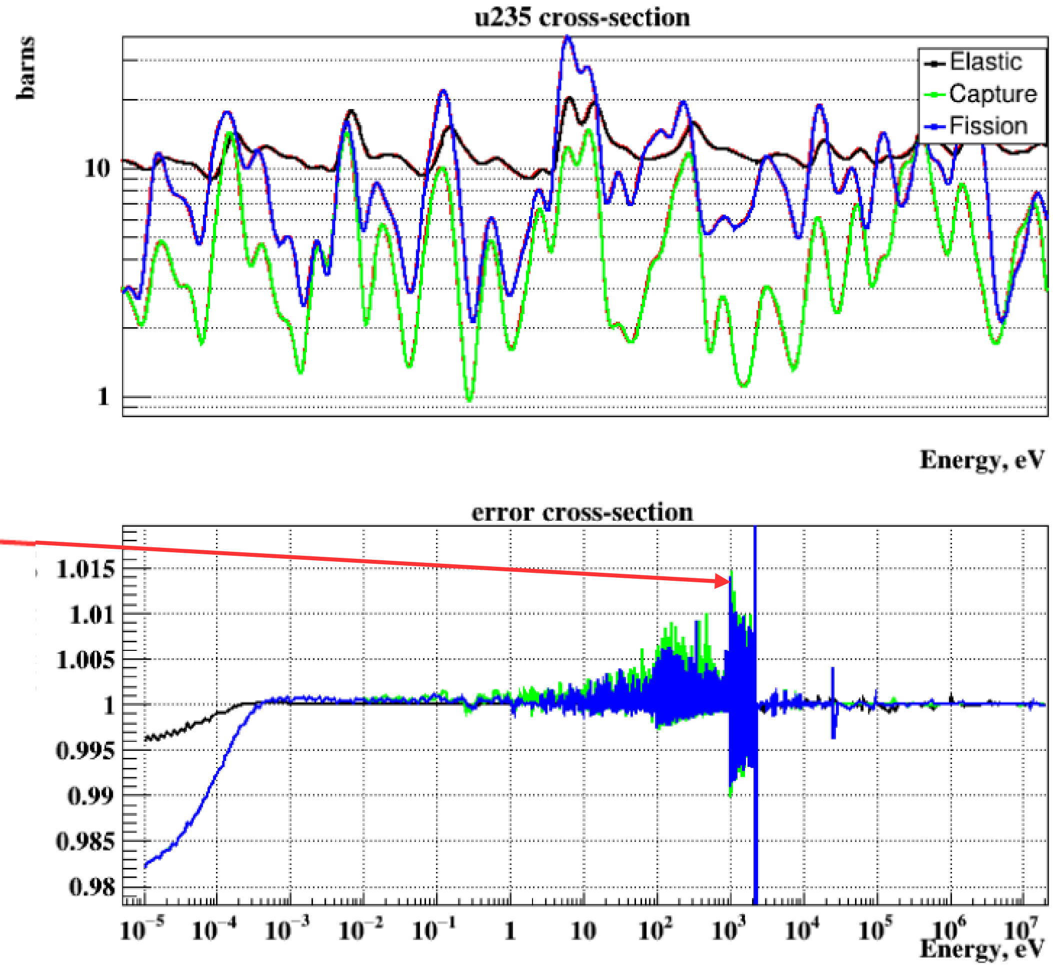


This is done before simulation into offline mode but one can do during simulation and go for a Day break

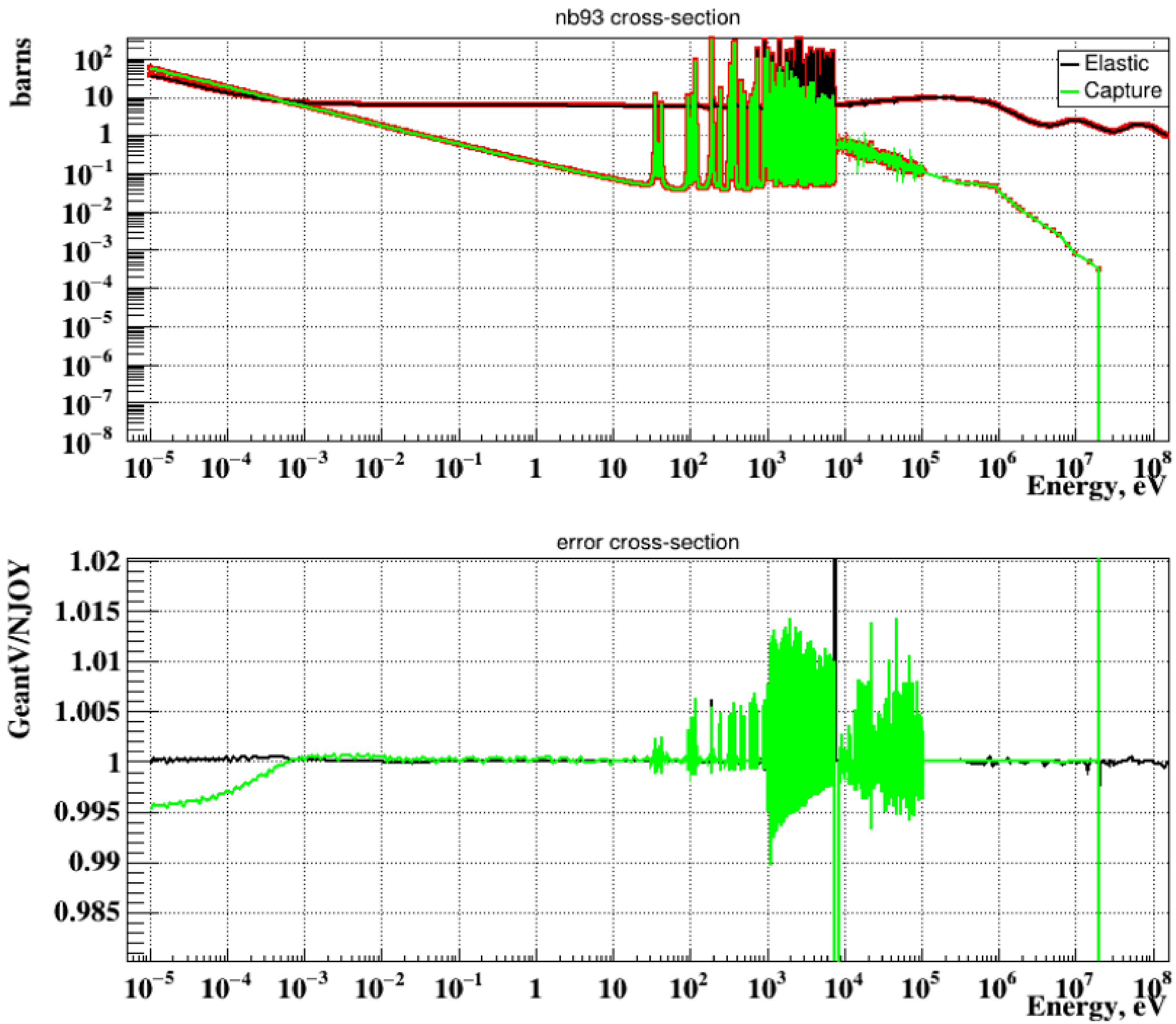
Reconstruction: U235 cross-sections

Closer look at maximum errors looks insignificant





Reconstruction: Nb93 cross-sections



Reconstruction: Doppler broadening

Maxwellian velocity

Distribution is used

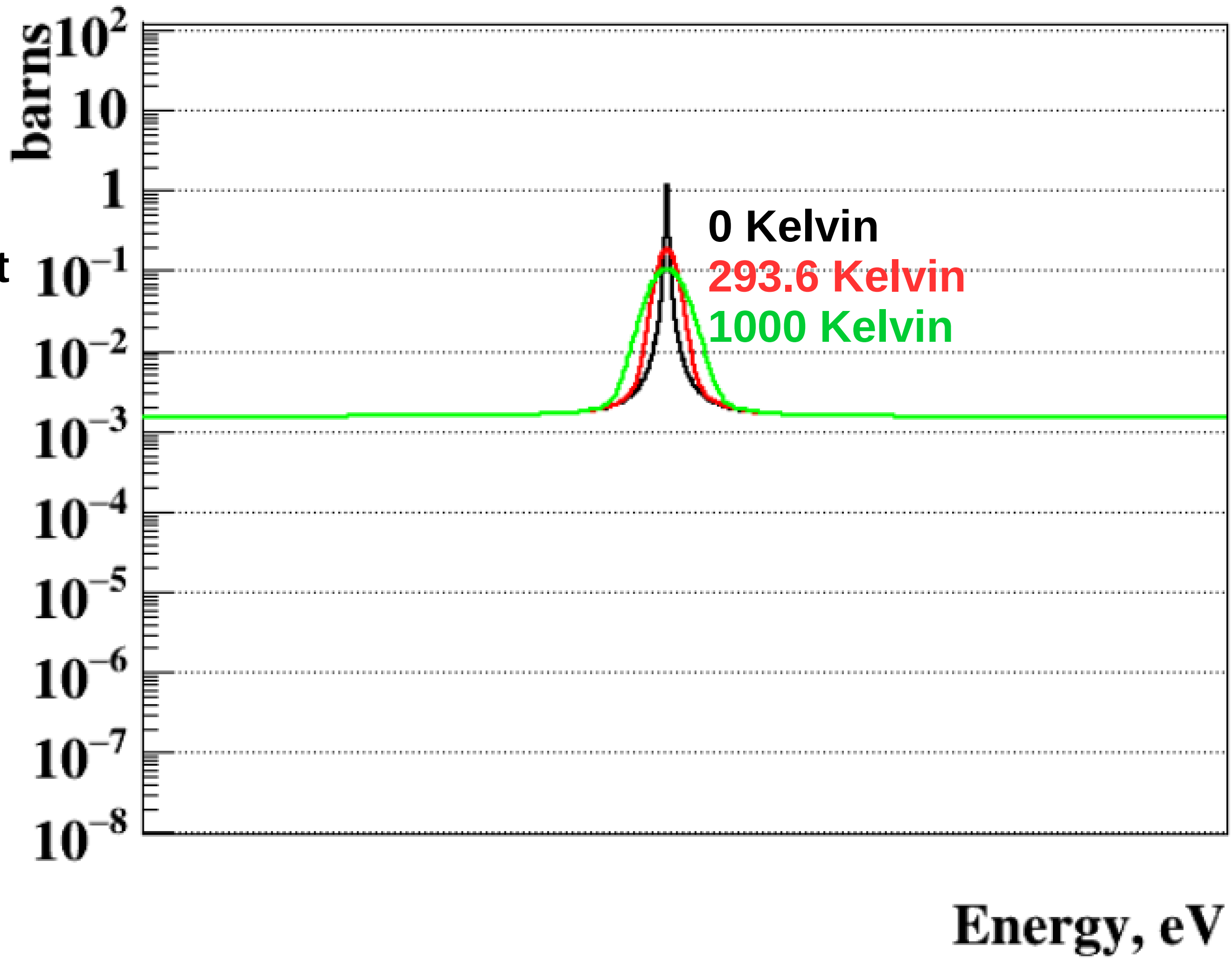
For the target atoms at

different temperatures

It is adopted from

Federico's fortran

version



Reconstruction: Angular Distributions

- Angular distributions are given in terms of Legendre coefficients and probability tables
- Data are given mostly for few energies
- Cumulative distribution and PDF are used to get the angle

$$f(\mu, E) = \frac{2\pi}{\sigma_s(E)}\,\sigma(\mu, E) = \sum_{l=0}^{\mathrm{NL}} \frac{2l+1}{2}\, a_l(E)\, P_l(\mu)$$

Legendre coefficients

$$E_i < E_{in} < E_{i+1}$$

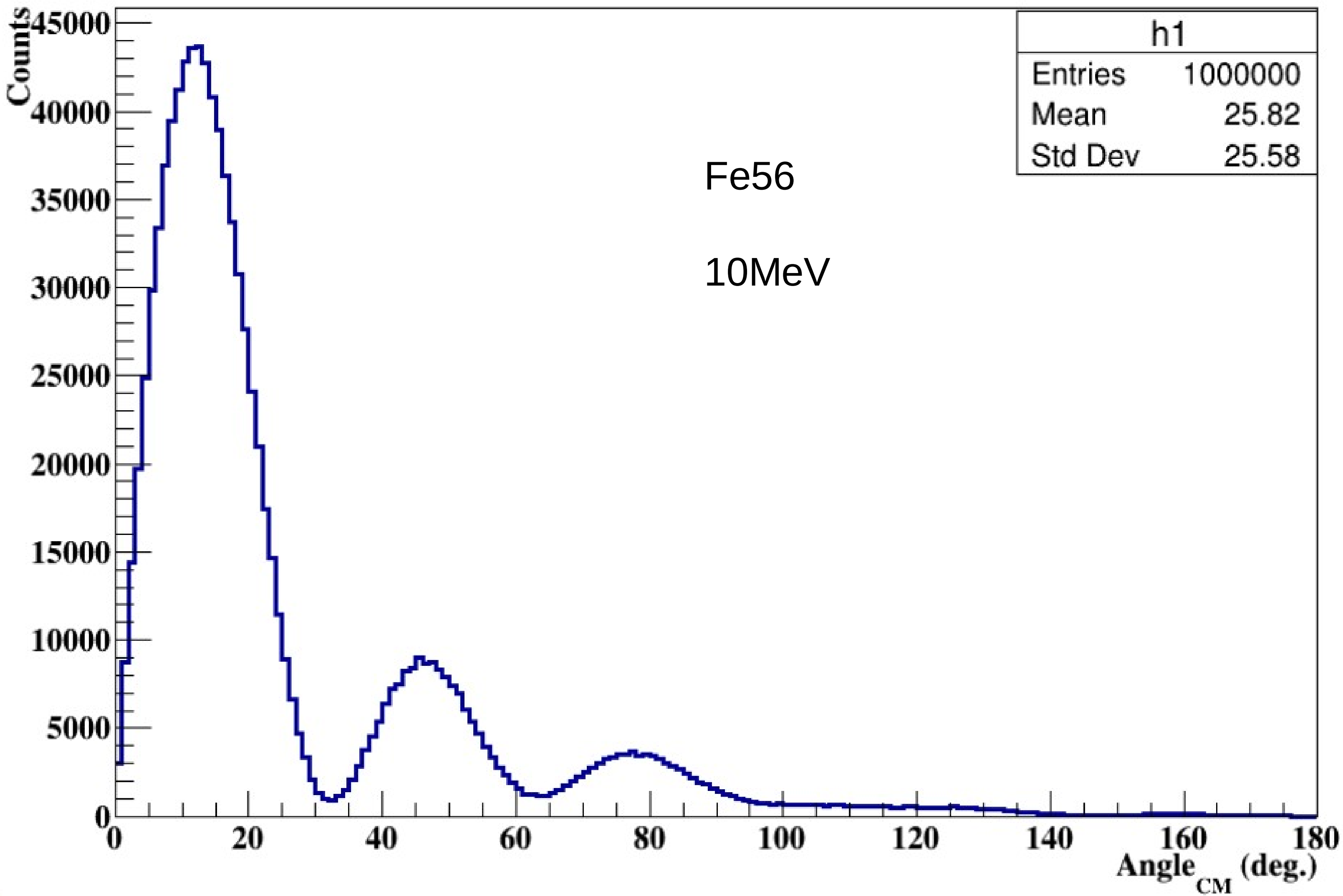
$$E_{in} = E_i + r(E_{i+1} - E_i)$$

$$c_{l,k} < \xi_1 < c_{l,k+1}$$

$$\mu' = \mu_{l,k} + \left\{ \frac{\sqrt{P^2_{l,k} + 2\left[\frac{p_{l,k+1} - p_{l,k}}{\mu_{l,k+1} - \mu_{l,k}}\right](\xi_1 - c_{l,k})} - p_{l,k}}{\left[\frac{p_{l,k+1} - p_{l,k}}{\mu_{l,k+1} - \mu_{l,k}}\right]} \right\}$$

The making of probability tables are done at initialization and we plan to shift to offline
Otherwise one can have a chat

Reconstruction: Elastic Angular Distribution



Reconstruction: Energy Distributions

- Energy distributions are given by tabular data or 5-6 different formulations
- We make all formats into probability tables
- Cumulative distribution and PDF are used to get the energy

One of the formulation for energy spectra

$$f(E \to E') = \frac{1}{2}\left[g(E', E_F(L)) + g(E', E_F(H))\right]$$

$$g(E', E_F) = \frac{1}{3\sqrt{(E_F T_M)}}\left[u_2^{3/2}\mathrm{E}_1(u_2) - u_1^{3/2}\mathrm{E}_1(u_1) + \gamma\left(\frac{3}{2}, u_2\right) - \gamma\left(\frac{3}{2}, u_1\right)\right]$$

$$u_1 = \left(\sqrt{E'} - \sqrt{E_F}\right)^2 / T_M$$

$$u_2 = \left(\sqrt{E'} + \sqrt{E_F}\right)^2 / T_M$$

$E_F(X)$ are constant, which represent the average kinetic energy per nucleon of the fission fragment; arguments L and H refer to the average light fragment (given by the parameter EFL in the file) and the average heavy fragment (given by the parameter EFH in the file), respectively.

T_M parameter tabulated as a function of incident neutron energy,

$\mathrm{E}_1(x)$ is the exponential integral,

$\gamma(a, x)$ is the incomplete gamma function. The integral of this spectrum between zero and infinity is one. The value of the integral for a finite integration

Probability tables are made at initialization and we plan to shift to offline Otherwise one can have one more chat

Reconstruction and sampling

Read data and Store in ROOT file

Resonance Parameters

No Resonance Parameters

Reconstruct resolved resonances

Reconstruct Unresolved resonance

Add Higher energy data

Linearization

Unionization

Angular distribution

Energy distribution

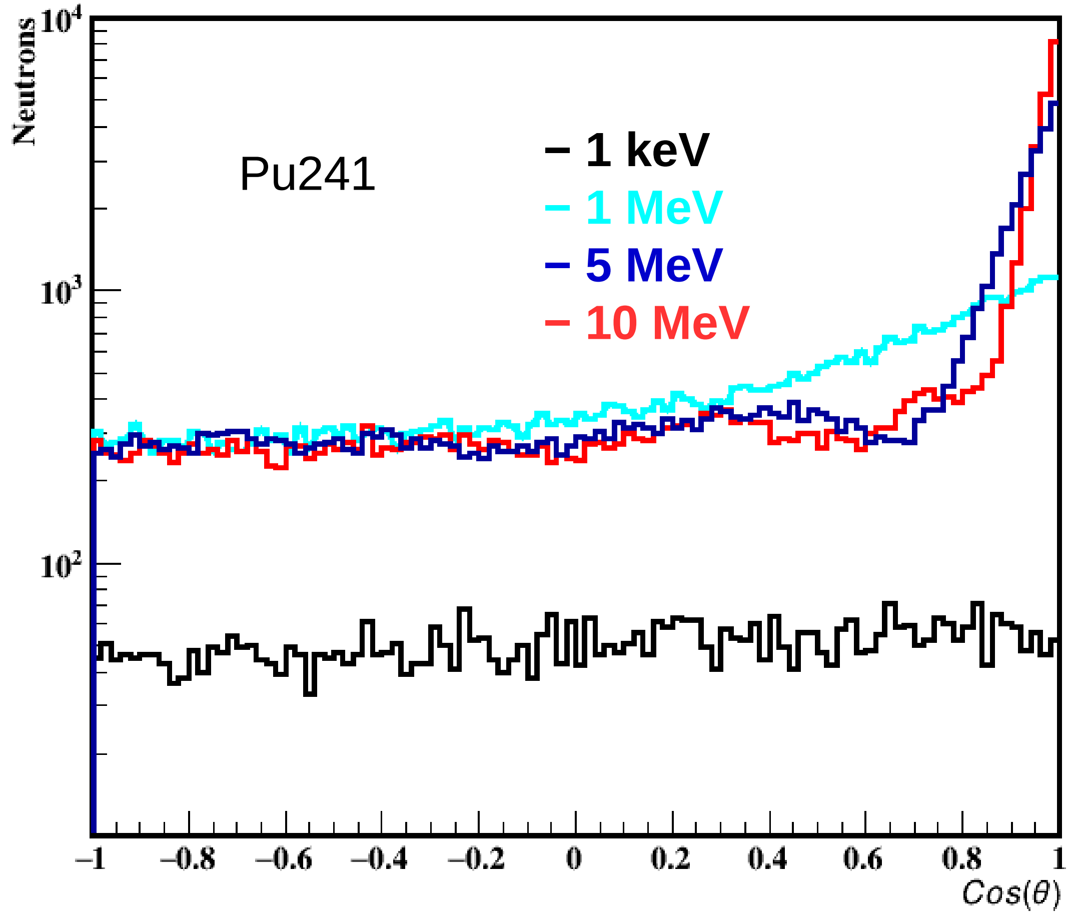
Fission fragments, fission neutrons, heat

Sample reactions, Secondaries

All is to be Done before simulation

Sampling: Elastic Angular Distribution

- Data are given mostly for few energies
- Bilinear interpolation
- Isotropic behavior for keV neutrons and forward peaking at higher energies
- 1 Milllion events are simulated

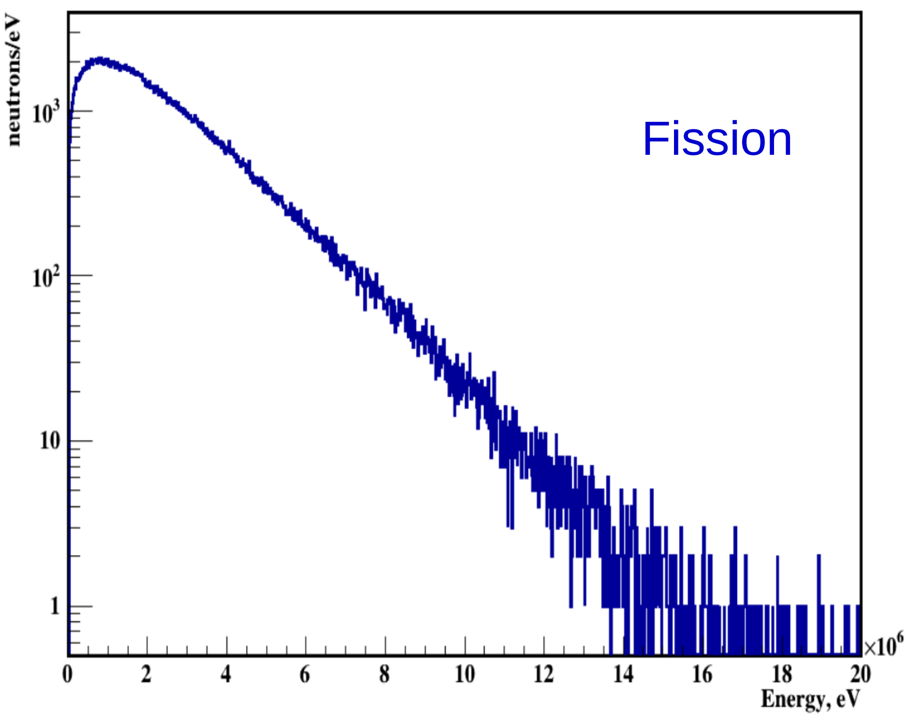


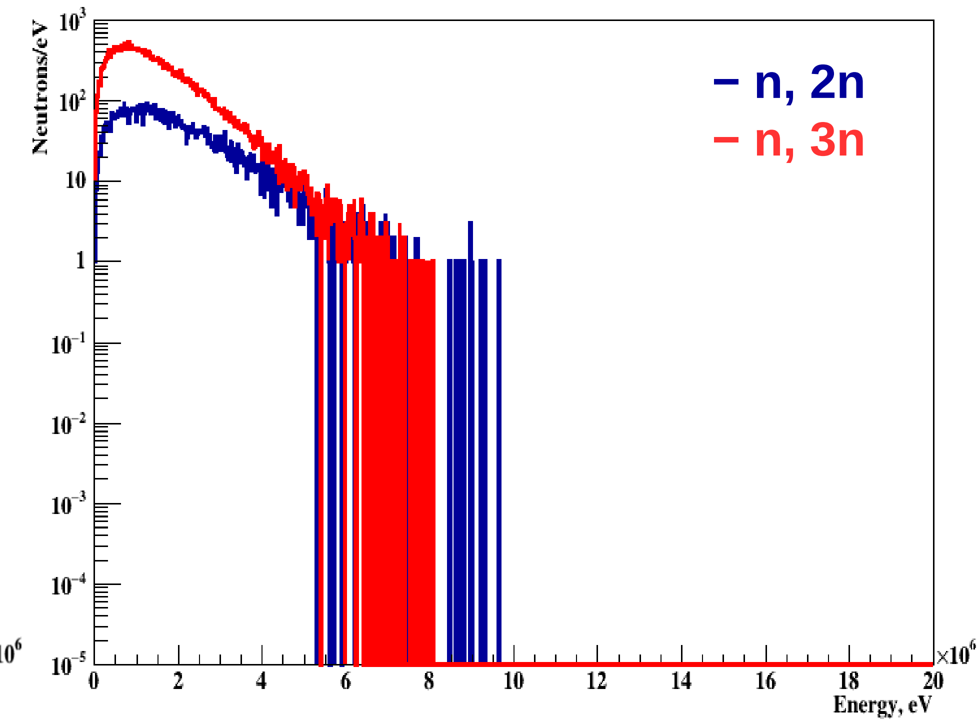
Sampling: Energy Distribution

In case of Fission second or third or higher number of neutrons are sampled from the same distribution

Second neutron from n,2n reaction can have Total - 1st neutron energy – recoil energy

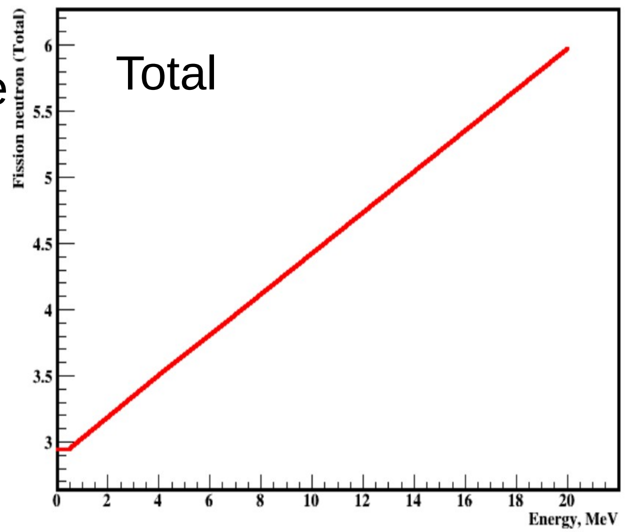
Energy conservation exist but without correlation until such data are given

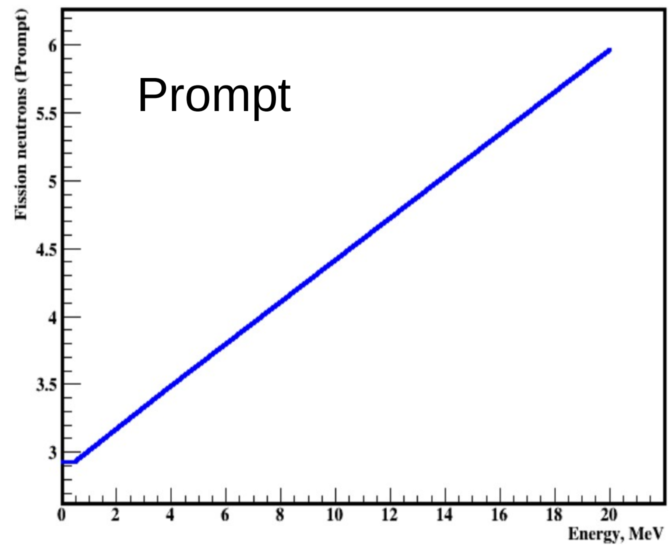


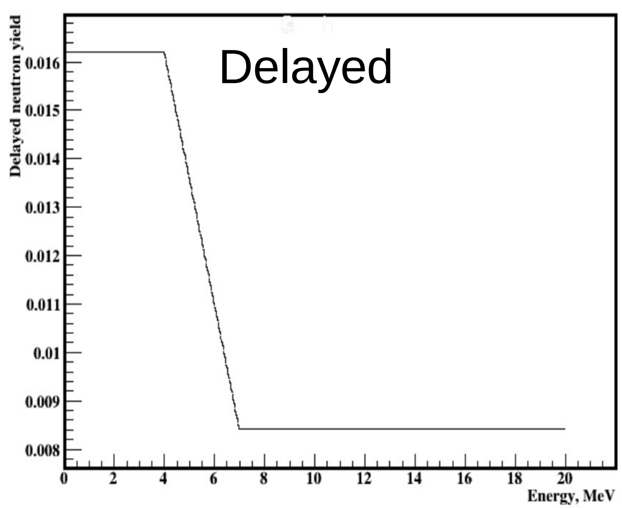


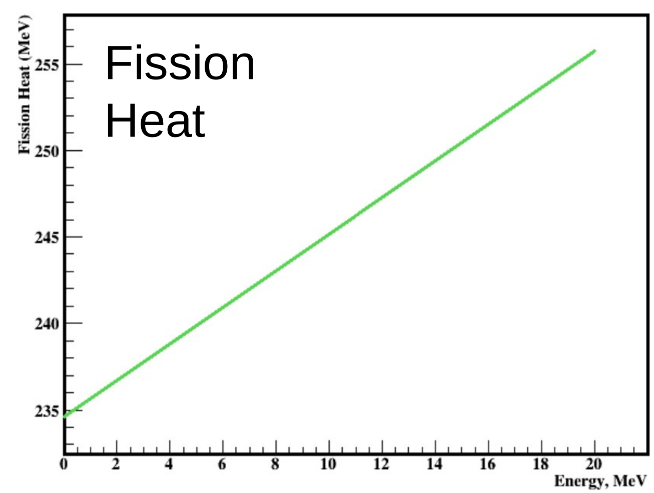
Sampling: PU-241 Fission neutrons

Sampling of average fission neutrons i.e. 2.56 is done based one Poissonian distribution



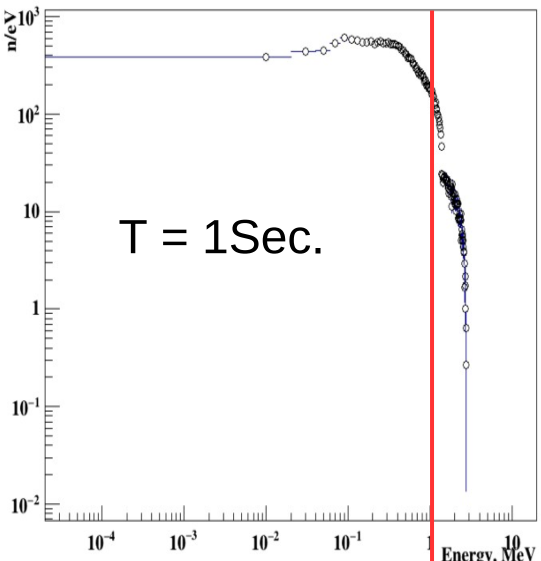


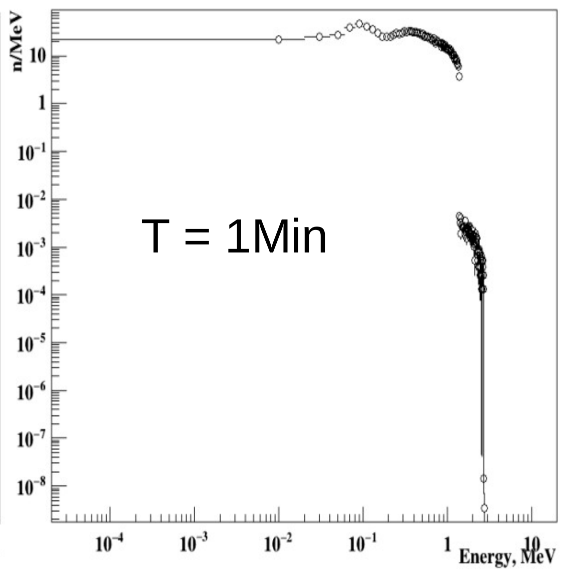


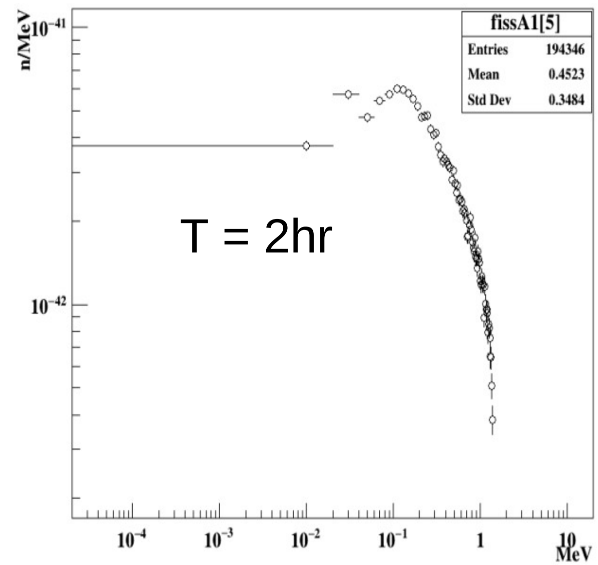


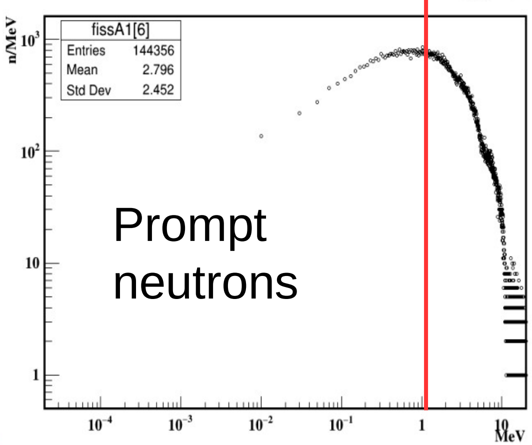
Sampling: PU-241 Delayed Fission neutrons

Delayed neutrons emitted by 6 precursor families. Mean time of decay is up to 100 seconds.





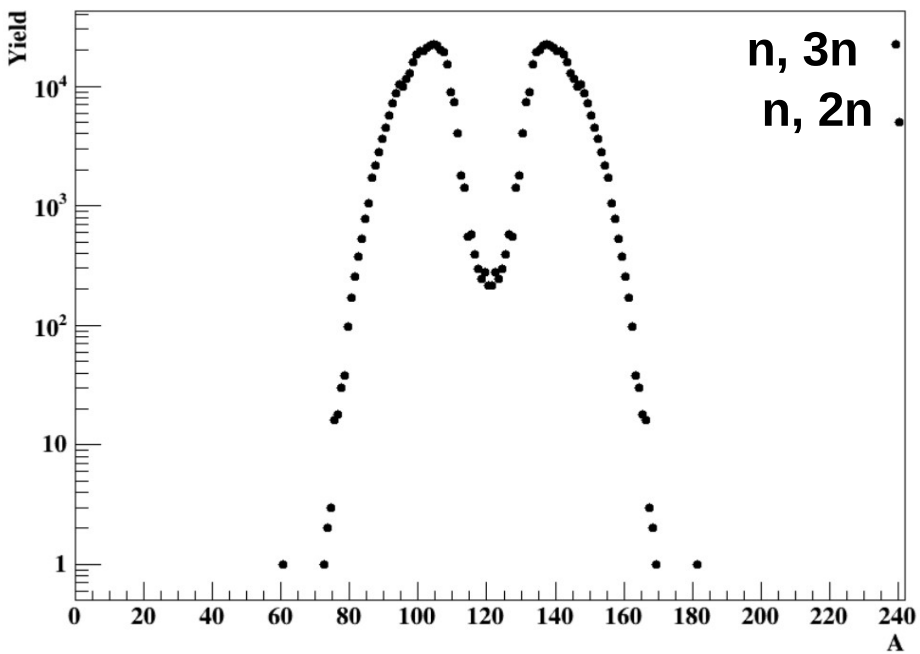


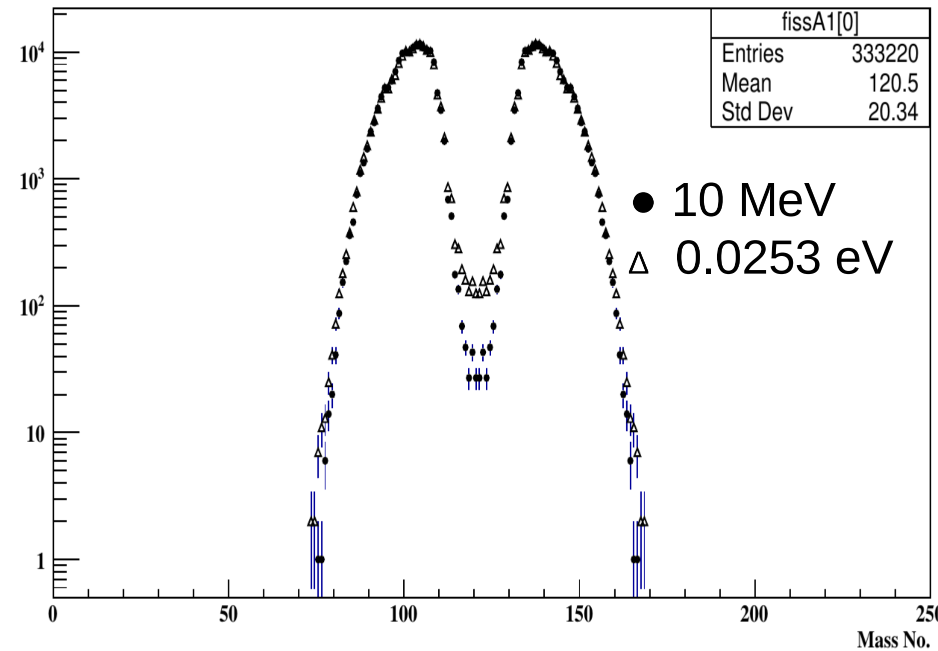


Prompt neutron spectrum is harder than delayed neutron spectrum

Sampling: PU-241 Fission fragments

- Data are given mostly for 2-3 energies (0.0253 eV, 0.5MeV, 14MeV).
- Interpolate for intermediate intervals.





Summary

- Neutron cross-sections are reconstructed and agreement with NJOY data is good.
- Angle and energy distributions are well described.
- Fission fragments and fission neutron multiplicity are validated.
- Doppler broadening at various temperature is too many sets of data points (every 50Kelvin)
- One should make effort to parameterize the data for temperature dependence and use them for given temperature (300k-3000K).

Future work

- Transport and Validation for the multiplicity, distributions
- Validation of photon distributions
- Include thermal scattering data
- Atomic relaxation data
- Optimize sampling technique
- Include variance reduction techniques
- Optimize for vectorized architecture

धन्यवाद

Thank you for your attention!