Point Wise Neutron treatment for FLUKA v4

G4 hadronic meeting
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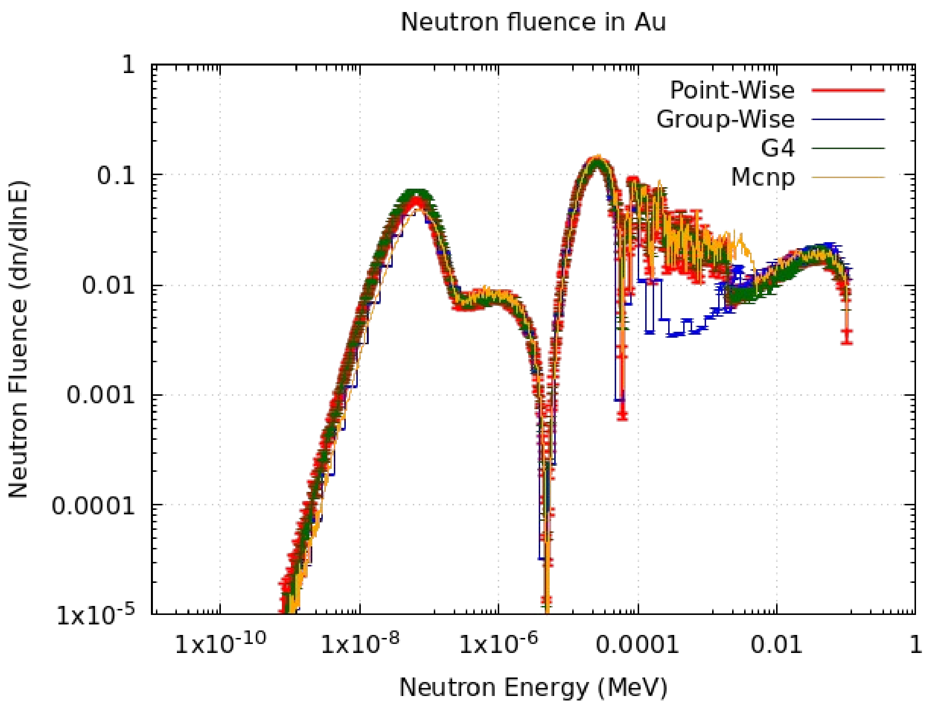
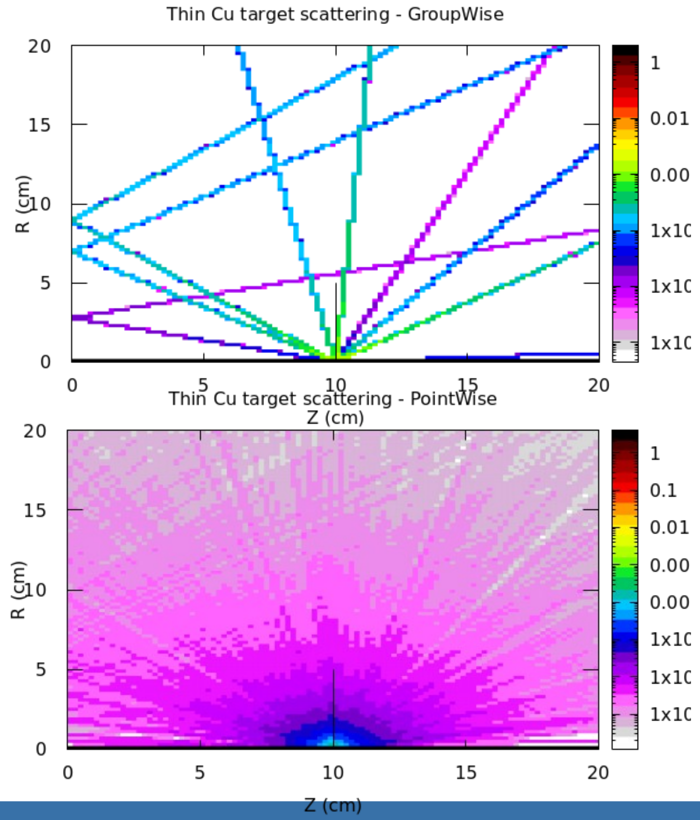
Motivation

- A major drawback of FLUKA was the transport of low energy neutrons ($E_n \leq 20$MeV) using a multi-group approach.

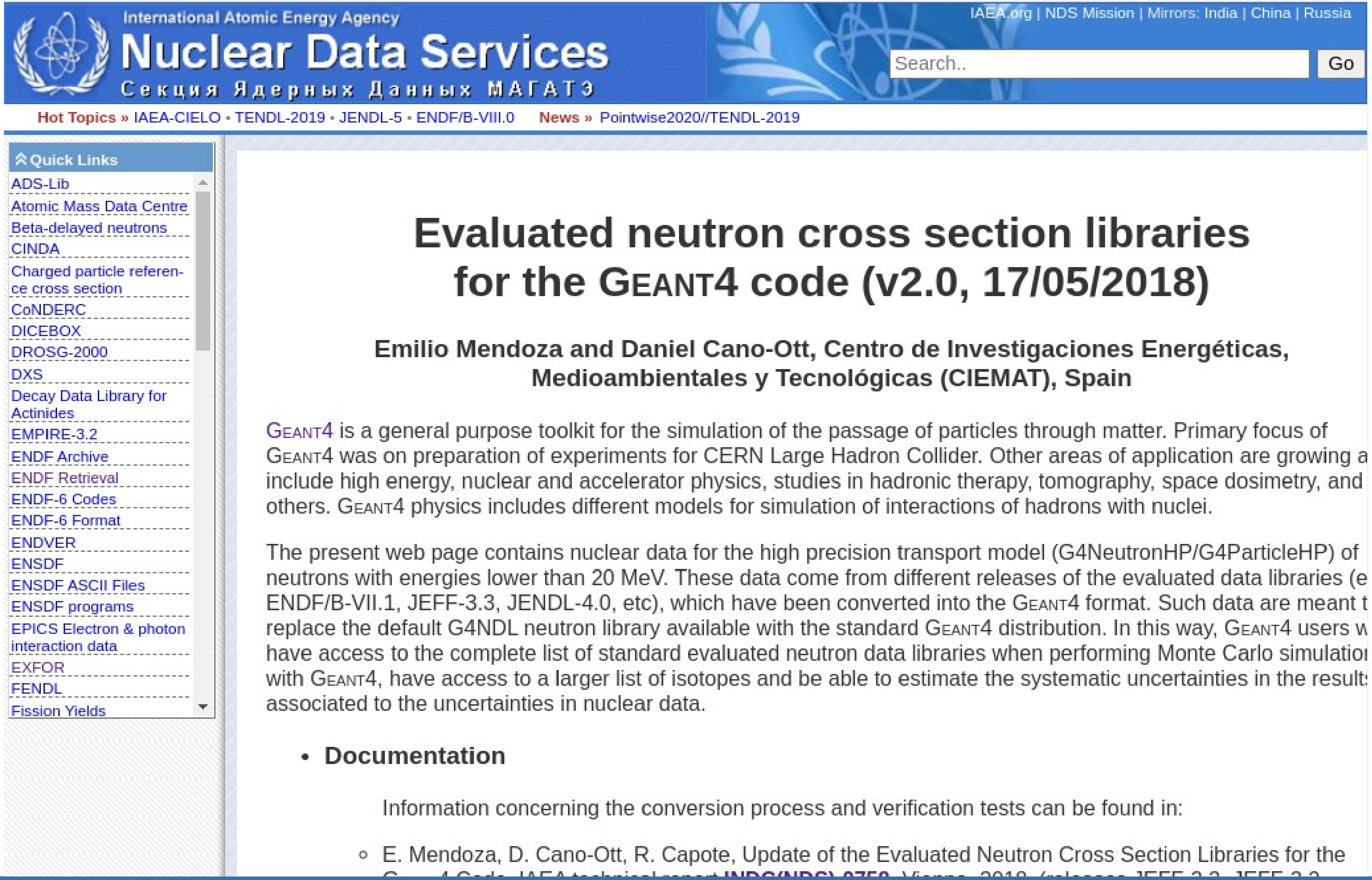




Motivation

- A major drawback of FLUKA was the transport of low energy neutrons ($E_n \leq 20$MeV) using a multi-group approach.
- The main difficulties for going pointwise were:
  1. the processing of the evaluated neutron interaction libraries (ENDF…) It requires time, critical judgment, verification, implementation of adhoc codes for formatting and testing
  2. the plethora of channels and the multitude of laws to describe these interactions
  3. the inclusive spectra providing uncorrelated information of the ejectiles
  4. performance issues, both in speed and huge memory footprint of the data

Geant4 DB Freely distributed from IAEA



Evaluated neutron cross section libraries for the GEANT4 code (v2.0, 17/05/2018)

Emilio Mendoza and Daniel Cano-Ott, Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT), Spain

GEANT4 is a general purpose toolkit for the simulation of the passage of particles through matter. Primary focus of GEANT4 was on preparation of experiments for CERN Large Hadron Collider. Other areas of application are growing a include high energy, nuclear and accelerator physics, studies in hadronic therapy, tomography, space dosimetry, and others. GEANT4 physics includes different models for simulation of interactions of hadrons with nuclei.

The present web page contains nuclear data for the high precision transport model (G4NeutronHP/G4ParticleHP) of neutrons with energies lower than 20 MeV. These data come from different releases of the evaluated data libraries (e ENDF/B-VII.1, JEFF-3.3, JENDL-4.0, etc), which have been converted into the GEANT4 format. Such data are meant t replace the default G4NDL neutron library available with the standard GEANT4 distribution. In this way, GEANT4 users w have access to the complete list of standard evaluated neutron data libraries when performing Monte Carlo simulatio with GEANT4, have access to a larger list of isotopes and be able to estimate the systematic uncertainties in the result associated to the uncertainties in nuclear data.

- **Documentation**

  Information concerning the conversion process and verification tests can be found in:

  - E. Mendoza, D. Cano-Ott, R. Capote, Update of the Evaluated Neutron Cross Section Libraries for the

Current Status [1/2]

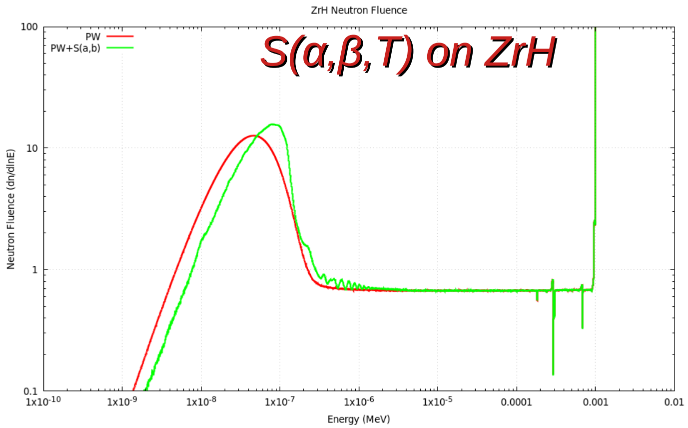
After ~1y of intensive implementation the work is **complete**

i. Modern implementation in **C++** with emphasis on:
  - physics results
  - optimization:
    a) by caching a lot of necessary information
    b) using adaptive algorithms to improve performance
    e.g. for the online exact Doppler broadening of the cross sections at any temperature
    c) improved sampling of secondary distributions
    d) An innovative idea: making a fast indexing of cross sections using a CPU-cheap $\log_2$ approximation by bit-shifting the internal representation of a IEEE754 floating point number,
    → greatly sped by a huge factor the cross section sampling.
  - “low” memory consumption

ii. Loading all G4NDL information including S(α,β,T)

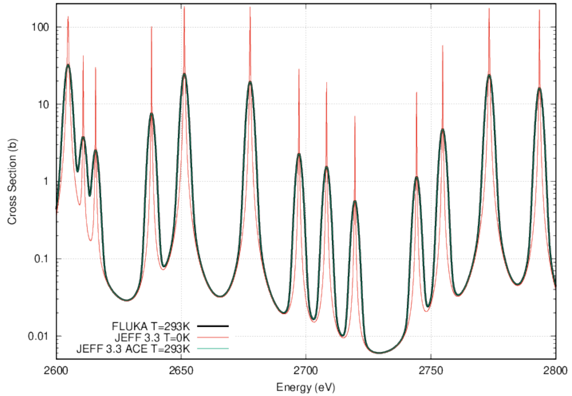
iii. Doppler broadening at any temperature on loading

iv. Perform “fully” correlated emission of reaction products by treating an N-body final state as a subsequent 2-body emission (kinematics gradually constraining database distributions)



S(α,β,T) on ZrH

Doppler broadening example



Current Status [2/2]

iv. Using FLUKA γ-de-excitation model to reproduce all known levels

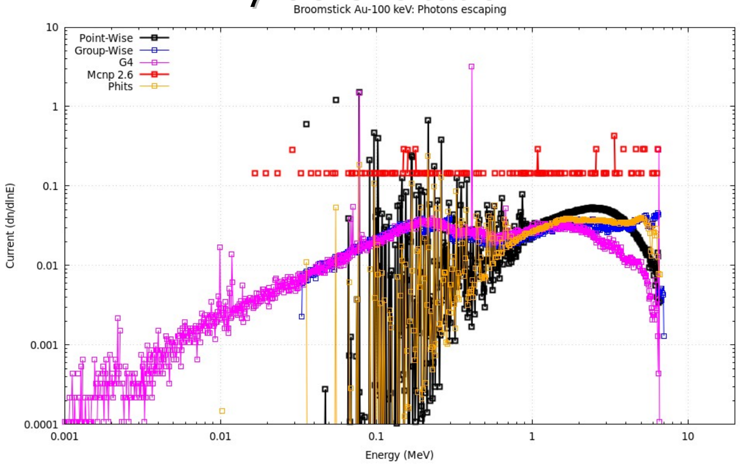
v. Ability to run mixed-calculations PW + GW

vi. Fission yields from databases and when not existing, sample from Wahl systematics

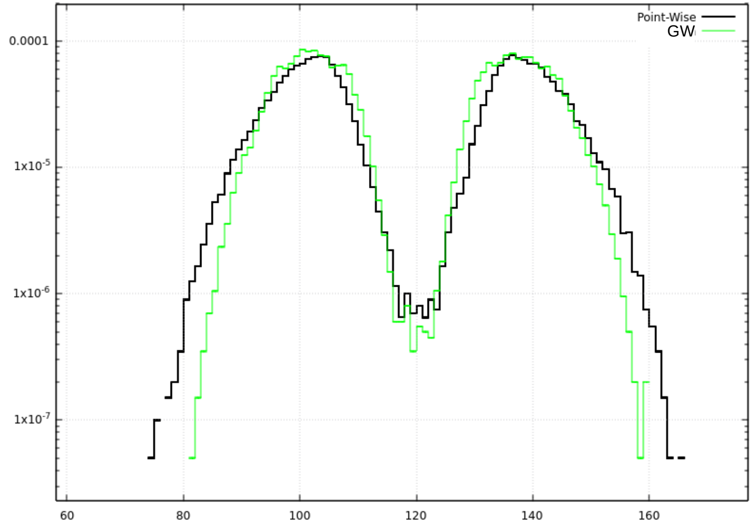
vii. Q-value correction per channel on loading

viii. Extensive testing/validation campaign (including all available databases)

γ-de-excitation



Fission yield from Wahl



Doppler broadening

- Doppler broadening is performed during initialization for all channels

$$\sqrt{E}\,\sigma\left(E,T_2\right)=C\int_0^{\infty}\sigma\left(x,T_1\right)\sqrt{x}\left[e^{-\alpha\left(\sqrt{E}-\sqrt{x}\right)^2}-e^{-\alpha\left(\sqrt{E}+\sqrt{x}\right)^2}\right]dx$$

$$a=\frac{A}{k\left(T_2-T_1\right)} \qquad C=\frac{1}{2}\frac{\sqrt{\frac{a}{\pi}}}{E}$$

- Using “*adaptive*” numerical integration, ensuring a precision higher than the initial cross section data=0.1%
- Pretty fast: about 20s on 3GHz single core to process all channels of the 550 isotopes

Hierarchical structure of XS

- The latest ENDF datasets contains the data for all isotopes (no more natural elements)
- On loading **total** cross sections are reconstructed for
  - per isotope ← from all channels (elastic, capture, fission, inelastic, S(α,β))
  - Natural element ← from the total of each isotope
- Random selection of element in material followed
  - by the isotope
  - 4 main channels (elastic, capture, inelastic, fission)
    - Elastic
      - 3 channels for S(α,β,T),
    - Inelastic
      - 36-channels for inelastic
      - up to 50 discrete composite channels (n,n'), (n,p),...(n,α)
    - Fission
      - 4-sub-channels for fission

Cross Section Sampling

- A huge CPU fraction, about 2/3 of the total time in neutronics is spent in sampling cross sections
- Cross sections are given as list of pairs $(E_i, \sigma i)$…
- Some channels can have up to half-million (E_i, σ_i) pairs e.g. $^{238}U(n,f)$
- Searching is time-consuming
  - e.g. material like CASTLEAD in nTOF spallation target having 12 natural elements (about 30 isotopes) requires on every step 4x30 ~ 120 XS searches
  - Each search is done by bisection
  - followed by a linear interpolation

Cross Section Searching algorithms

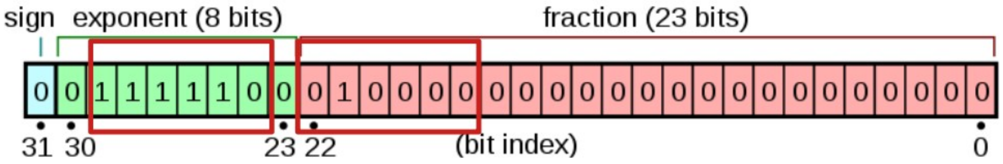
- Linear search O(n)
  Very slow
- Bisection O($\log_2$(n))
  Good performance
- Unionizing energies O(1)
  Very fast but huge memory needed
- Fractional Cascade O($\log_2$(n) + m*O(2))
  Good performance + 1/3 extra memory needed
- Indexing O(log + $\log_2$(fraction-of-n))
  Costly log(),exp() functions

where:

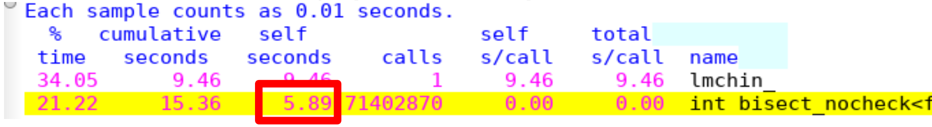
n is the number of *(E,σ)* pairs per channel
m is number of *channels*isotopes* to search

Innovative idea

→ calculate an approximate *$\log_2$(E)* indexing using only bit operations

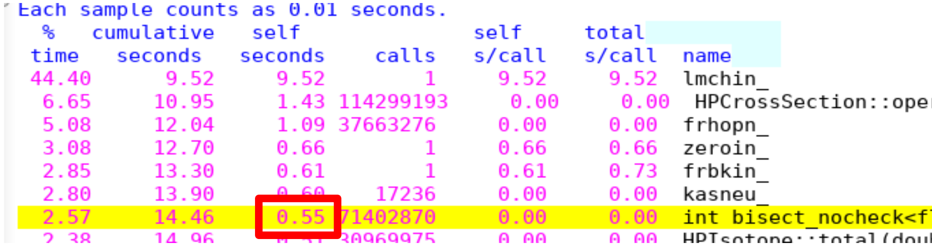


With no indexing (bisection)



```
Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls   s/call   s/call  name
 34.05      9.46     9.46        1     9.46     9.46  lmchin_
 21.22     15.36     5.89 71402870     0.00     0.00  int bisect_nocheck<f
```

With indexing (12bits ≈ 2156 entries/channel)



```
Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls   s/call   s/call  name
 44.40      9.52     9.52        1     9.52     9.52  lmchin_
  6.65     10.95     1.43 114299193     0.00     0.00  HPCrossSection::ope
  5.08     12.04     1.09 37663276     0.00     0.00  frhopn_
  3.08     12.70     0.66        1     0.66     0.66  zeroin_
  2.85     13.30     0.61        1     0.61     0.73  frbkin_
  2.80     13.90     0.60    17236     0.00     0.00  kasneu_
  2.57     14.46     0.55 71402870     0.00     0.00  int bisect_nocheck<f
  2.38     14.96     [illegible] 30969975     0.00     0.00  HPIsotope::total(dou
```

Gain x10

Elastic Scattering

Free Gas approximation

- Above few kT (~10eV) the target nucleus is assumed at stand still
- Below the target is sampled from a Maxwell Boltzmann distribution
  - Special attention is payed that to avoid kinematically impossible situations
  - Using a “constant” cross section model (valid for most of the elements)

Molecular Binding effects S(α,β,T)

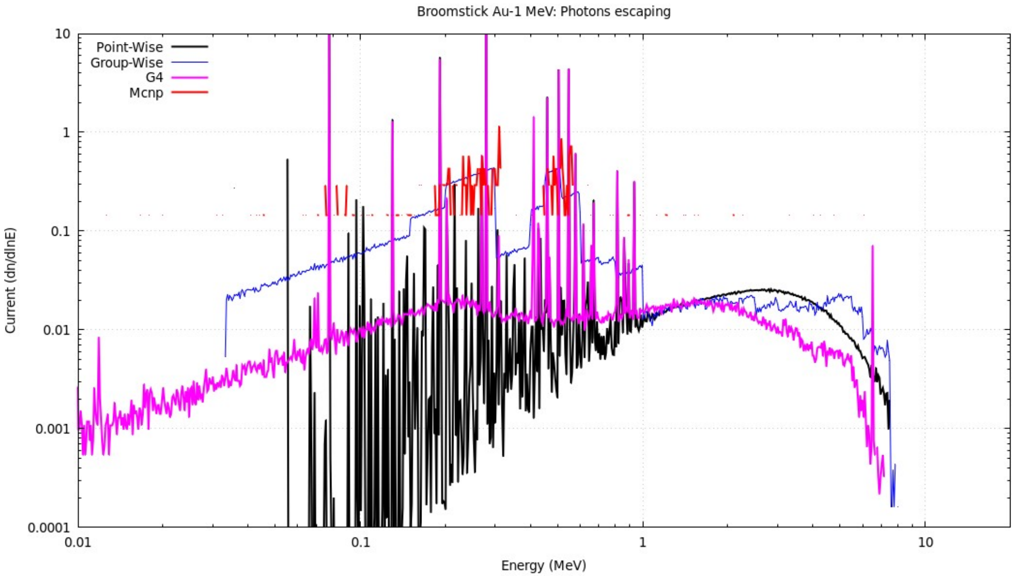
- Below 4eV the S(α,β,T) model is used:
  - Elastic scattering
    - Coherent
    - Incoherent
  - Inelastic scattering
- The supplied 3D tabulations are “*stretched*” in E to avoid aliasing effects produced by the sharp peak at $E_{in} = E_{out}$

Radiative capture

γ-lines are generated either:

1) from the FLUKA evaporation γ-de-excitation model (including all known levels and their correlations

2) sampling from the provided database distributions

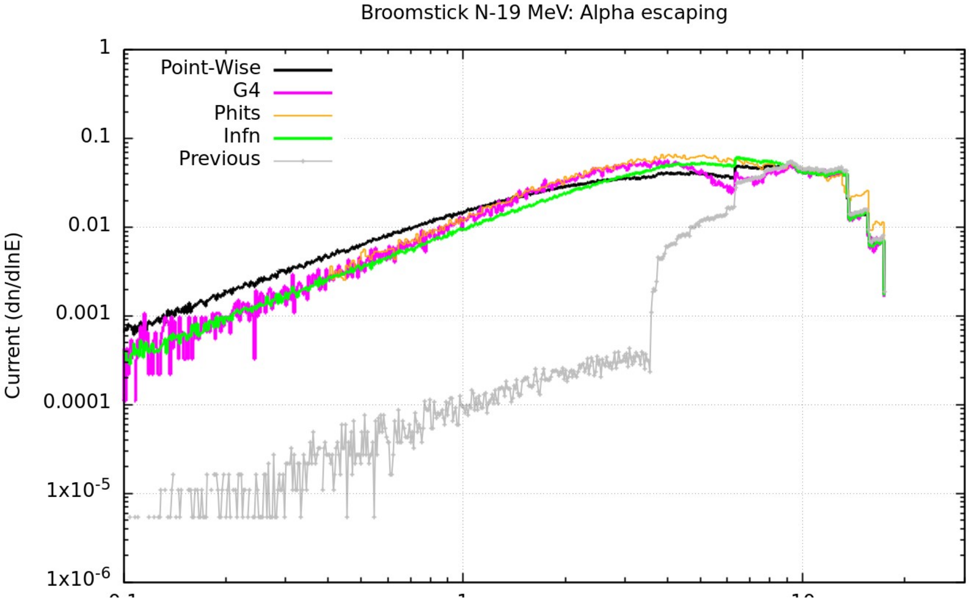


Inelastic channels

- All inelastic channels / secondary laws are handled giving priority to the emitted neutron.
- There are numerous protections for kinematically impossible situations and/or database artefacts
- If after several tries the interactions cannot close kinematically e.g. improper threshold energy vs Q-value (especially for natural elements), the code aborts the interactions and resamples another channel

Channels with missing information

- For very few isotopes some channels were missing any secondary particle information
- **(n,n')** to the continuum
  → replaced with a flat probability sampling from the highest level to the maximum allowable energy
- **(n,cp)** (charged particle)
  → replaced with n-body phase space distribution up to a max energy of allowed by the kinematics
- **(n,xn)** (+ neutron as ejectile)
  → replaced with an evaporation spectrum with an average temperature T=1MeV

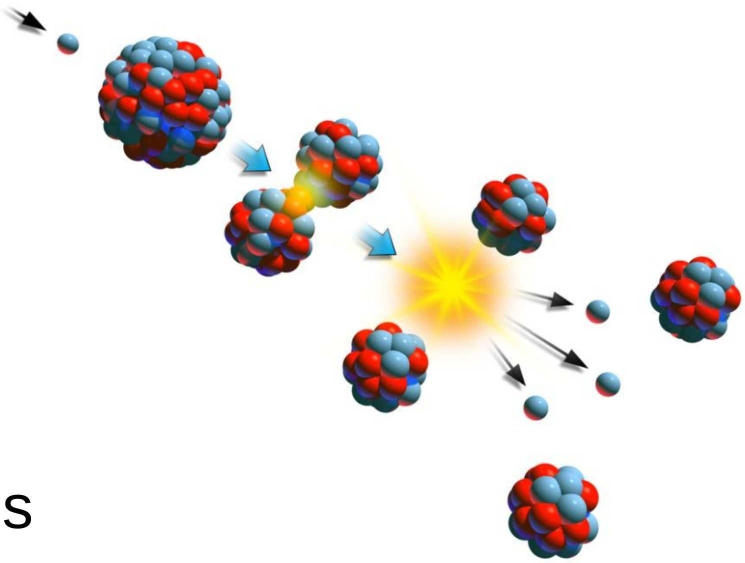


$$P_i^{\mathrm{CM}}(\mu, E, E') = C_n \sqrt{E'}\,(E_i^{\max} - E')^{(3n/2)-4}$$

$$f(E \rightarrow E') = \frac{E'}{I} e^{-E'/\theta(E)}$$

Fission timeline

1. Compound nucleus n+(Z,A) → (Z,A+1)
2. ~10% neutrons emitted pre-scission
   if kinematically possible
3. Scission → Split into two ~~or three~~ fragments
4. Excited fragments emit prompt neutrons
   proportionally to their neutron excess and
   gammas from the database distribution
5. Fragments can further emit delayed neutrons
   not implemented!
6. Beta decay and neutrino emission of fission
   fragments

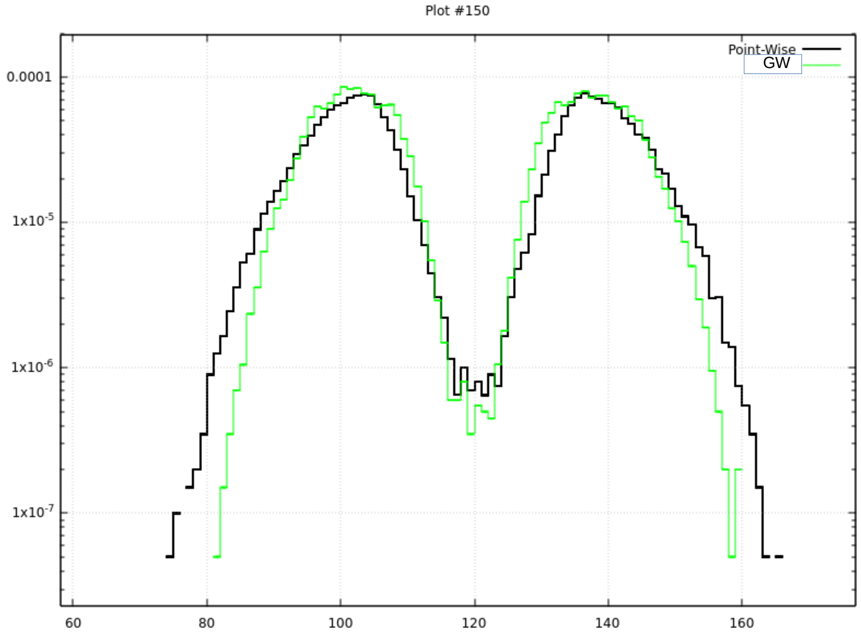


Mass/Charge distribution

- past: FLUKA for the high energy fission uses a simplistic model with two Gaussian distributions

- current: sample from the yield distribution if available, else use WAHL systematics:
  A fit of 7 Gaussian’s with their parameters depending on the isotope, kinetic energy of the incoming neutron etc.. They are described as a fit of the 11 isotopes where information exists.

- Z-charge per fragment is given as a Gaussian spread from the line of stability

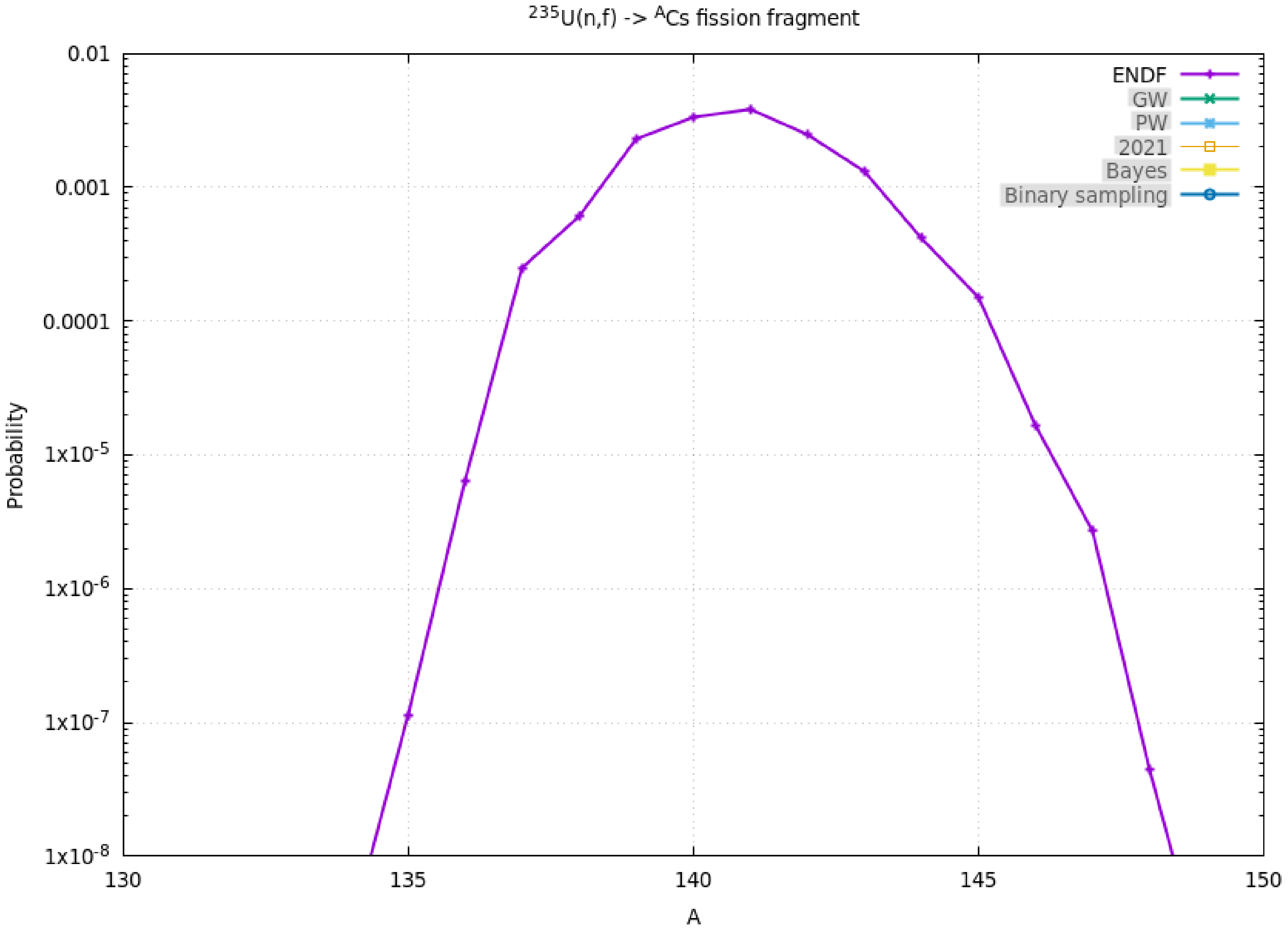


Artefact of correlated sampling

- Fission fragment from: ^{235}U(n,f) yield of ^{137}Cs
- GW: fission fragments are produced as residual nuclei from NJOY which gives directly the production probability of each (A,Z)
- PW:
  - Sample first FF from ENDF (A,Z)
  - Sample neutron multiplicity from a Poisson distribution
  - Calculate second fragment as:
    $Z_2 = Z - Z_1$
    $A_2 = A + 1 - A_1 - n$

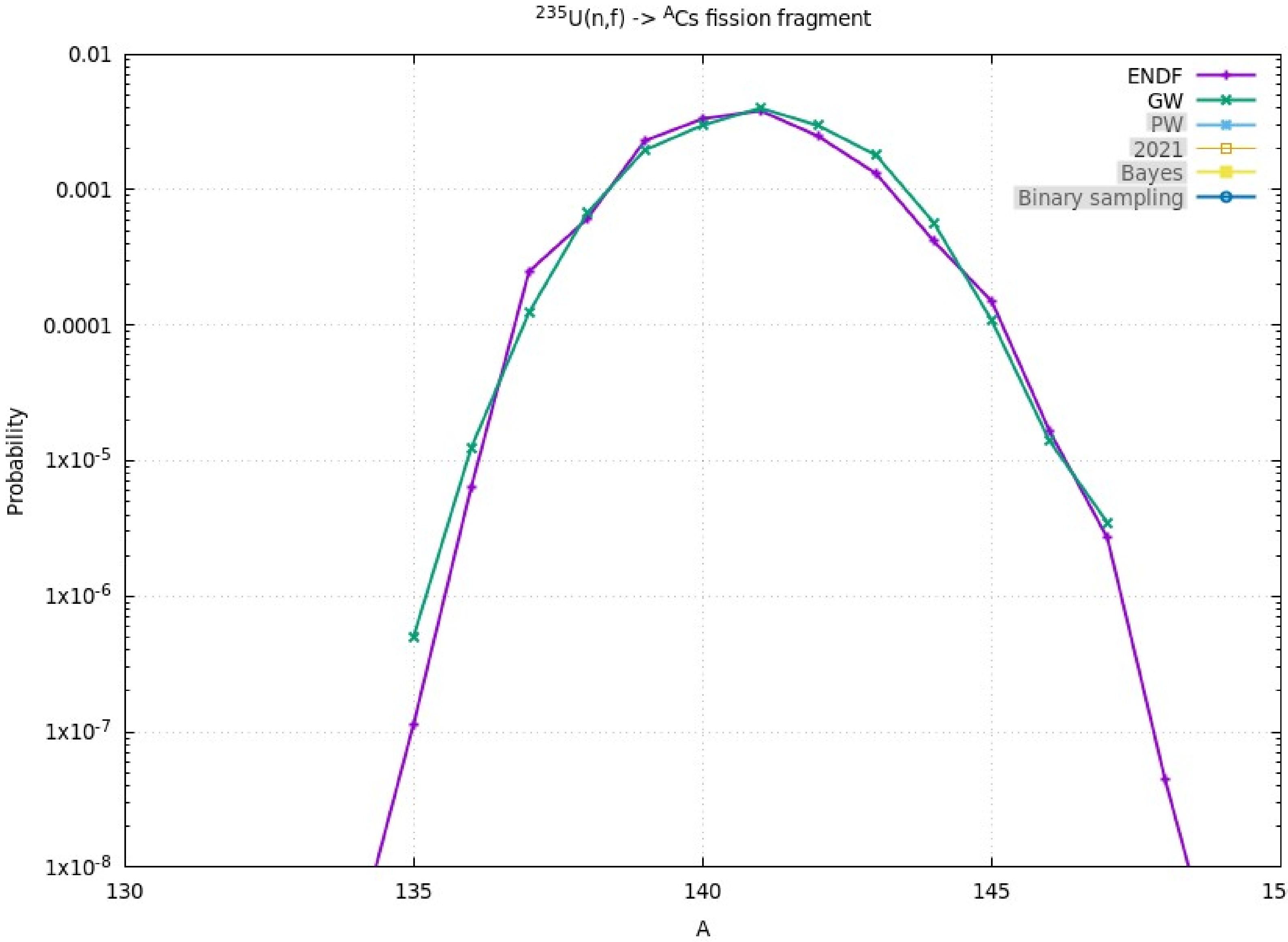
^{137}Cs

ENDF VIII.0
data



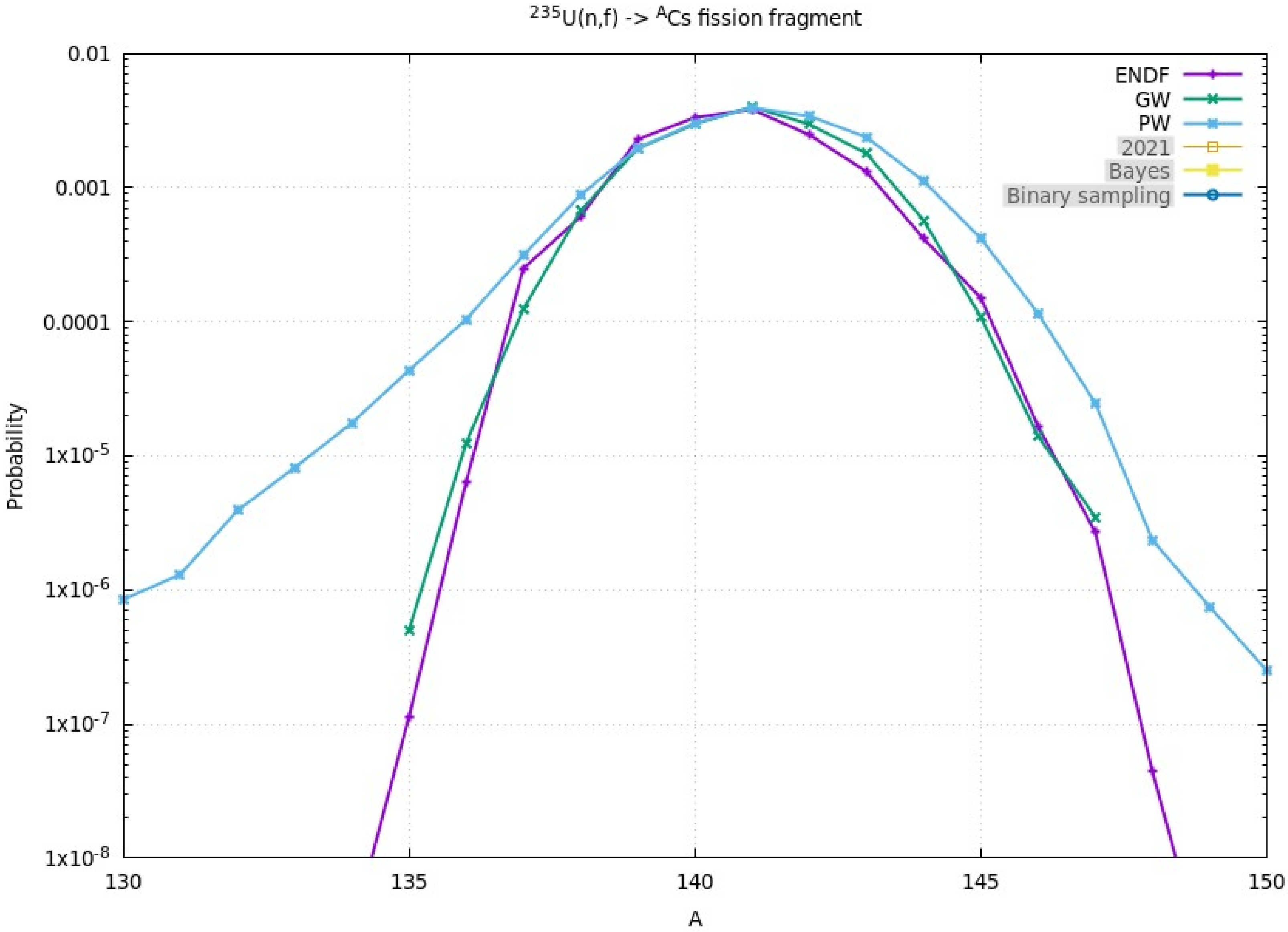
^{137}Cs

Group Wise sampling from ENDF-VI (or VII) data



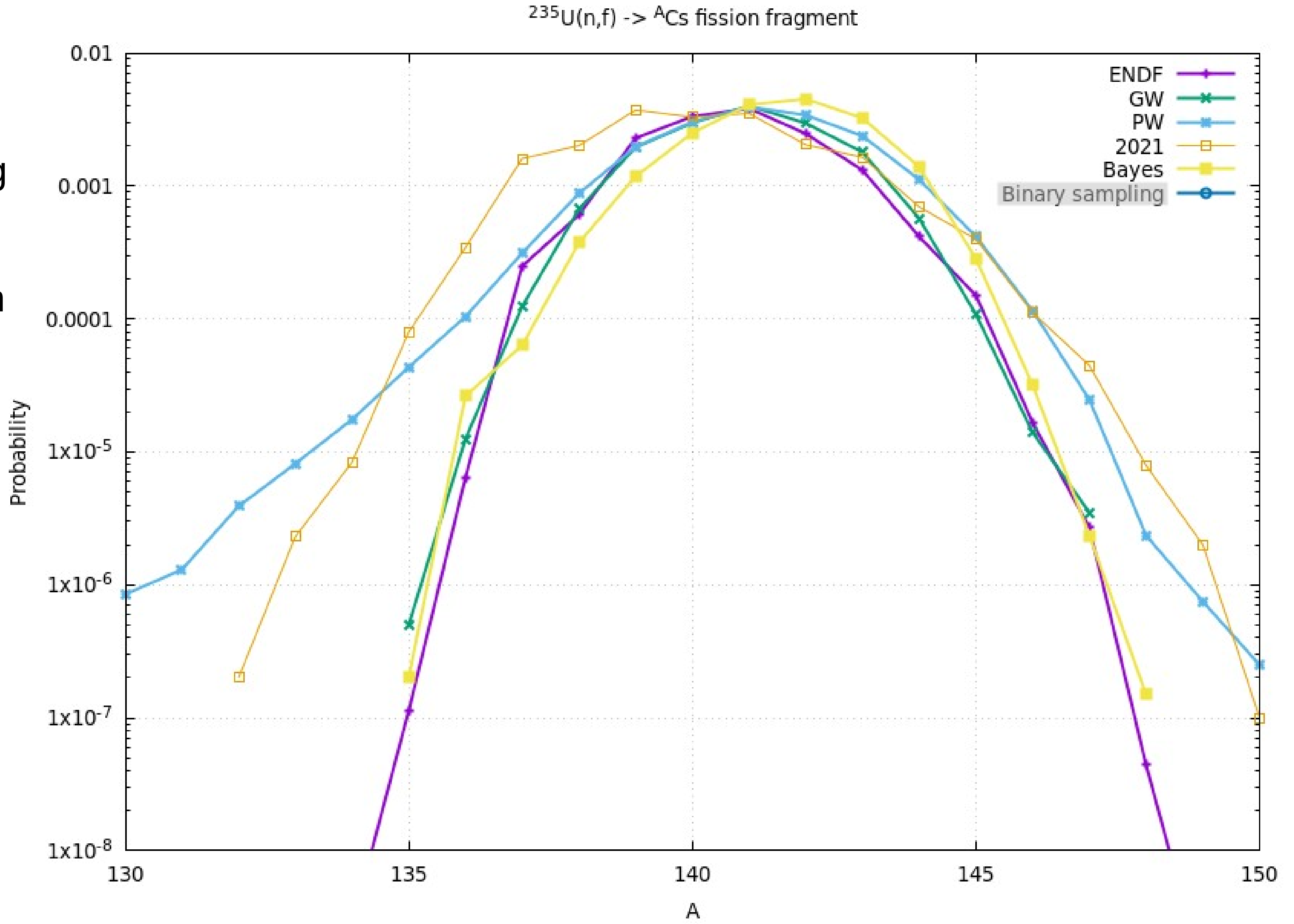
^{137}Cs

Actual implementation. Secondary FF is smoothed from the Poisson distribution sampling



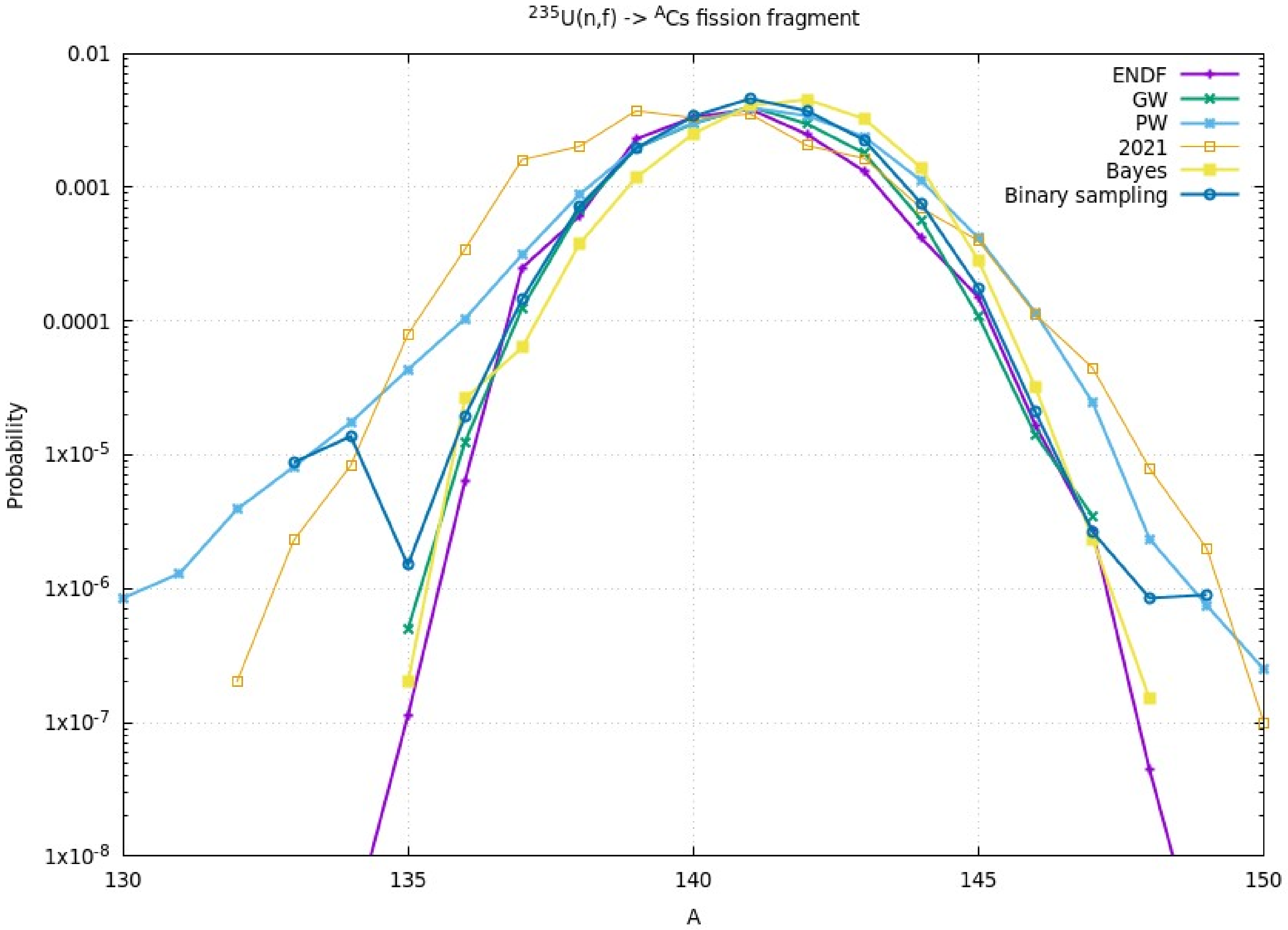
^{137}Cs

Altering secondary FF distribution using Bayes for the various P(n) assuming a Poisson distribution with multiplicity equal to the global one.



^{137}Cs

Sampling either |ν| or |ν|+1 as multiplicity



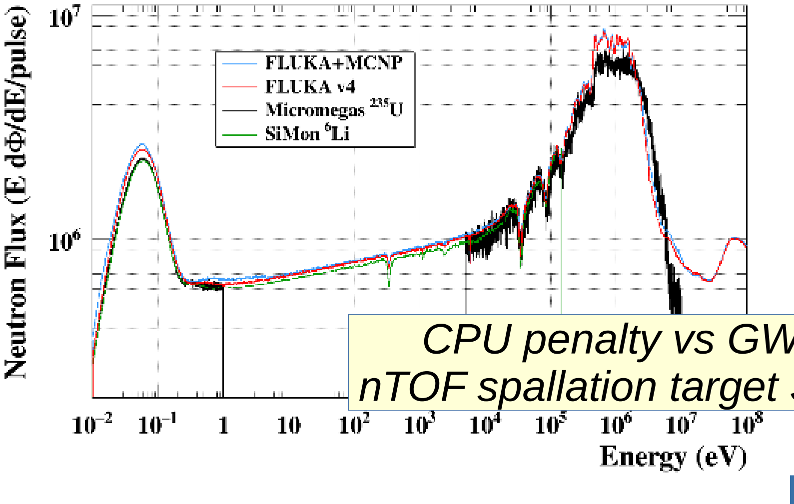
^{137}Cs

- Unfortunately Bayesian altering assumes the same neutron multiplicity for each FF, therefore it alters the final neutron multiplicity
  Reducing total multiplicity by: 33%!
  From 2.4 → 1.6 @ E_n=100keV
- "*Best approach*" was to use the binomial sampling
  - Respects the neutron multiplicity
  - Alteration of the FF spectrum is small
    Still generates some artifacts

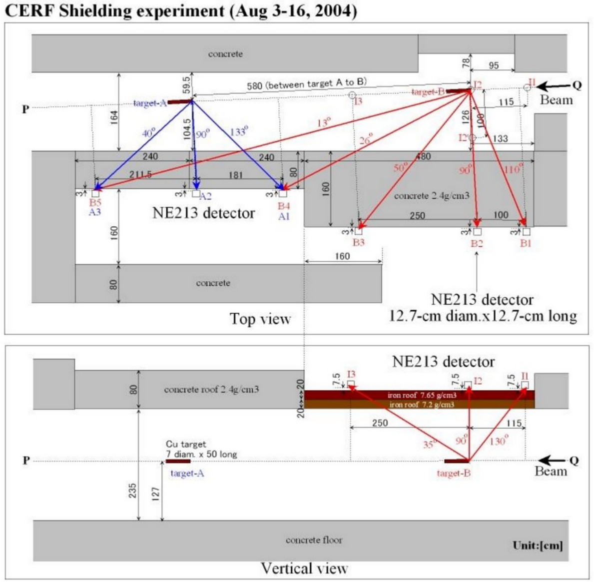
Performance and Validation

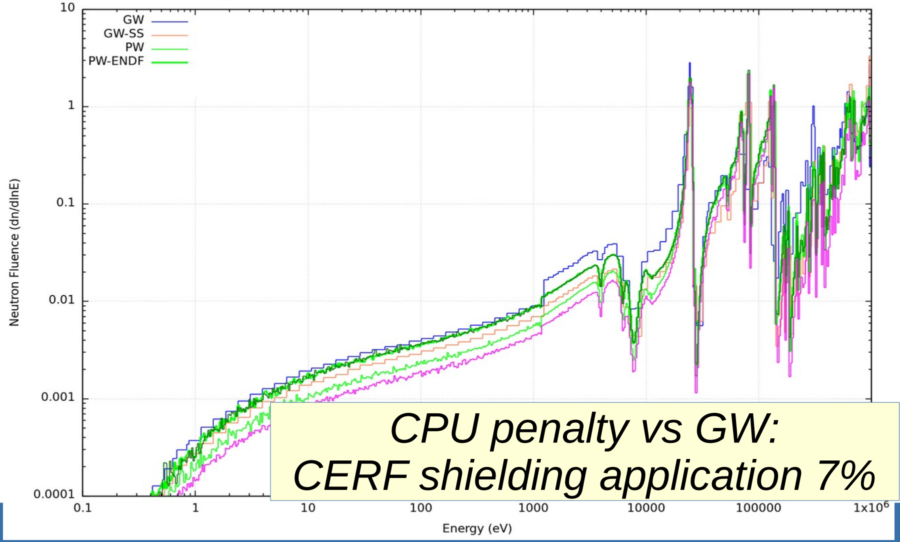
- An extensive testing campaign:
  - single interactions
  - secondary distributions
  - complex cases
- has validated both physics and CPU performances

nTOF EAR2 neutron flux



CPU penalty vs GW:
nTOF spallation target 30%





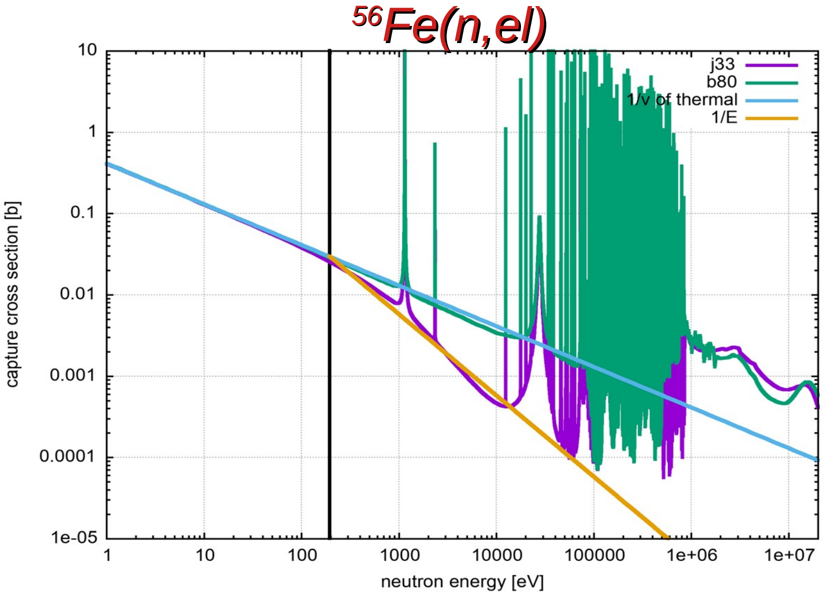
CPU penalty vs GW:
CERF shielding application 7%

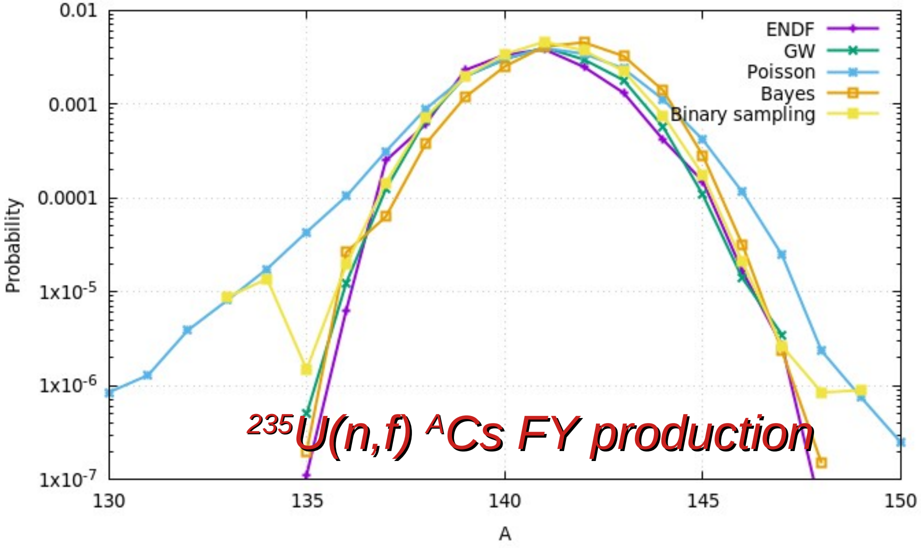
Problems

- Data issues:
  - Wrong or imprecise data
  - Inconsistent Q values
  - Uncorrelated description of secondary distributions
  - Artifacts in data: Non-physical structures or jumps in distributions

→ forces the use of adhoc solutions

- "*Correlation*" on inclusive data → biases the final distributions.





Summary

- FLUKA v4 neutron PW implementation is complete available from v4-3.0 (released on Sep 2022)
- Novel C++ implementation based on the Geant4 neutron processed data with emphasis:
  - Physics results
  - “Correlated” emission of interaction products
  - Performance → resulting in “small” CPU penalty

FLUKA