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Using EXFOR for Fission Product Yield Calculations

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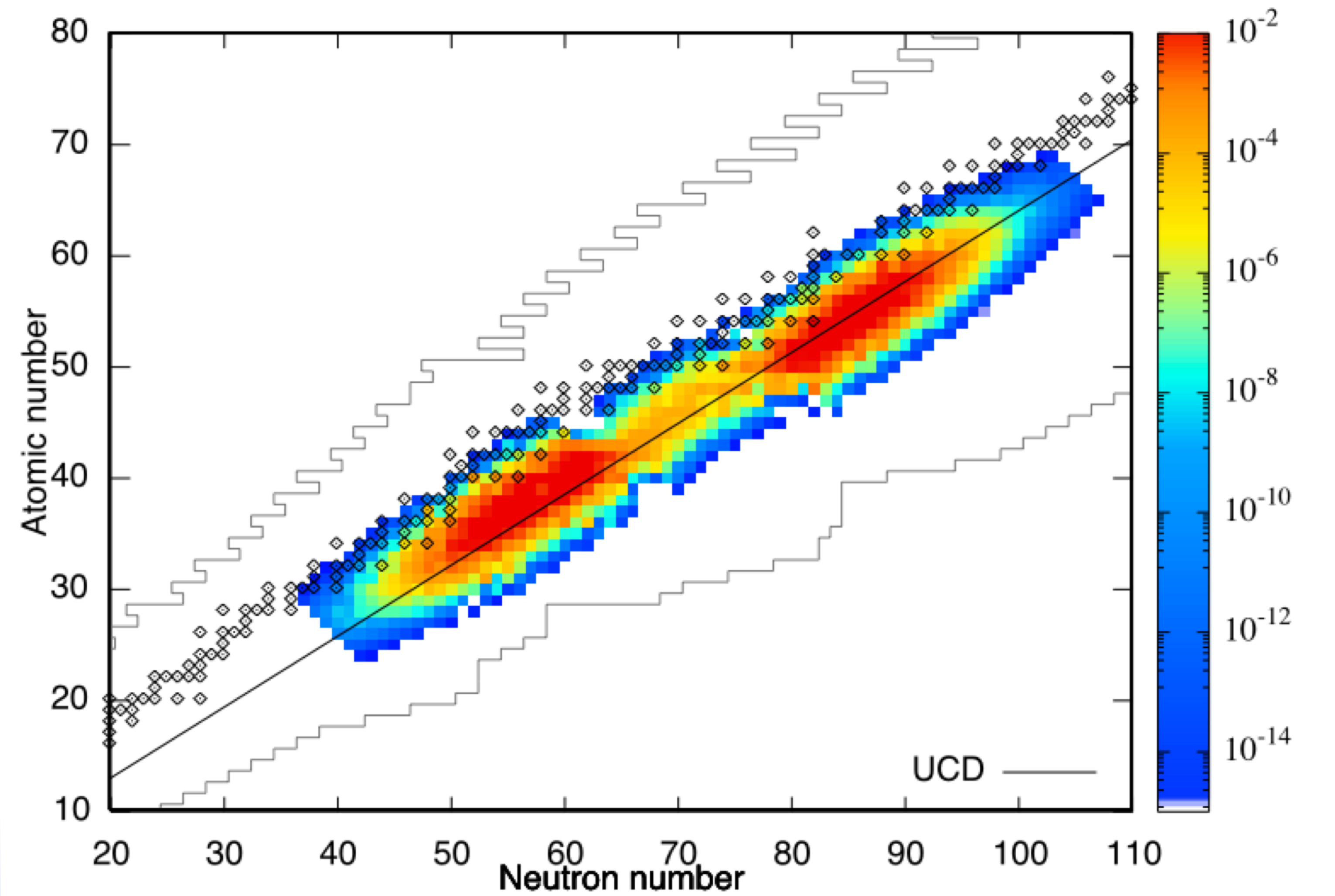
  6. Connection to the theoretical fission model (4D Langevin)

Fission product yield

- Wide variety of fission products (more than 1,000 nuclides) are produced during the fission process of actinides such as ^{235}U.

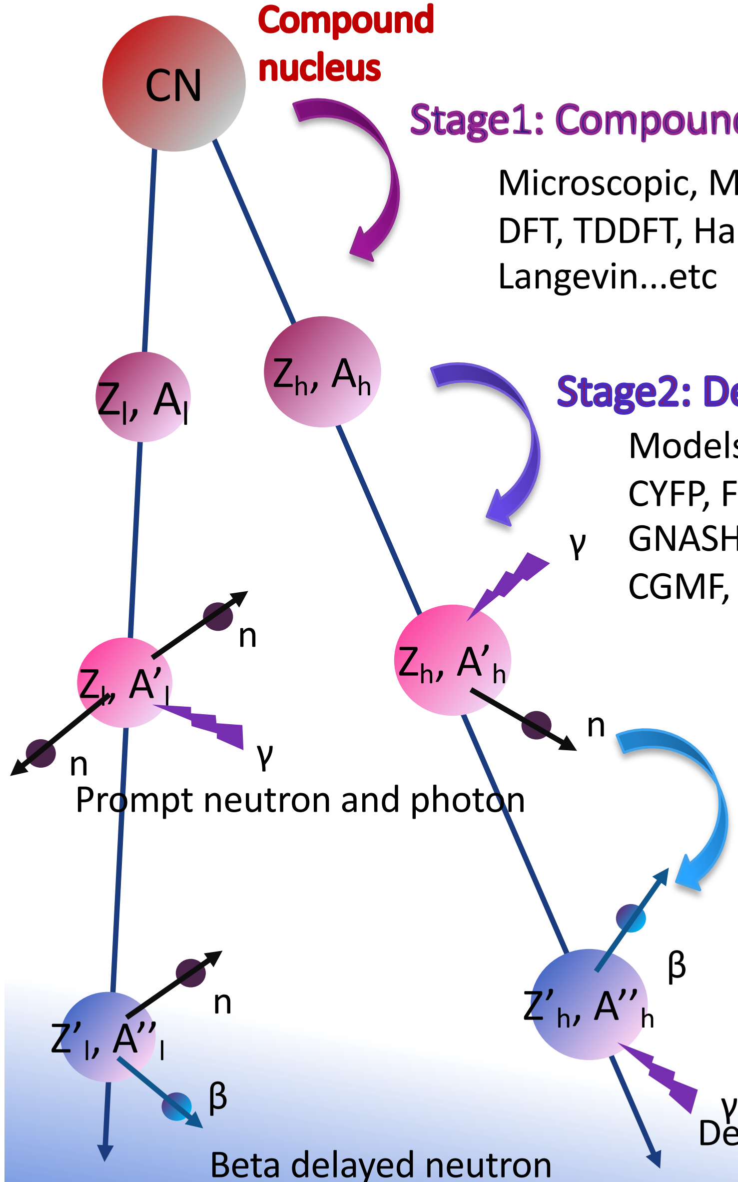


Well understood?

Independent yield of $^{235}U(n_{th},f)$ in JENDL-FPY/20111

Nuclear fission and decay processes

- An accurate prediction of fission observables by theoretical calculations are still remain difficult.



Stage1: Compound nucleus formation to scission

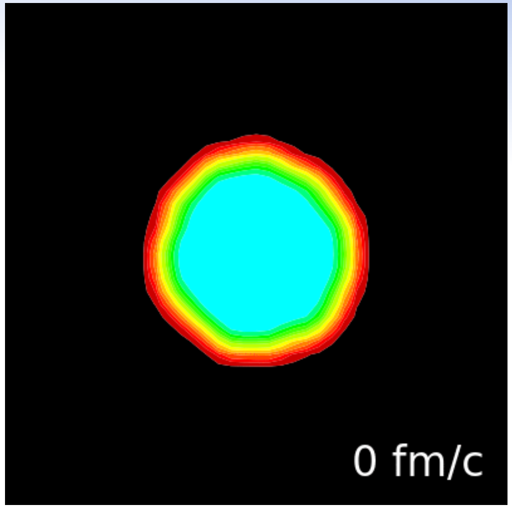
Microscopic, Macroscopic approaches:
DFT, TDDFT, Hartree-Fock-Bogoliubov, AMD, Langevin...etc

Stage2: De-excitation of fission fragments

Models and codes:
CYFP, FREYA, GEF, FIFRELYN, GNASH, EMPIRE, TALYS, CCONE, CGMF, CoH/BeoH, ..etc

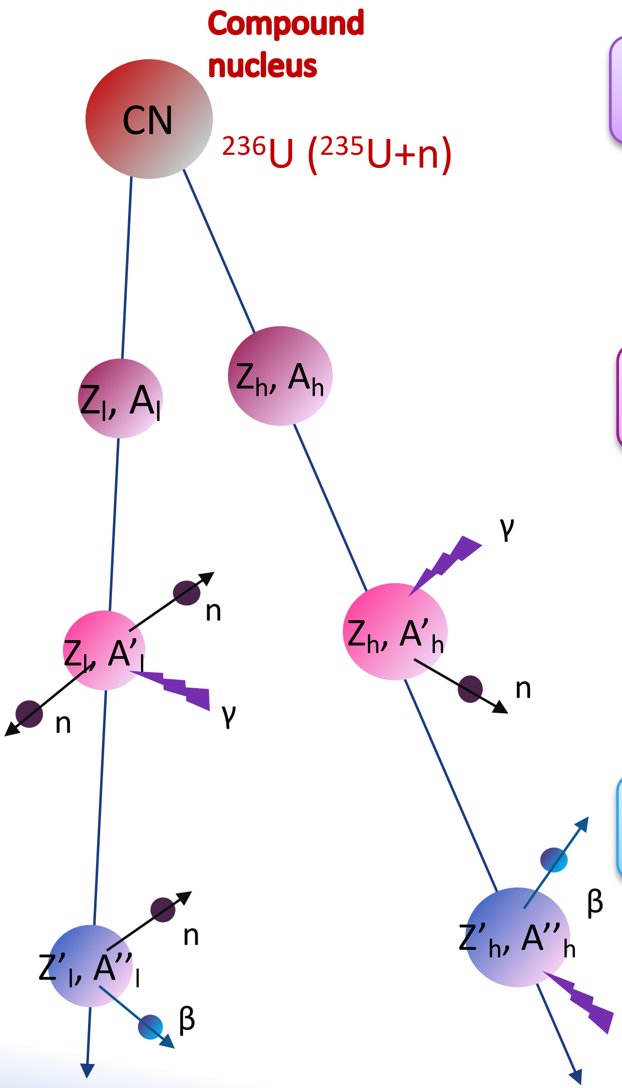
Stage3: Beta decay

Bateman equation, Gross theory, Summation calculation
Decay Data



By AMD simulation: Anti-symmetrized Molecular Dynamics (A. Etori and S. Chiba in Tokyo Institute of Technology, tba)

Definitions of FFY and FPY



Primary FFY

- $Y_P(Z,A,M)$

Neutron-rich atomic fragment just after scission

Independent FPY

- $Y_I(Z,A,M)$

Produced directory from fission, but after emission of prompt neutrons and photons, but before any radioactive decay.

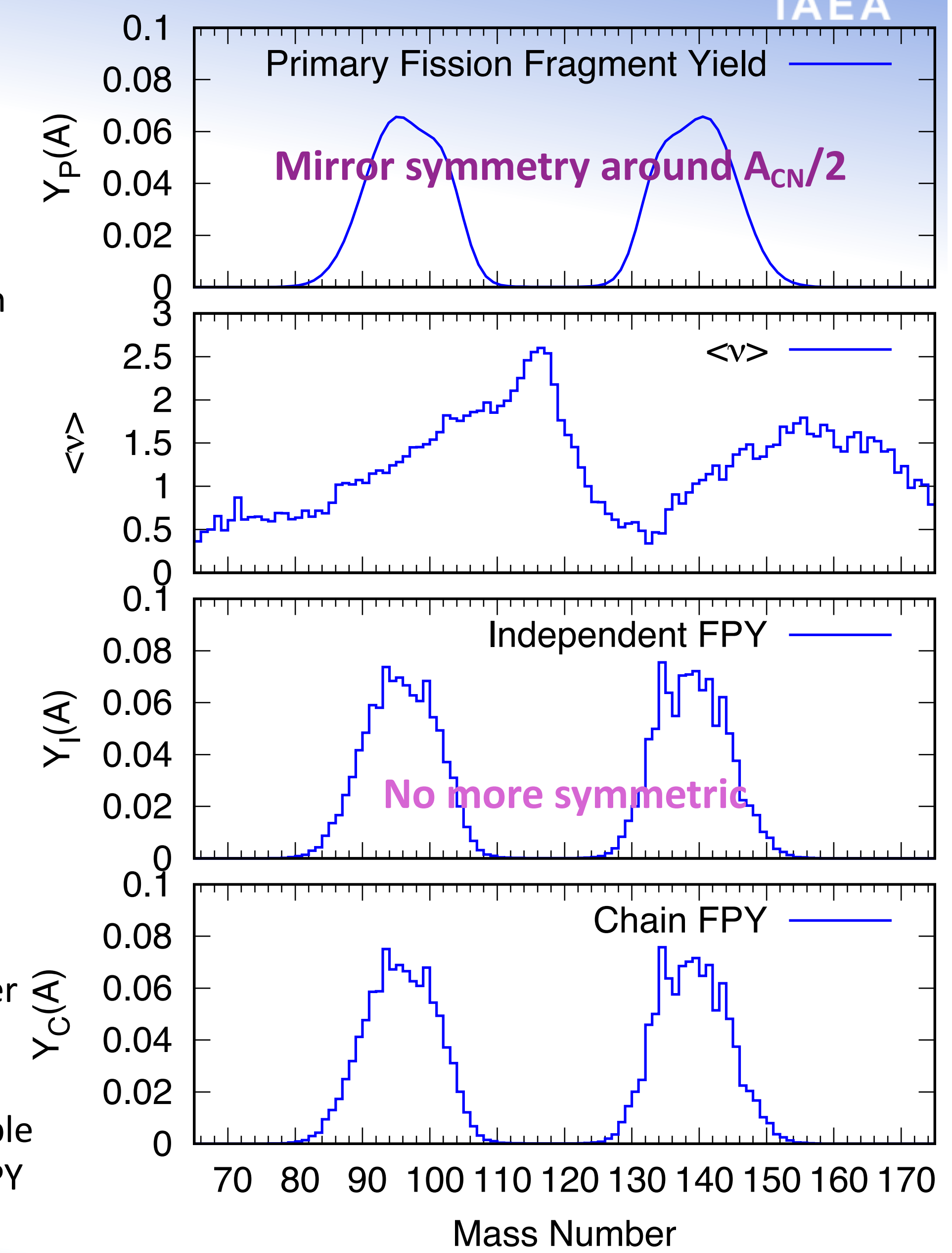
Cumulative FPY

- $Y_C(Z,A,M)$

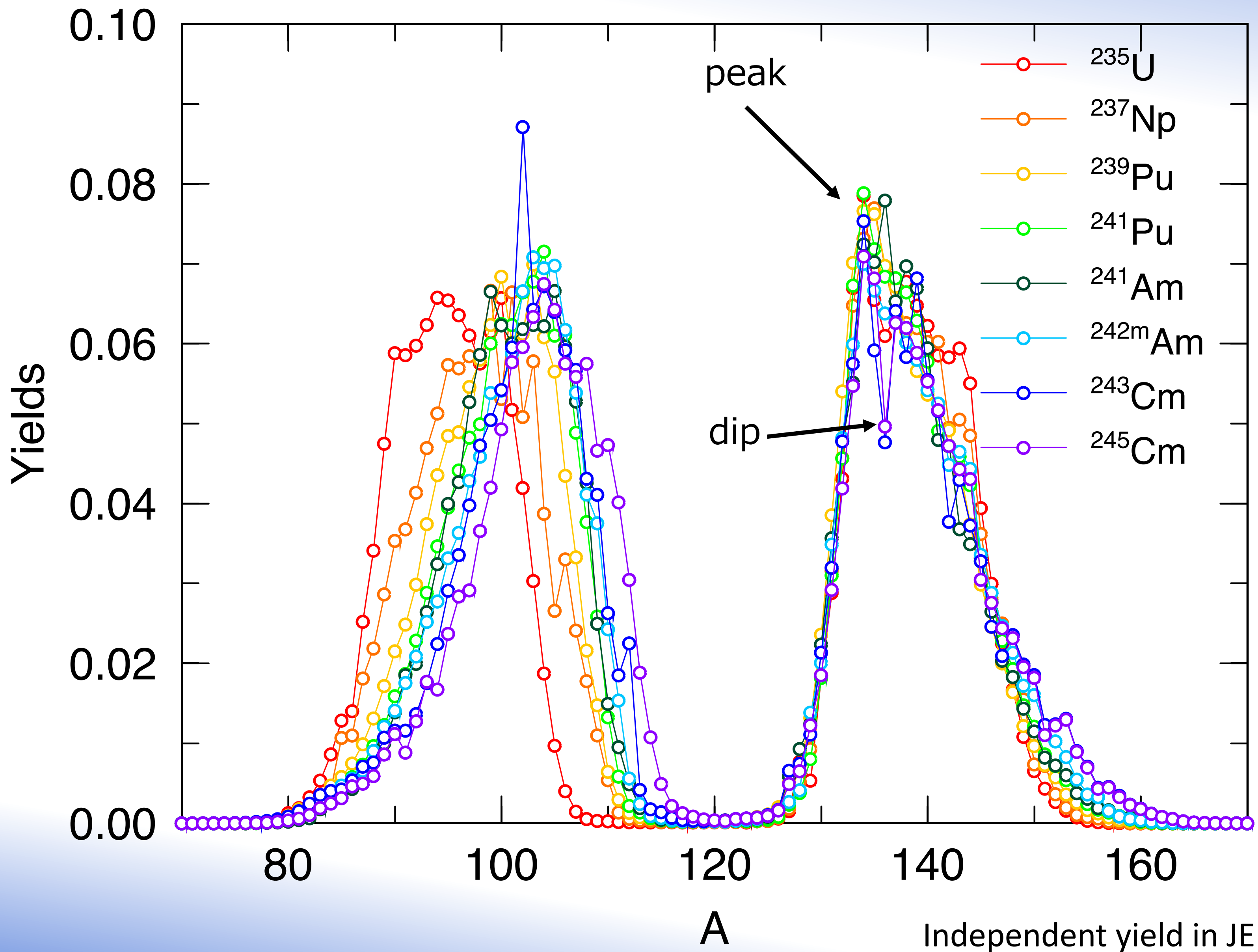
Produced over all time after one fission.

Chain FPY

Equal to the sum of all stable or long-lived cumulative FPY for a given mass chain.

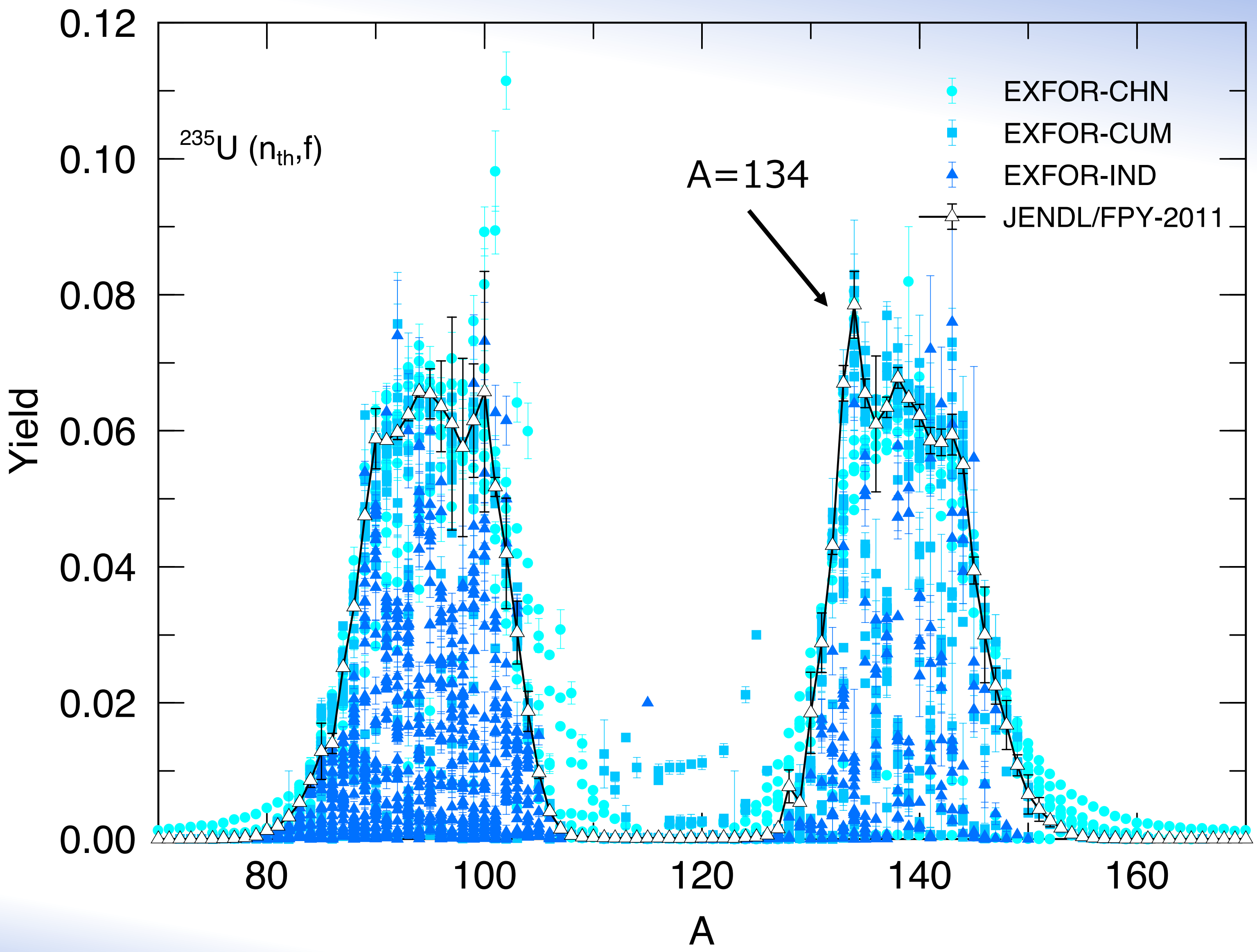


Mass distributions of independent FPY



Independent yield in JENDL-FPY/20111

Mass distribution of FPY



Comparison of $^{235}U(n_{th},f)$ FPY between JENDL/FPY-2011 and experimental data taken from EXFOR

Charge distribution of FPY

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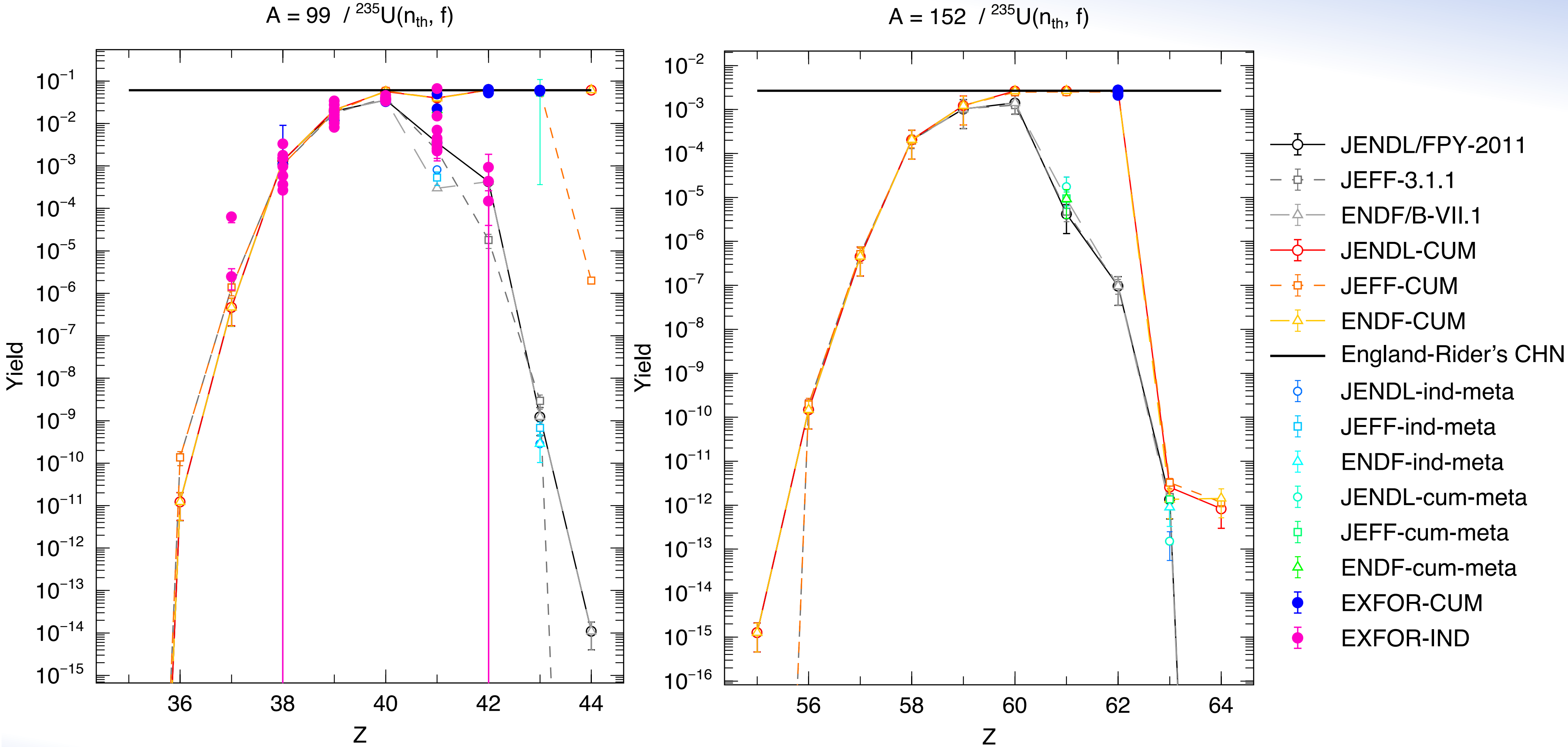
- Charge distributions are not well known in some mass ranges.

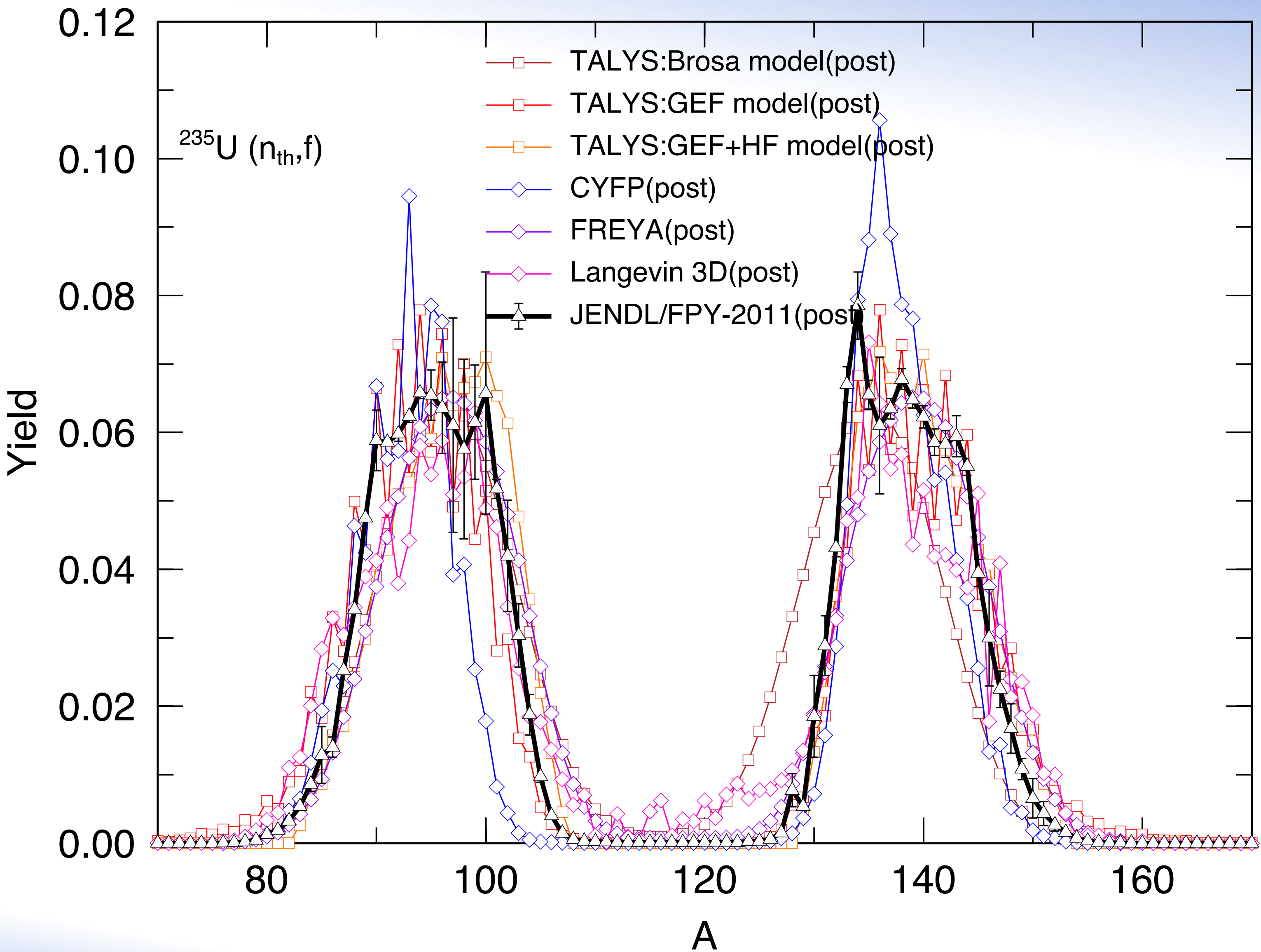


- Evaluated nuclear data libraries contains the charge distribution by Wahl systematics (Z_P model).

$$Z_P = \frac{A_c}{Z_c} A + \Delta Z$$

A.C. Wahl, Technical Report LA-13928,(2002).

Codes comparison

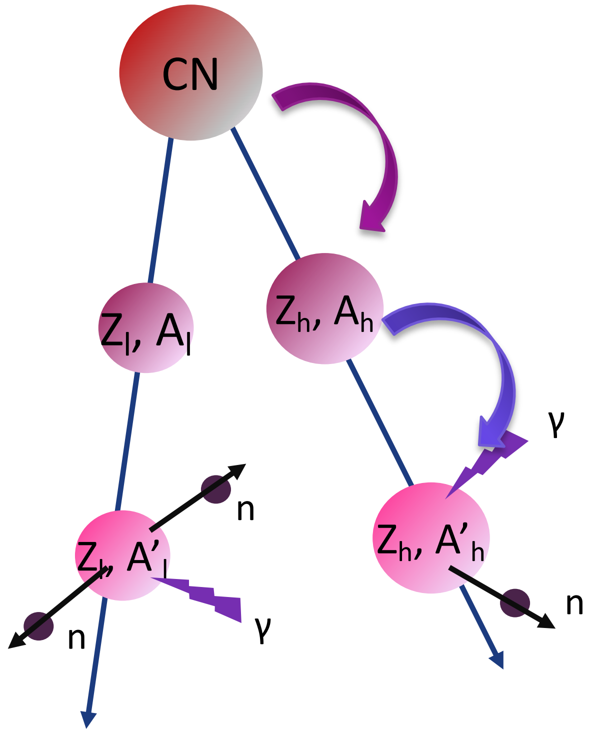


Comparison of $^{235}U(n_{th},f)$ FPY between JENDL/FPY-2011 and calculated

- No code reproduced the fine structure of $Y_I(A)$ perfectly.

Distributions of each decay stage

- Calculation of independent FPY require the stochastic distributions of primary fission fragments



Stage 1: Distributions of the primary fission fragments (Monte Carlo)

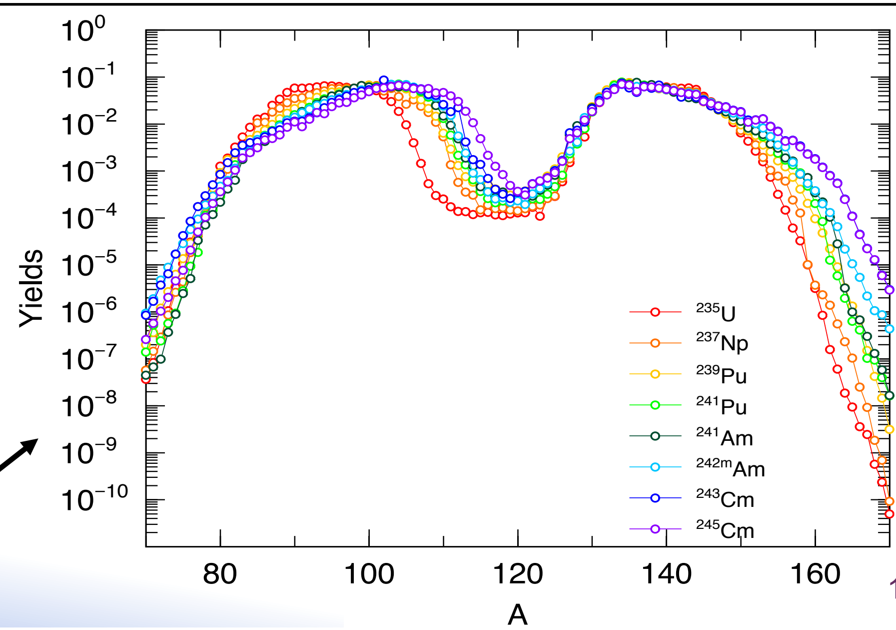
- Mass, charge $Y(Z, A)$ of fission fragments (just after the scission)
- Spin and parity distribution $R(J, \Pi)$ in the fission fragments
- Total kinetic energy (TKE) and total excitation energy (TXE)

Stage 2: Distributions in the evaporation process (MC, deterministic)

- Level density of all nuclei in the de-excitation chain
- Neutron and photon competition (strength functions) at each excited states

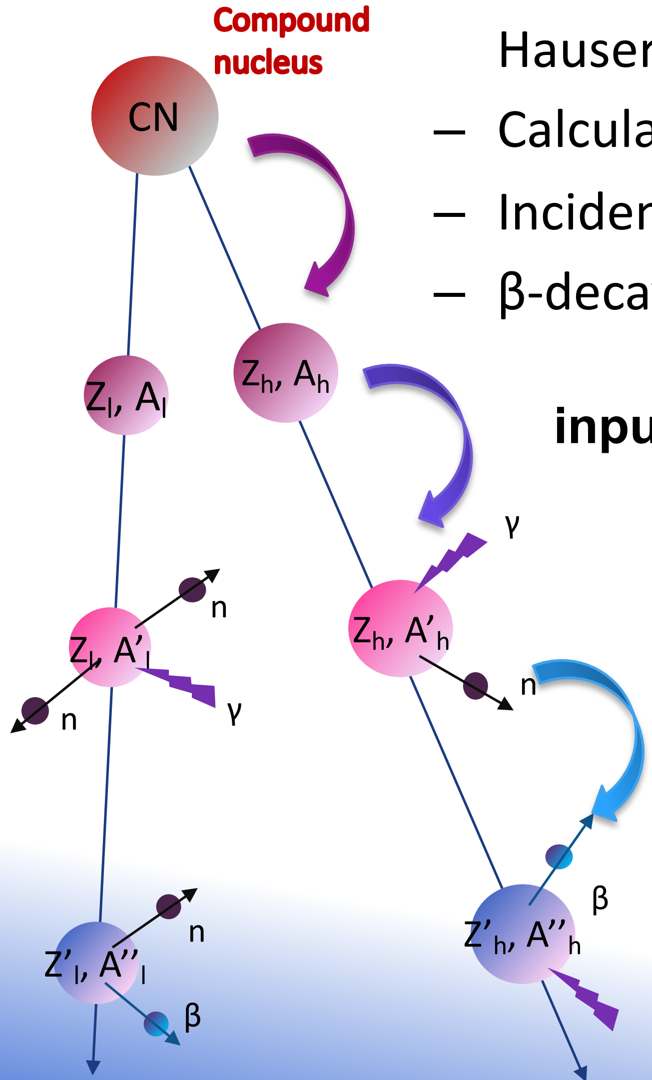
Calculation of the prompt fission neutron and γ-ray emissions requires to integrate (sum) over these distributions.

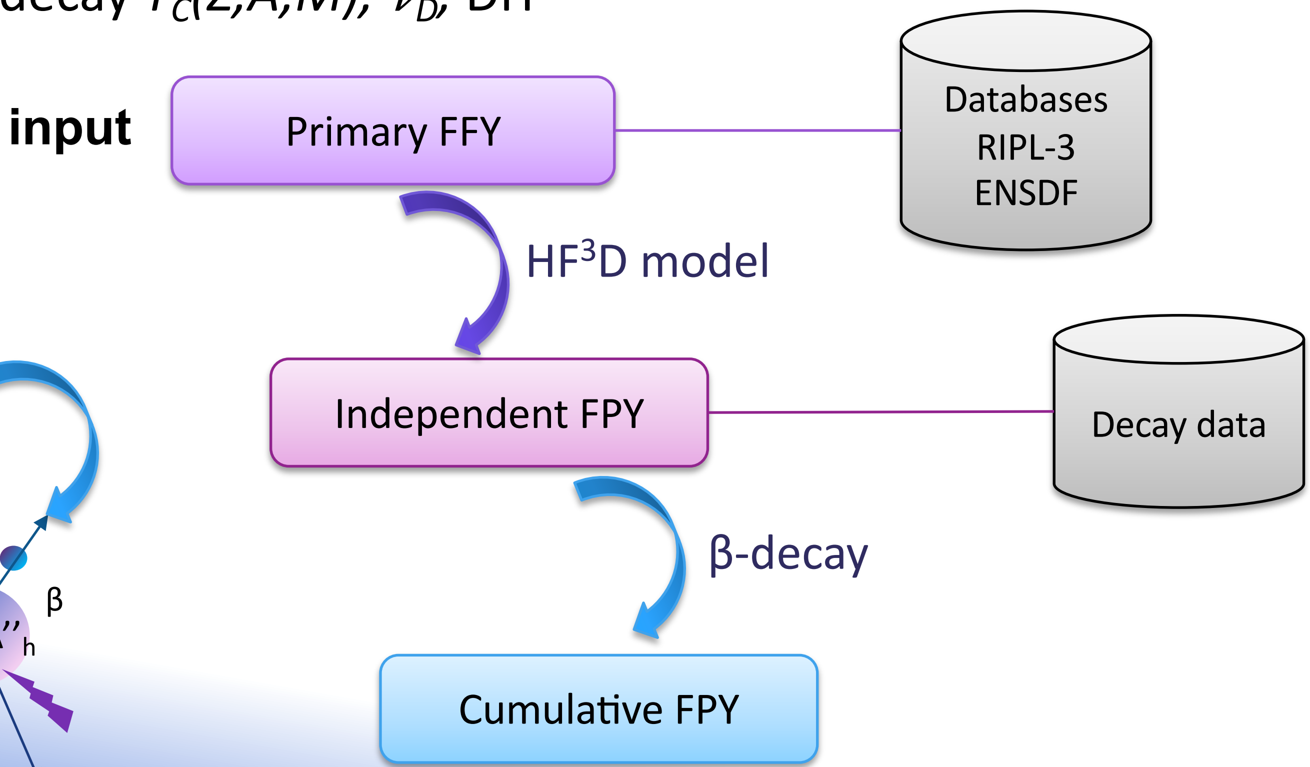
in the order of magnitude: 10^{-11} to 10^{-2}



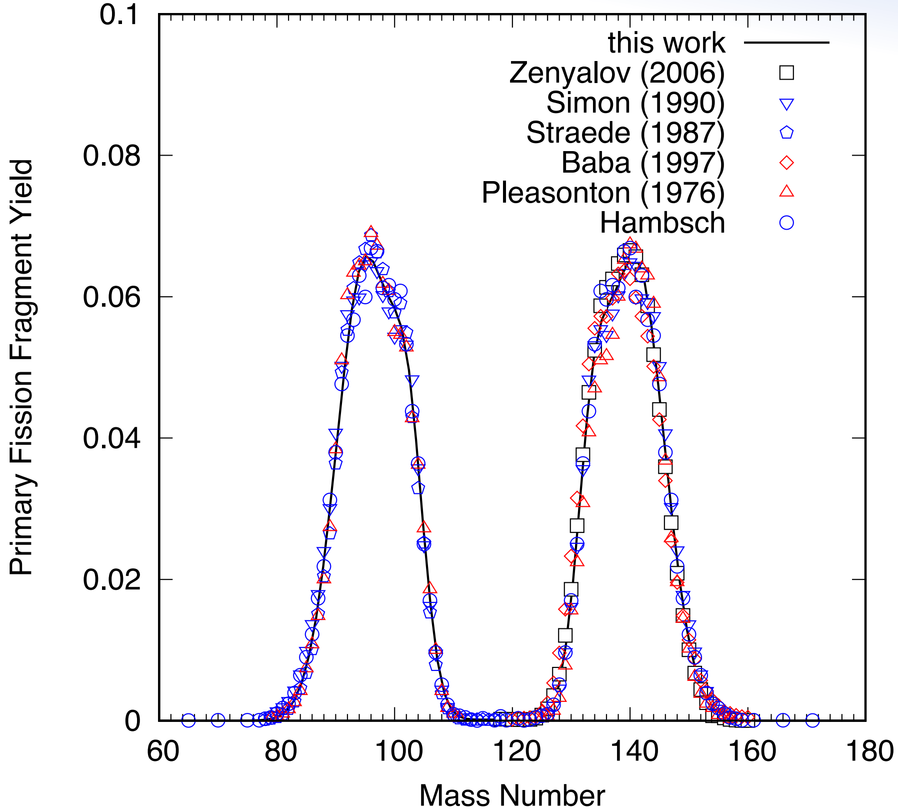
Deterministic Fission Fragment Decay model (HF^3D) + β-decay

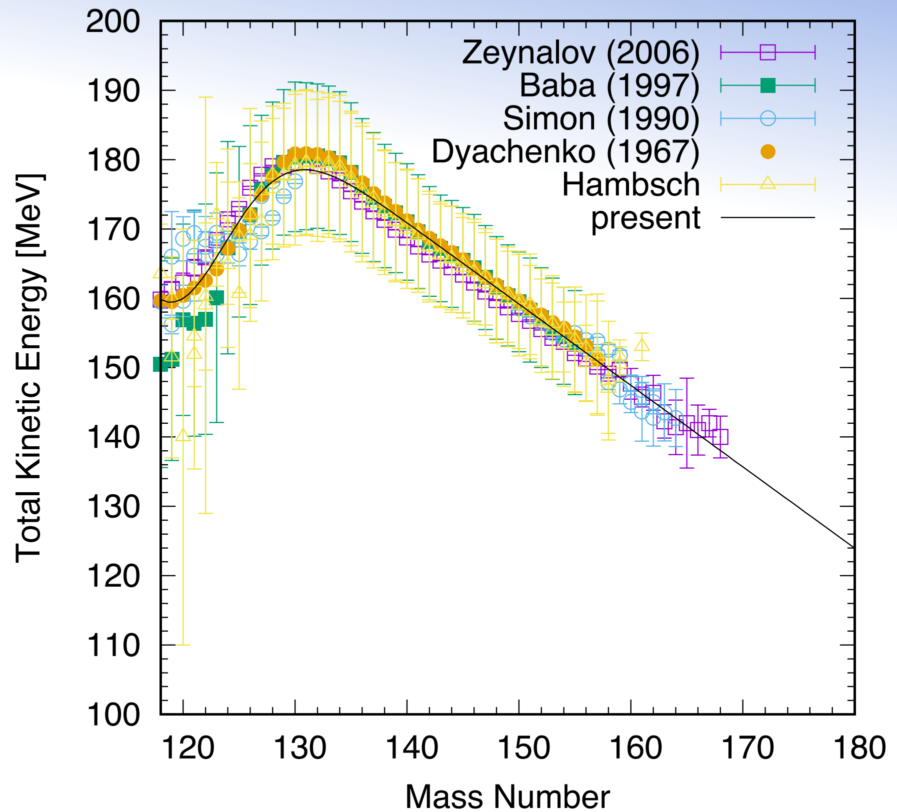
- Los Alamos and Tokyo Tech developed the deterministic way of the Hauser-Feshbach Fission Fragment Decay calculation model, HF^3D.
  - Treat a primary fission fragment as a compound nucleus for Hauser-Feshbach statistical decay
  - Calculate $\bar{\nu}$, $\bar{\gamma}$, $\chi(E)$, $Y_I(Z,A,M)$
  - Incident neutron energy (E_{in}) < 5 MeV
  - β-decay $Y_C(Z,A,M)$, ν_D, DH





Initial distribution of primary fission fragments (inputs)





Generating the distribution of primary fission fragment $Y_P(Z, A, TKE)$

$$Y(A) = \sum_{i=1}^{5} \frac{F_i}{\sqrt{2\pi}\sigma_i} \exp\left\{-\frac{(A - A_m + \Delta_i)^2}{2\sigma_i^2}\right\}$$

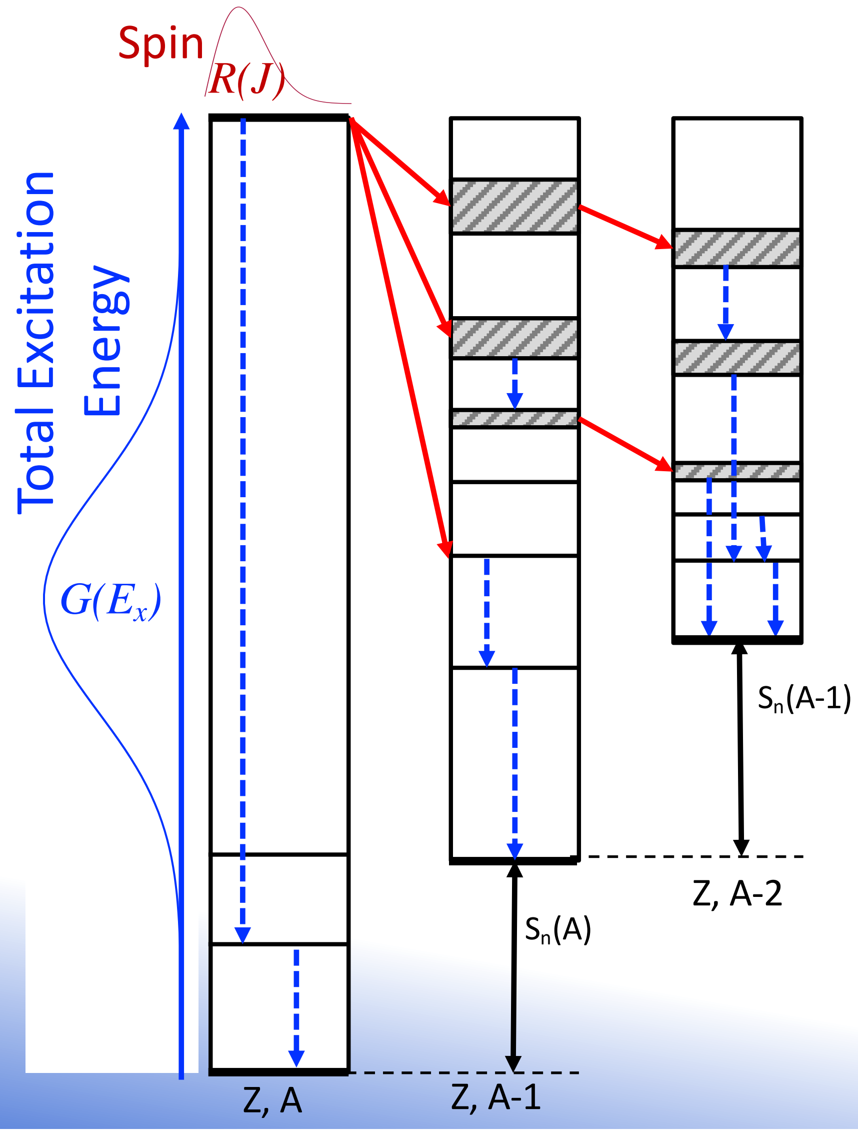
- The primary fission fragment mass distribution $Y_P(A)$ is approximated by five Gaussians.
- The charge distribution was generated based on Z_p model in Wahl's systematics.

$$\mathrm{TKE}(A_h) = (p_1 - p_2 A_h)\left\{1 - p_3 \exp\left(-\frac{(A_h - A_m)^2}{p_4}\right)\right\}$$

- Fit a simple analytic function to $TKE(A)$ experimental data at thermal energy.

Fission fragment decay

- Distributions of primary fission fragment characterized by $Y(Z, A, E_{ex}, J^{\Pi})$ are generated and integrated deterministically for all primary fission fragment pairs (no MC sampling - fast, but lost correlation)



<u>Neutron emission multiplicity</u>

$$\overline{\nu}^{(k)}_{l,h} = \int dE_x \sum_{J\Pi} \int d\epsilon \; R(J,\Pi) G(E_x) \phi^{(k)}_{l,h}(J,\Pi,E_x,\epsilon)$$

- Excitation energy distribution

$$G(E_x) = \frac{1}{\sqrt{2\pi}\delta_{l,h}} \exp\left\{ -\frac{(E_x - E_{l,h})^2}{2\delta^2_{l,h}} \right\}$$

$$\delta_{l,h} = \frac{\delta_{\mathrm{TXE}}}{\sqrt{E_l^2 + E_h^2}} E_{l,h}$$

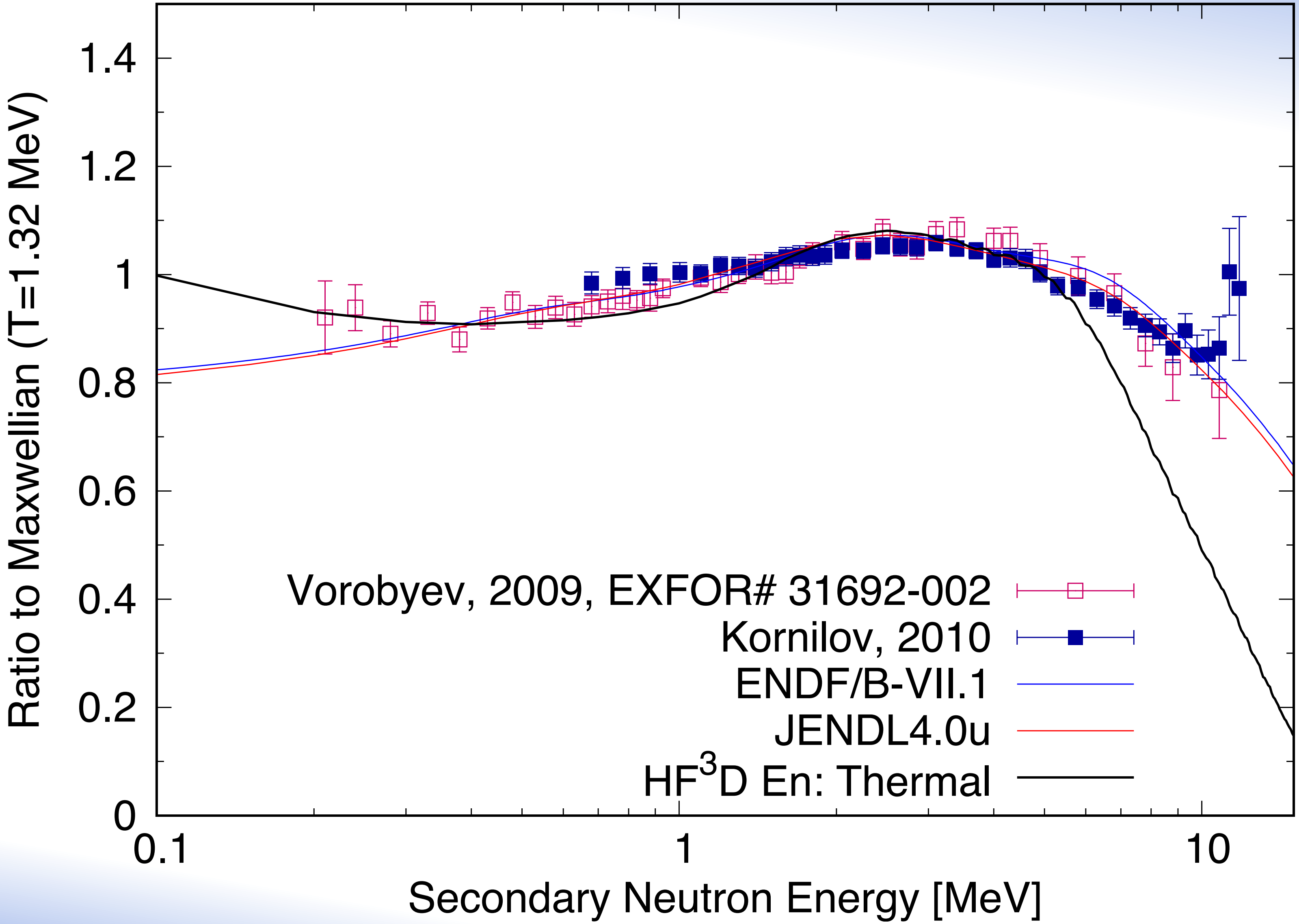
- Spin and parity distribution

$$R(J,\Pi) = \frac{J+1/2}{2f^2\sigma^2(U)} \exp\left\{ -\frac{(J+1/2)^2}{2f^2\sigma^2(U)} \right\}$$

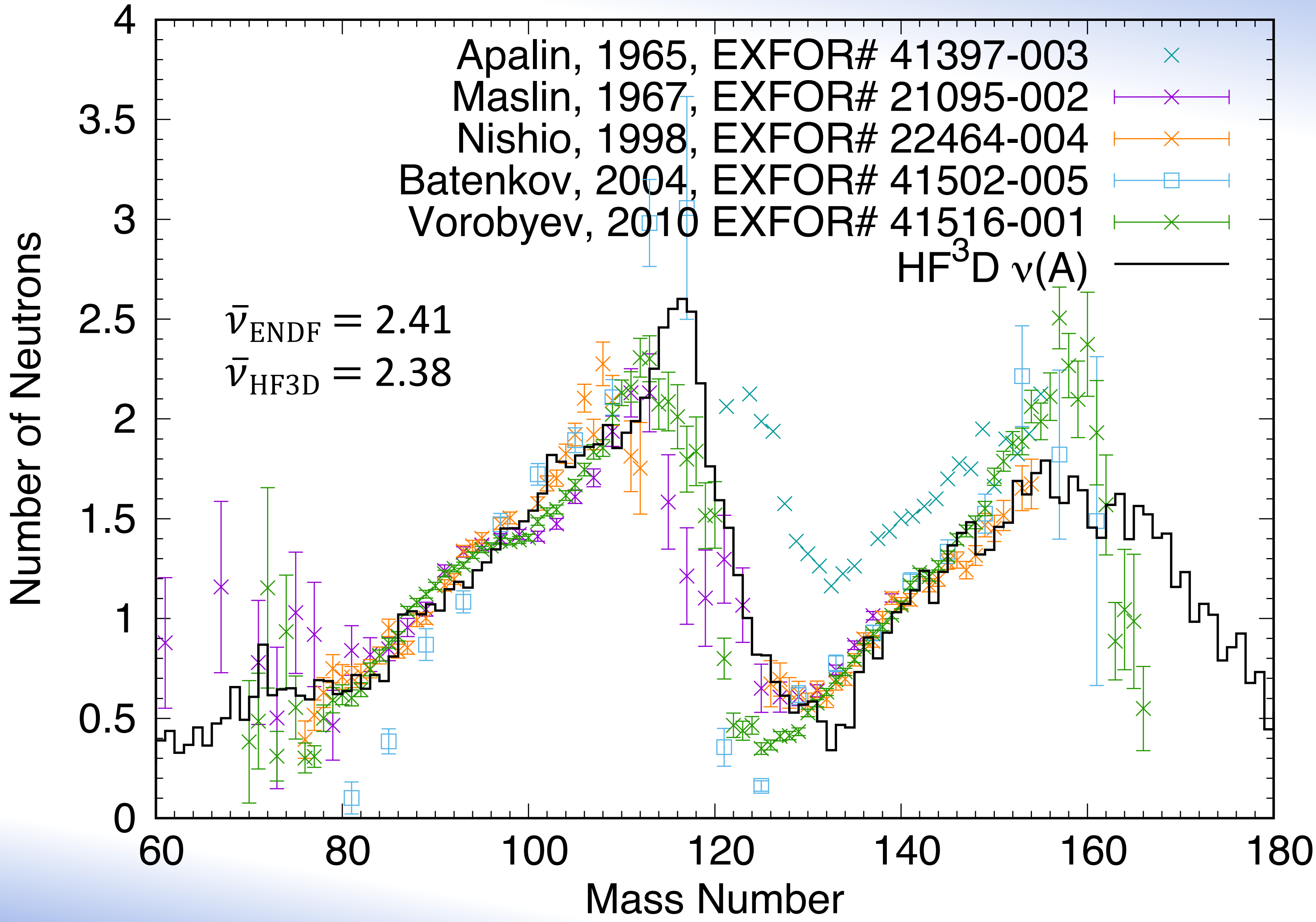
$\sigma^2(U)$: spin cut-off parameter
U: Excitation energy
f: scaling factor

Okumura et al. *J. Nucl. Sci. Technol.*,55,1009-1023,(2018).

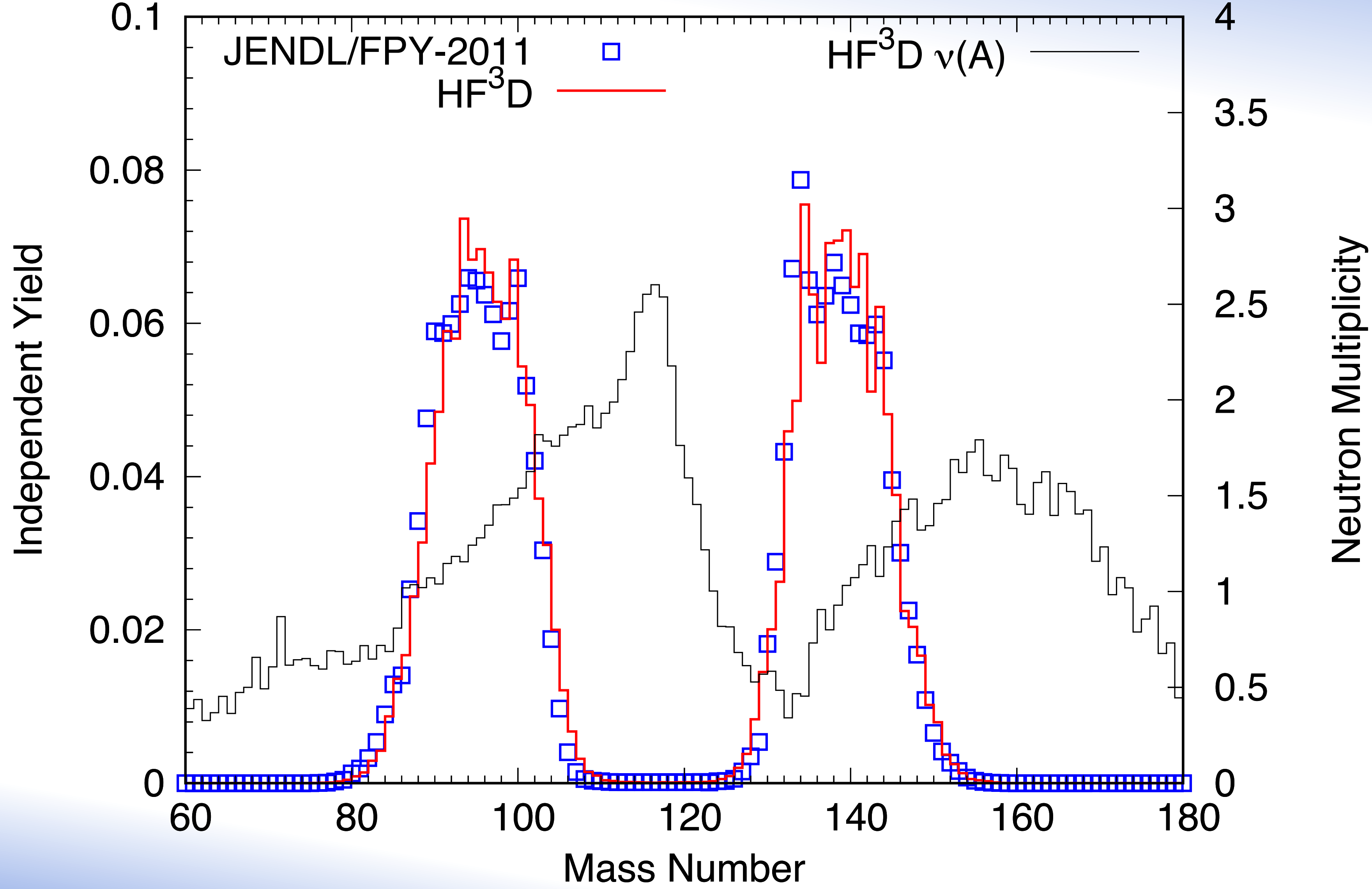
Result: Prompt fission neutron spectrum



Result: Prompt neutron multiplicity, ν(A)



Result: Independent FPY of $^{235}U(n_{th},f)$



Result: Independent FPY of $^{235}U(n_{th},f)$

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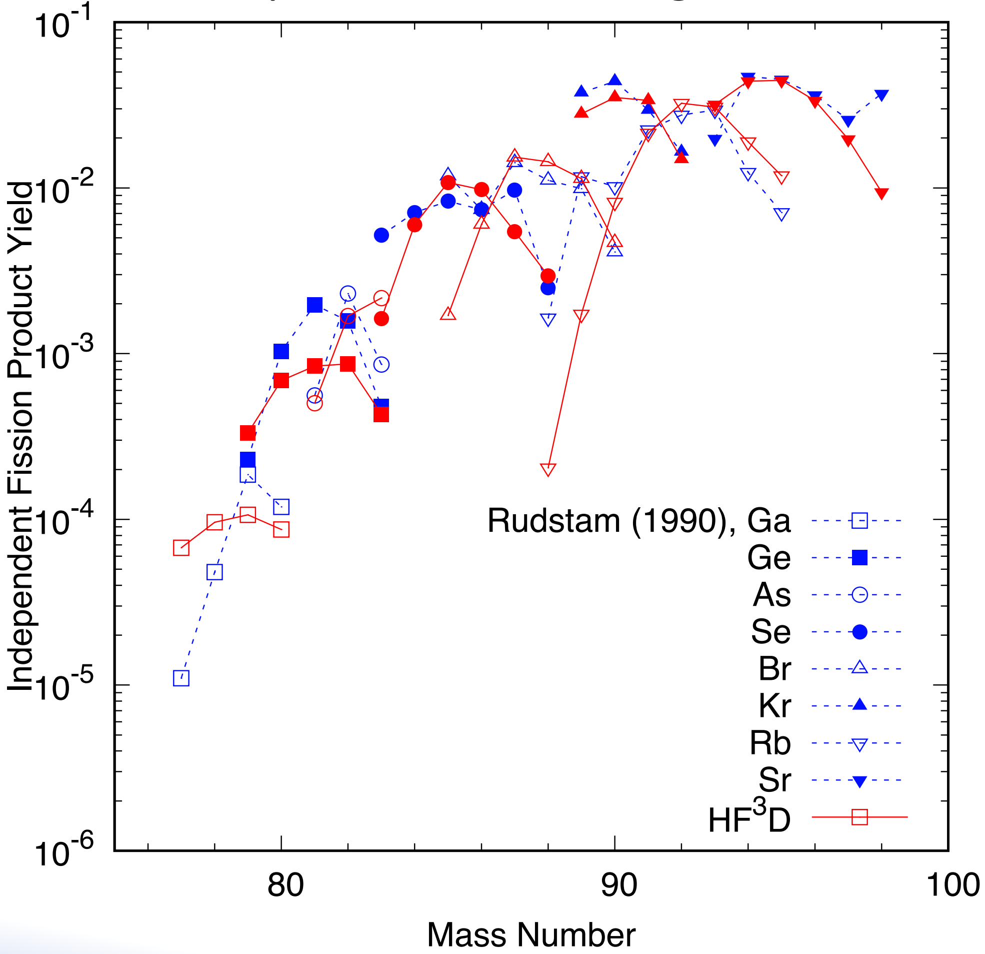
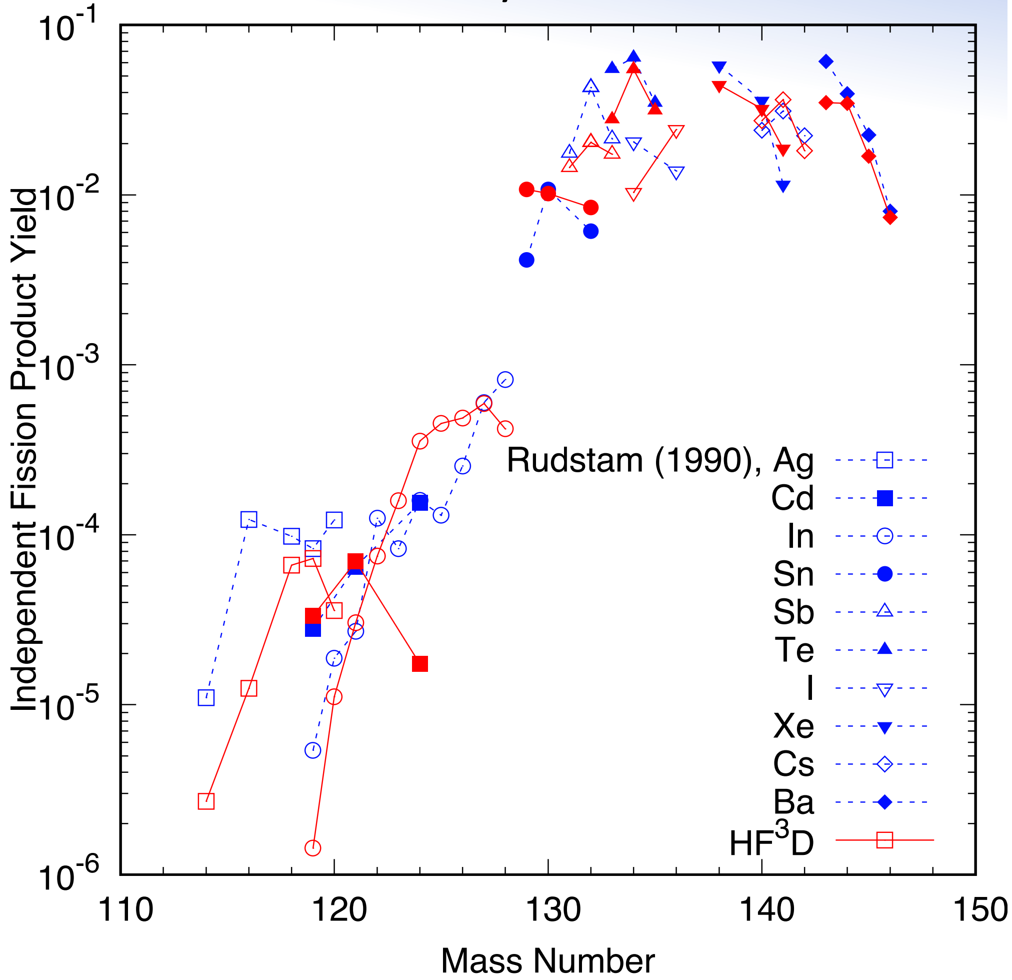
Isotope distribution of Light FPs



Heavy FPs



Rudstam G et. al., *Radiochimica Acta*.,49 (1990).
EXFOR# 22161-002

Result: Isomeric ratio

- ENDF (after B-VI) and JENDL 4.0 adopted isomeric ratios by Madland-England model.
- All the nuclides having the same $J_{m/g}$ and even/odd A will have the same isomeric ratio.

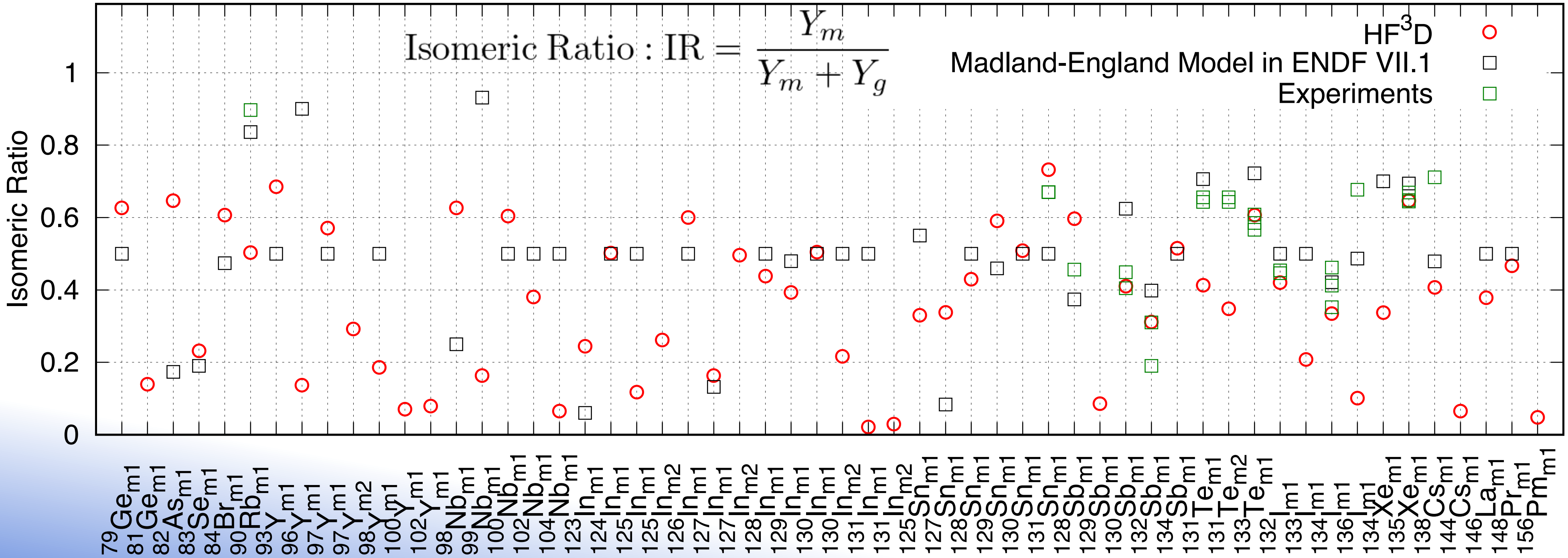
Madland-England model (Current ENDF VII.1 and JENDL 4.0)

- Even-odd of mass of FP nuclides
- Even-odd of spin difference of metastable, ground state FP nuclides (J_m-J_g)
- Spin of metastable, ground

D. G. Madland and T. R. England, Nulc. Sci. Eng., 64, 859-865, (1977).

Example in JENDL 4.0

Nuclide	J_g^{π}	J_m^{π}	IR
^{132}I	4^+	8^-	0.42
^{134}I	4^+	8^-	0.42
^{133}Xe	$3/2^-$	$11/2^-$	0.71
^{135}Xe	$3/2^-$	$11/2^-$	0.71



Experimental data is so scarce!!

Result: Cumulative FPY of $^{235}U(n_{th},f)$

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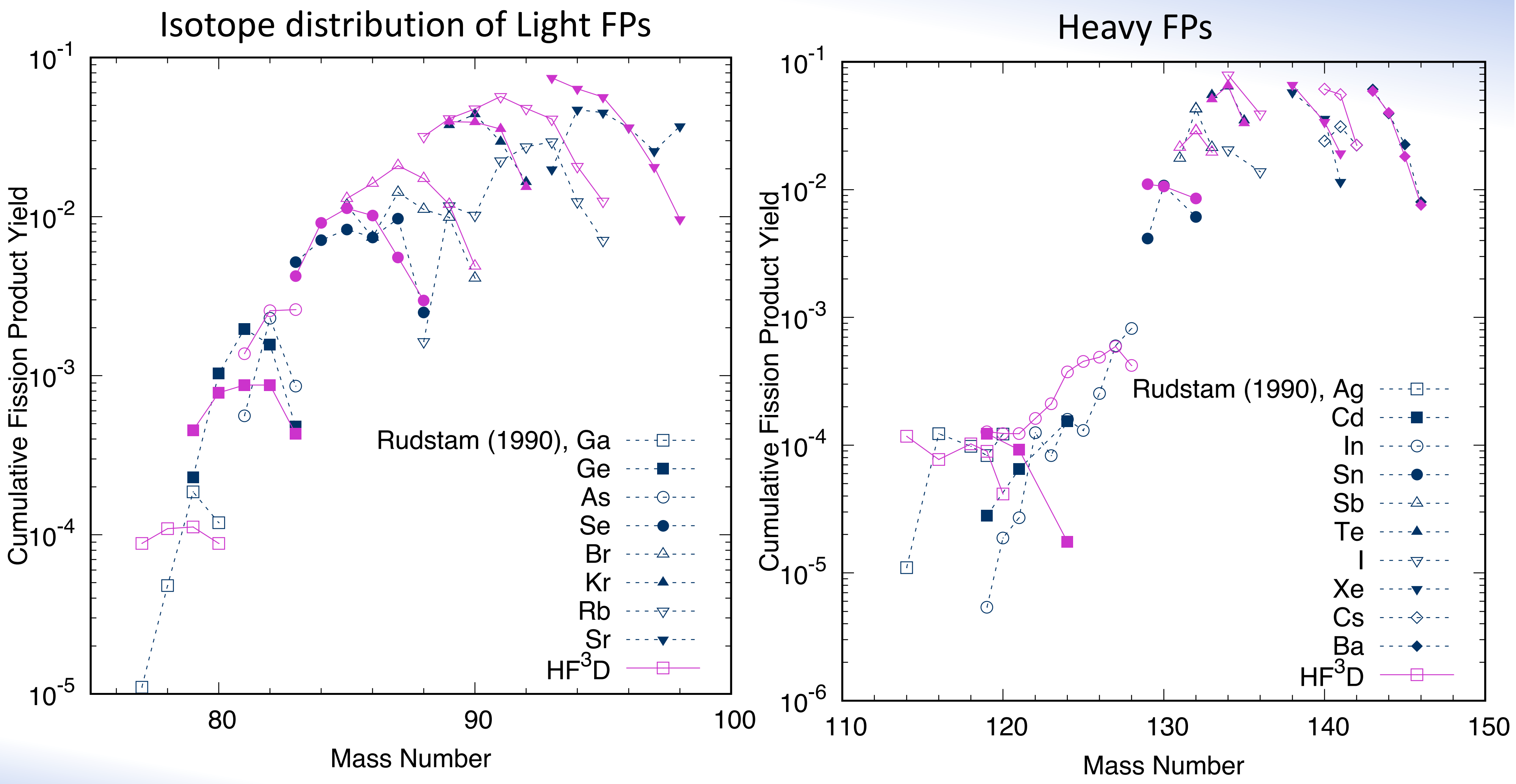
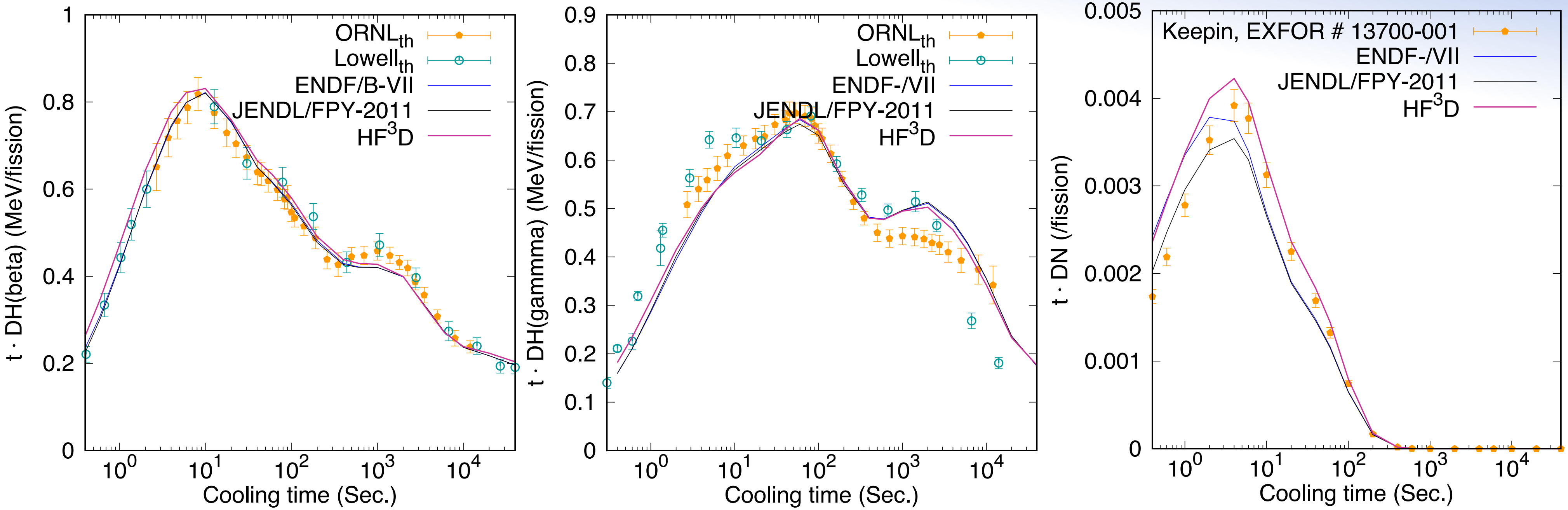


Rudstam G et. al., *Radiochimica Acta*.,49 (1990).
EXFOR# 22161-002

Result: Calculated decay heat and delayed neutron

- Summation calculation of beta decay using ENDF/B-VII decay data library



decay heat total (MeV/fission)

Isotope	HF³D	ENDF/B-VII	JENDL/FPY-2011
39-Y-98-0	1.0029E-01	6.2298E-02	2.9617E-02
38-Sr-97-0	7.1420E-02	6.0794E-02	6.0945E-02
39-Y-97-1	5.5401E-02	3.6437E-02	5.9791E-02
38-Sr-96-0	5.2162E-02	5.4041E-02	5.4186E-02
37-Rb-95-0	4.9638E-02	3.0397E-02	3.0479E-02
39-Y-99-0	3.7535E-02	3.1491E-02	3.1468E-02
40-Zr-99-0	3.1358E-02	2.8238E-02	2.8297E-02
55-Cs-142-0	2.5797E-02	3.2072E-02	3.2160E-02
37-Rb-92-0	2.5157E-02	2.4540E-02	2.4606E-02
36-Kr-93-0	2.3157E-02	1.0814E-02	1.0843E-02

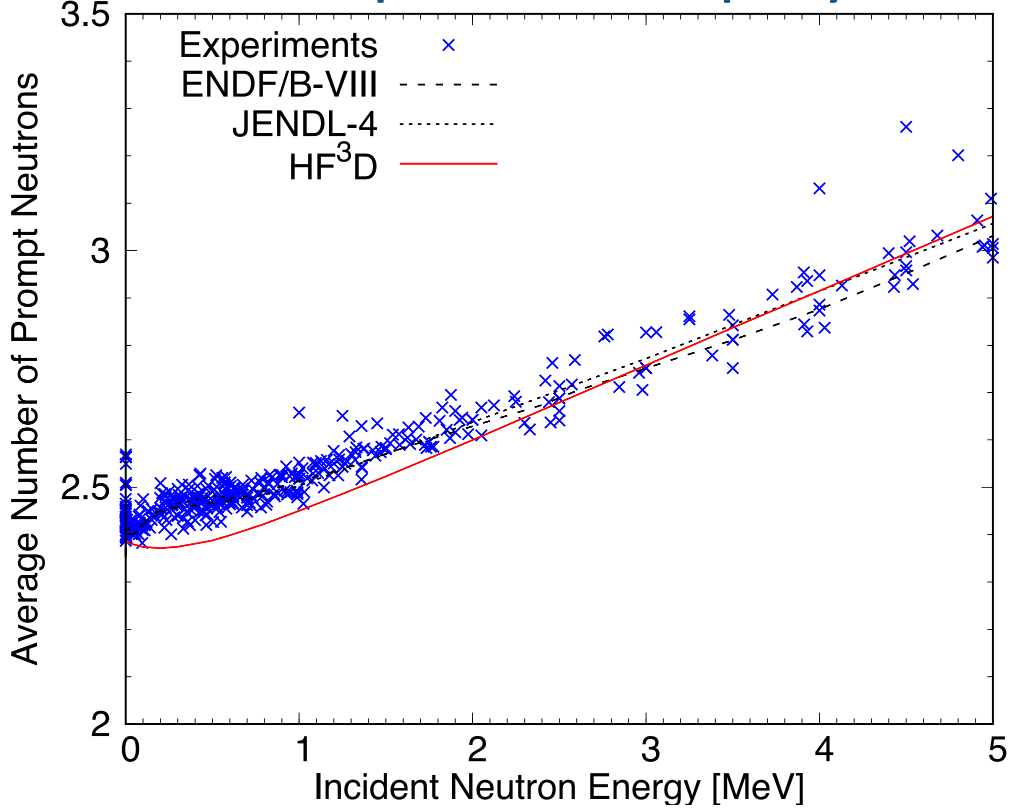
delayed neutron

Isotope	HF³D	ENDF/B-VII	JENDL/FPY-2011
37-Rb-95-0	9.6787E-04	5.9269E-04	5.9428E-04
37-Rb-94-0	4.9311E-04	3.9672E-04	3.9778E-04
35-Br-90-0	3.8195E-04	4.4369E-04	4.4488E-04
35-Br-91-0	3.3934E-04	3.4418E-04	3.4510E-04
37-Rb-96-0	3.2717E-04	2.5629E-04	2.5698E-04
35-Br-89-0	2.3806E-04	2.1677E-04	2.1735E-04
37-Rb-97-0	2.3125E-04	7.7580E-05	7.7789E-05
33-As-85-0	2.0059E-04	2.7429E-04	2.1779E-04
53-I-139-0	1.8703E-04	2.0876E-04	2.0932E-04
39-Y-99-0	1.6211E-04	1.3601E-04	1.3591E-04

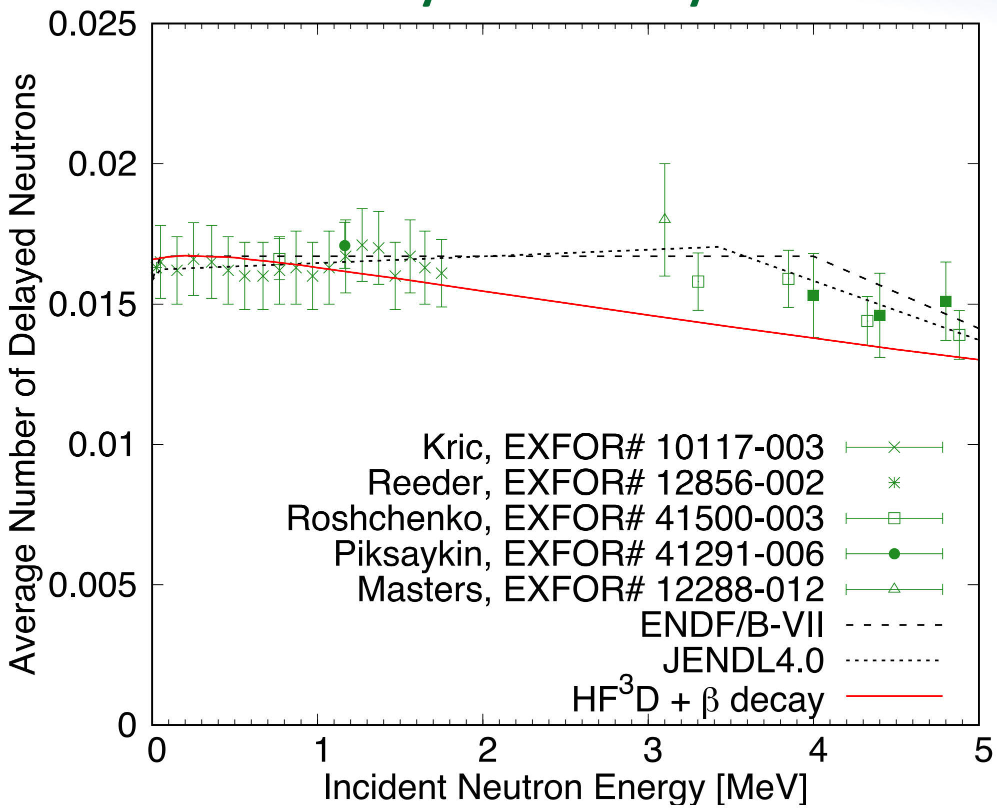
Result: Energy dependence of prompt/delayed neutron

- Neutron emissions are directory related to the FPY.

Prompt neutron multiplicity

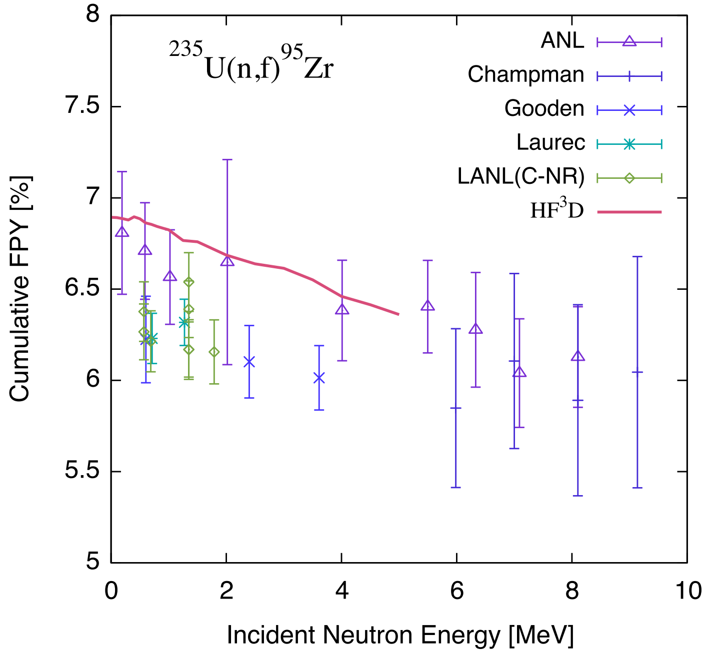


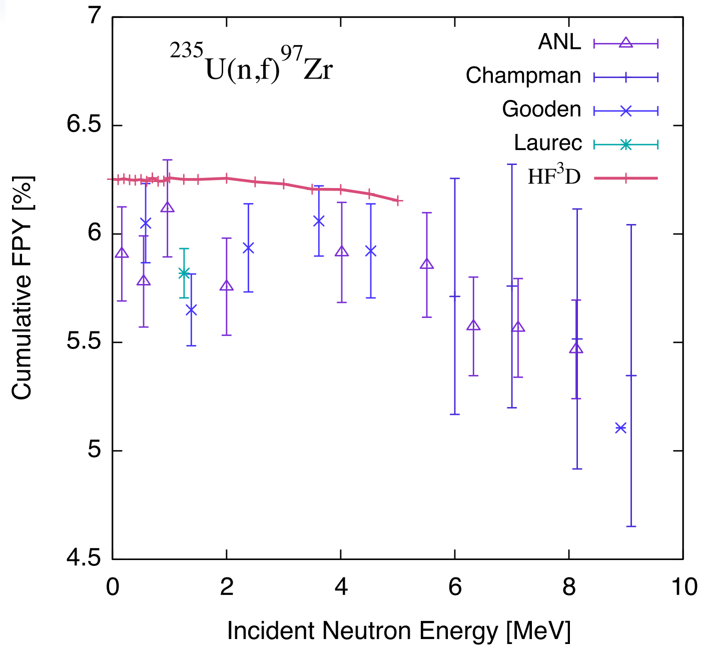
Delayed neutron yield

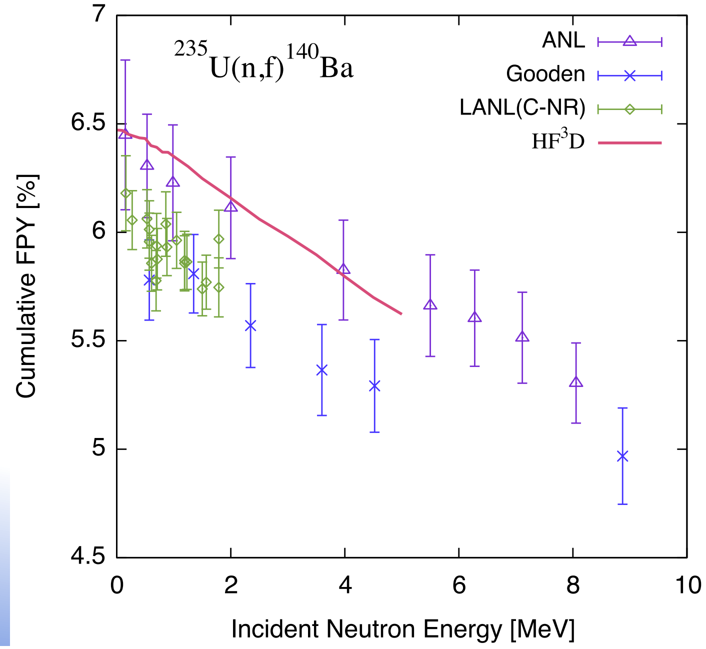


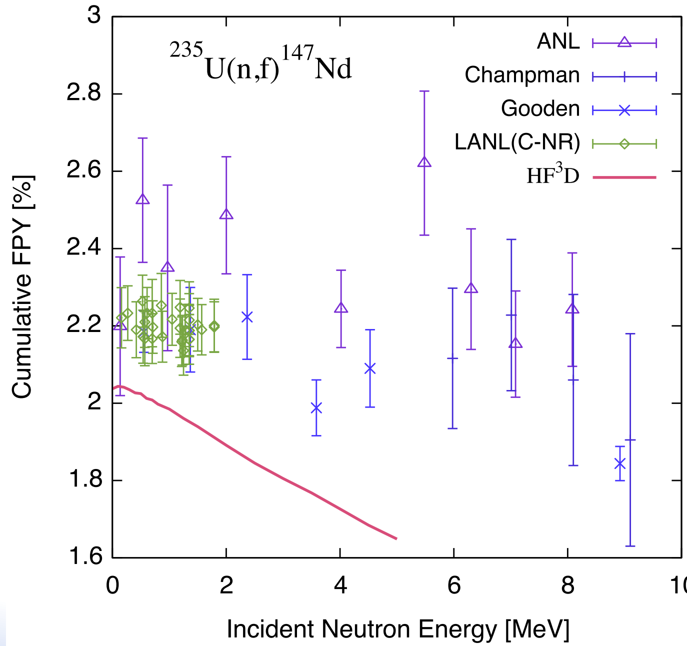
- These observables could be a guideline to check whether the calculations are reasonable or not.

Result: Energy dependency of cumulative FPY

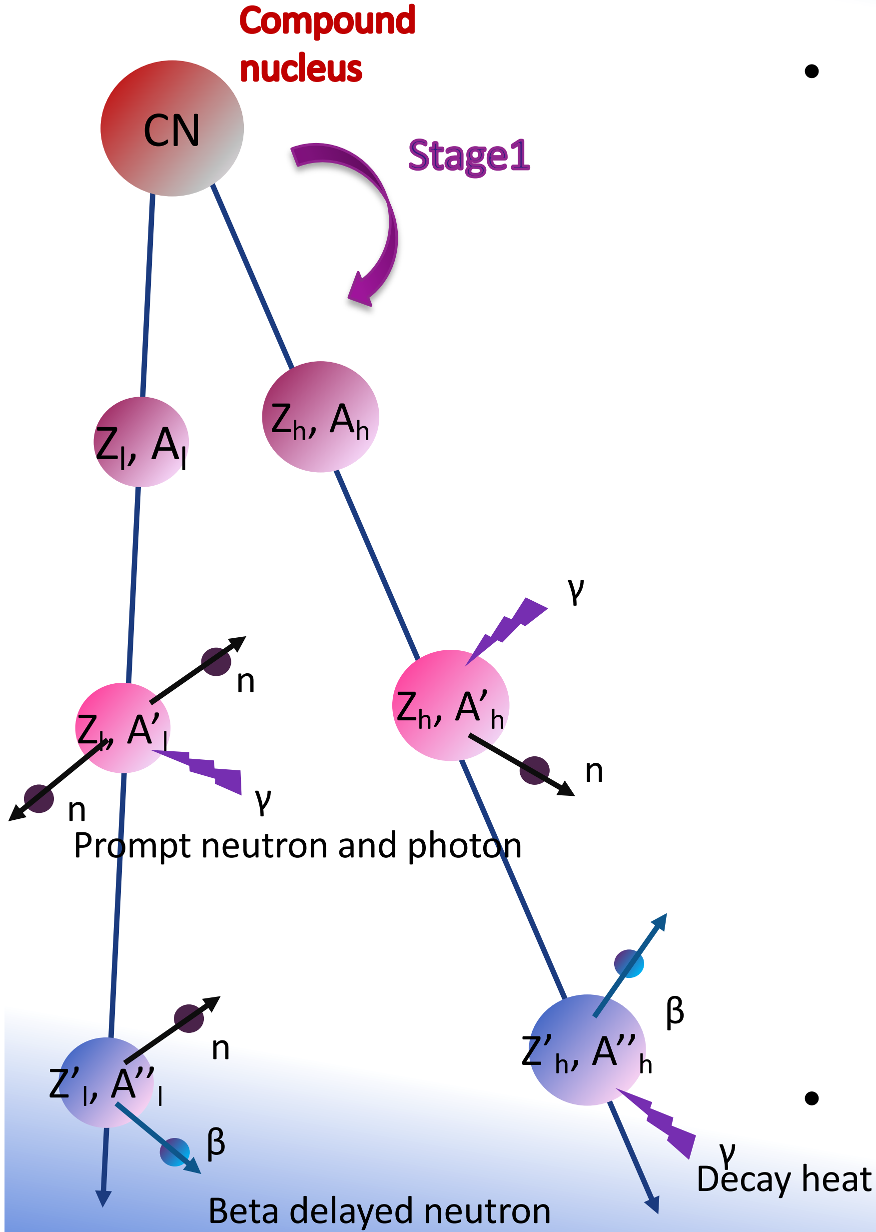




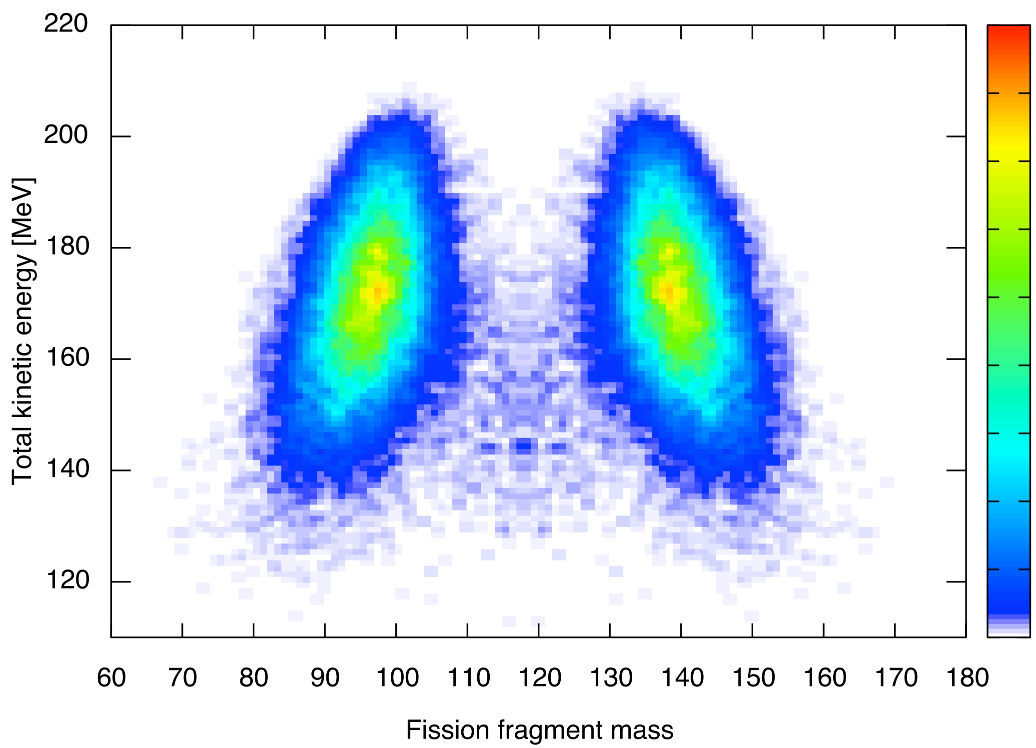




Connection with fission fragment distributions by 4D Langevin model



- Theoretical calculations will give primary fission fragment distributions.

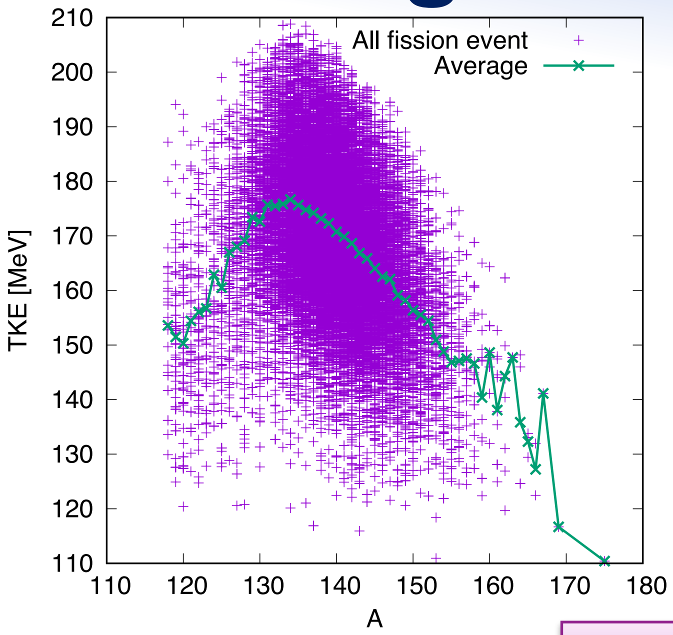


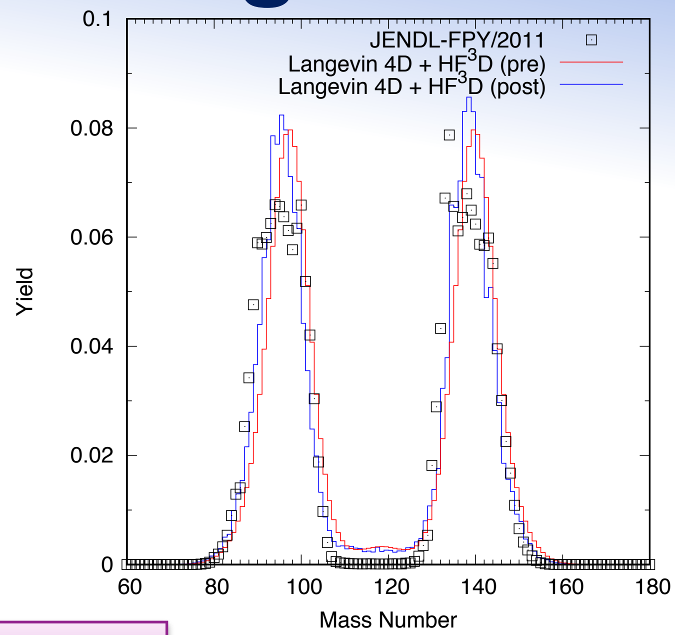
TKE distribution of ^{236}U (E_{ex} = 7MeV) with 4D Langevin model

Ishizuka C, et al. *Phys. Rev. C*. 96:064616(2017).

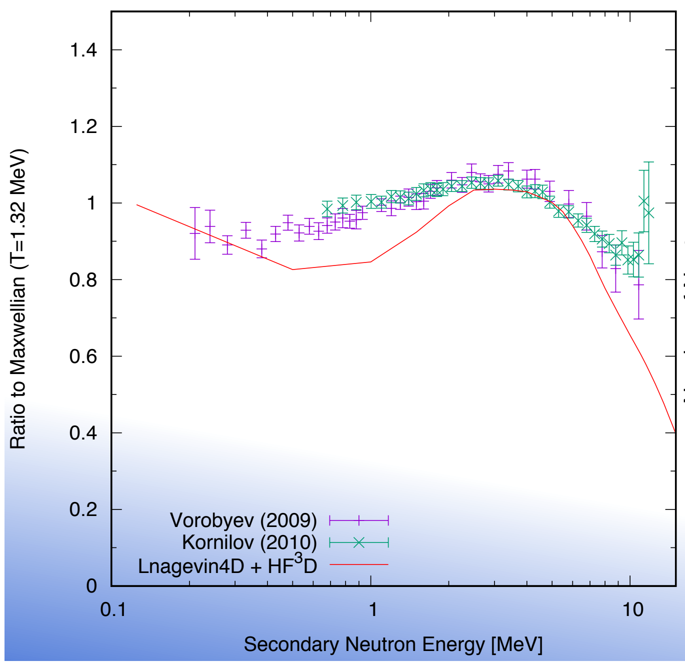
- How to compare with the experimental data?

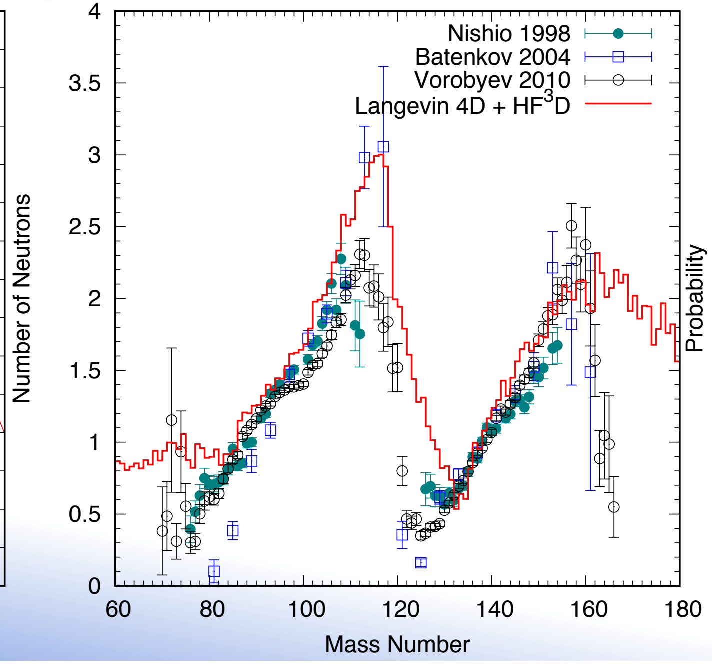
4D Langevin + fragment decay

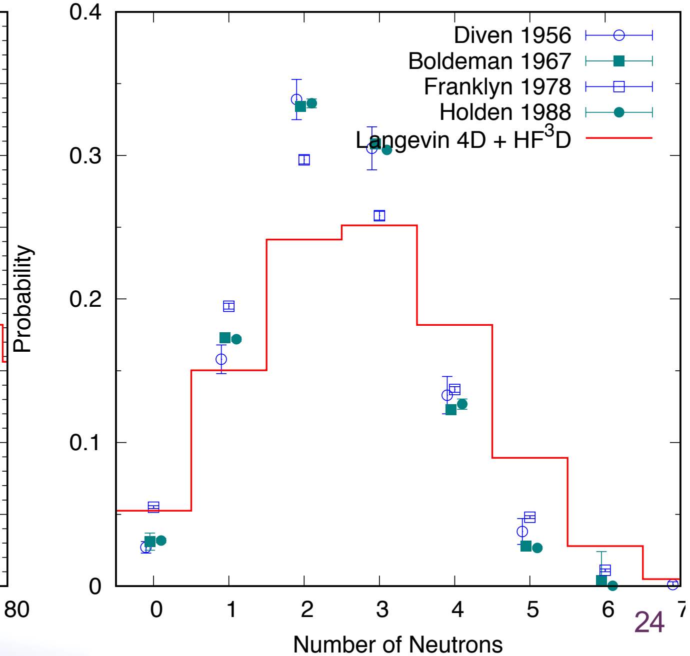




- Mass and TKE distributions from 4D Langevin model as inputs
- Comparison between calculated and experimental data of many fission observables tells the model accuracy







Summary

- Developed the Hauser-Feshbach Fission Fragment decay model for the fission fragment decay and combined it with beta decay and the summation calculation

- Simultaneously reproduces some fission observables starting from one fission fragment distribution
  e.g. $\bar{\nu}$, $Y_I(A, Z, M)$, isomeric ratio, $Y_C(A,Z,M)$, ν_d, DH

- Energy dependent calculations up to 5 MeV

- Connection with microscopic and macroscopic models (primary fission fragment (Y(A) and TKE)) feasible

- The optimization of fission yield to reproduce all fission observables precisely can allow us to use this model for the evaluation of nuclear data in the future

- More experimental data helps to improve fission theories and models