Prompt-fission observable and fission yield calculations for actinides by TALYS

Tokyo Tech.[1], Uppsala University[2], CEA[3], IAEA[4]

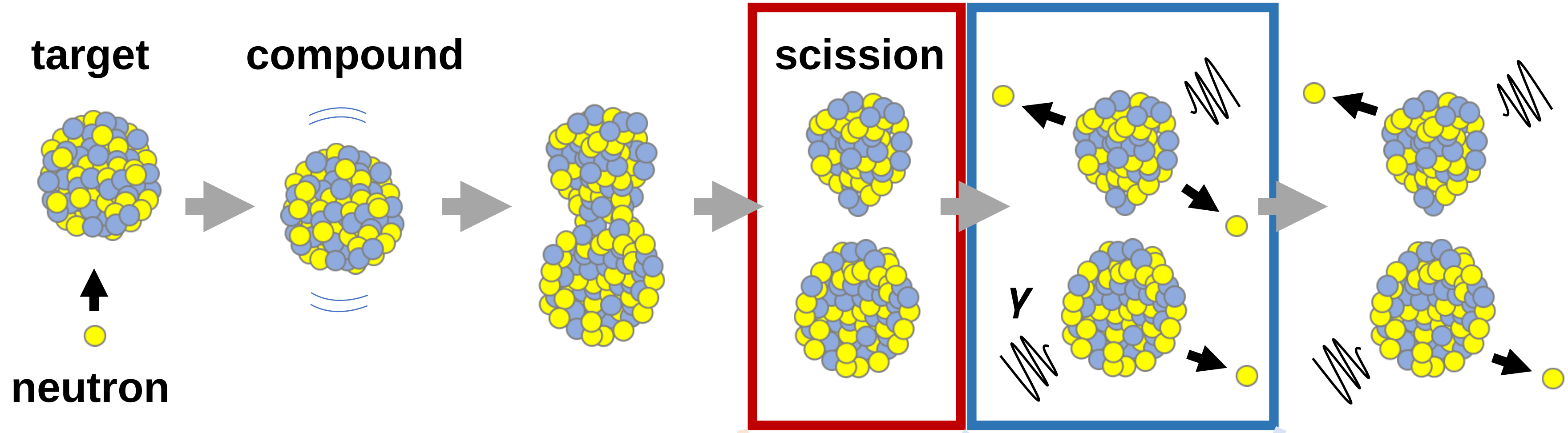
Kazuki Fujio[1], Ali Al-Adili[2], Fredrik Nordström[2], Jean-François Lemaître[3], Shin Okumura[4], Satoshi Chiba[1], Arjan Koning[4]

This presentation is supported by Grant-in-Aid for Scientific Research (B), MEXT, Japan, and by Japan Society for the Promotion of Science (JSPS) KAKENHI Grant Number 21H01856.

Outline

- **Hauser-Feshbach statistical decay calculation implemented in TALYS**
- **Sensitivity study of fission observables based on ^{235}U + thermal neutron reaction**
- **Application to neutron-induced fission of ^{235}U from thermal up to 5 MeV**
- **Global study on actinides at 1 MeV incident neutron reaction**
- **Conclusions**

New approach implemented in TALYS



Fission fragment information

- Fission fragment yield $Y_{\rm ff}(Z, A)$
- Total Kinetic Energy $\rm TKE$
- Mean excitation energy $\bar{E}_x$
- Width of the excitation energy distribution σ_{E_x}

Hauser-Feshbach statistical decay

- Independent fission product yield
- Isomeric yield ratio
- Neutron / γ-ray multiplicity
- Prompt Fission Neutron Spectrum / Prompt Fission γ-ray Spectrum

TALYS contains fission fragment information from several theoretical codes.

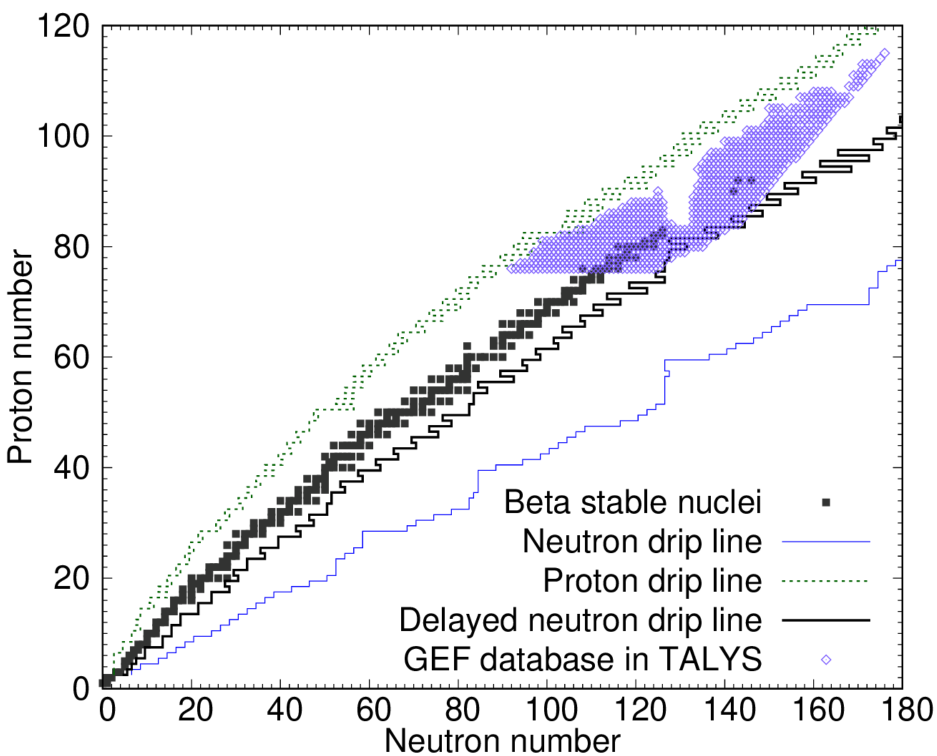
Fission fragment database in TALYS

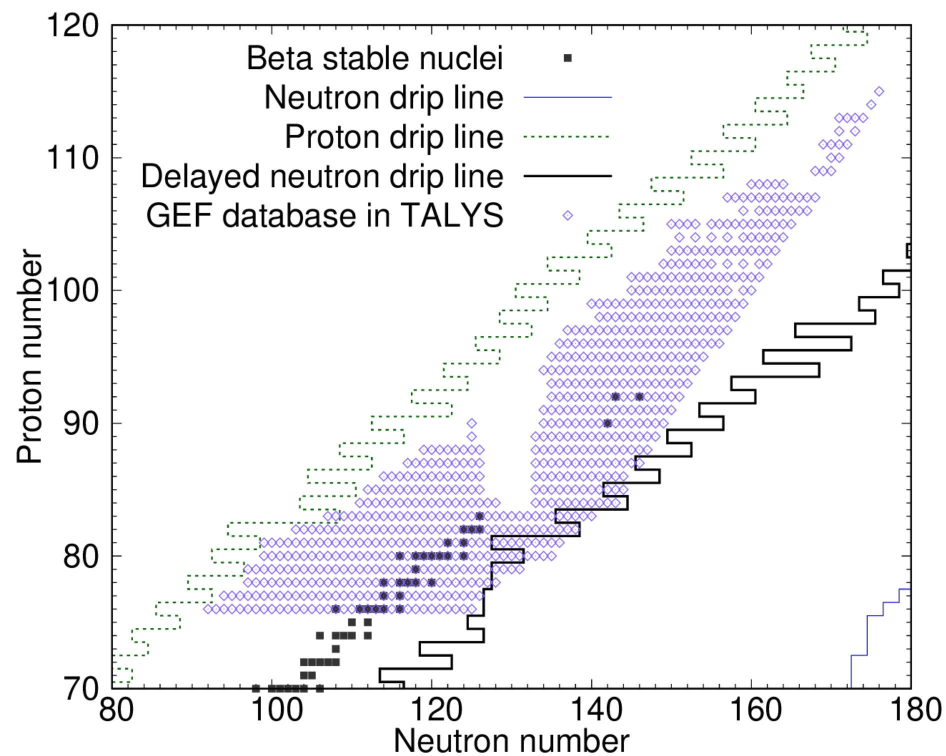
GEF Monte Carlo-based phenomenological fission model gives fission observables data not only after decays but also pre-neutron data.

K. –H. Schmidt, B. Jurado, C. Amouroux, C. Schimitt, Nuclear Data Sheets, 131, 107-221 (2016).

- TALYS contains 737 fissioning nuclei ranging from $_{76}$Os to $_{115}$Mc

F. Nordström, Technical Report UPTEC ES21016, Uppsala university (2021).





Fission fragment database in TALYS

HF³D Designed with a fully deterministic technique with fitting functions

S. Okumura, T. Kawano, P. Jaffke, P. Talou, and S. Chiba, JNST, 55(9), 1009-1023 (2018).

- For neutron-induced fission of ^{235}U, ^{238}U, and ^{239}Pu

Mass distribution of primary fragments

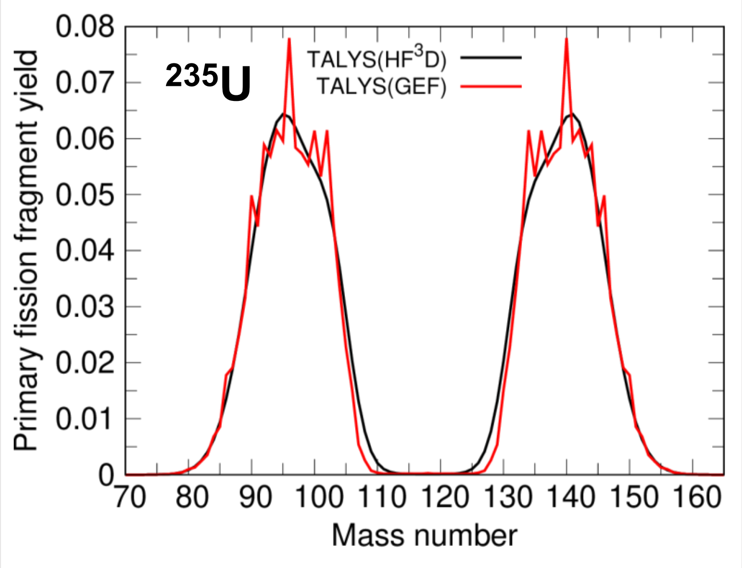
$$Y(A) = \sum_{i=1}^{5} \frac{Y_i}{\sqrt{2\pi}\sigma_i} \exp\left\{ -\frac{(A - A_m + \Delta_i)^2}{2\sigma_i^2} \right\}$$

$$A_m = A_c/2$$

A_c : mass number of compound nucleus

σ_i, Δ_i : Gaussian parameters

$Y_{1,5}$: yield (i = 1~5)



TKE distribution of primary fragments

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

p_i : fitting parameters $\varepsilon_{\mathrm{TKE}}$: correction term to ensure the average TKE

- Charge distribution is obtained from Wahl's Z_p model
- R_T model is used for the excitation energy partition
  R_T = 1.29 at thermal energy and R_T = 1.00 as R_T approaches 5 MeV.

Fission fragment table

Z = 92
A = 236
Ex (MeV) = 6.55e+00
Ntotal = 207

$\bar{E}_x$ σ_{E_x}

Zl	Al	Zh	Ah	Yield	TKE[MeV]	TXE[MeV]	El[MeV]	Wl[MeV]	Eh[MeV]	Wh[MeV]
28	72	64	164	1.7222e-06	1.4140e+02	2.1593e+01	9.0083e+00	3.3421e+00	1.2584e+01	4.6688e+00
29	73	63	163	3.3249e-06	1.4256e+02	2.2054e+01	9.1763e+00	3.3591e+00	1.2877e+01	4.7139e+00
30	73	62	163	1.5739e-06	1.4514e+02	2.0166e+01	8.7278e+00	3.5748e+00	1.1438e+01	4.6847e+00
29	74	63	162	1.6362e-06	1.4375e+02	1.9948e+01	7.9037e+00	3.2017e+00	1.2044e+01	4.8788e+00
30	74	62	162	1.0661e-05	1.4634e+02	2.2937e+01	1.0050e+01	3.6535e+00	1.2887e+01	4.6847e+00

Excitation energy distribution

$$G(E_x) = \frac{1}{\sqrt{2\pi}\sigma_{E_x}} \exp\left\{ -\frac{(E_x - \bar{E}_x)^2}{2\sigma_{E_x}^2} \right\}$$

$\bar{E}_x$: mean excitation energy

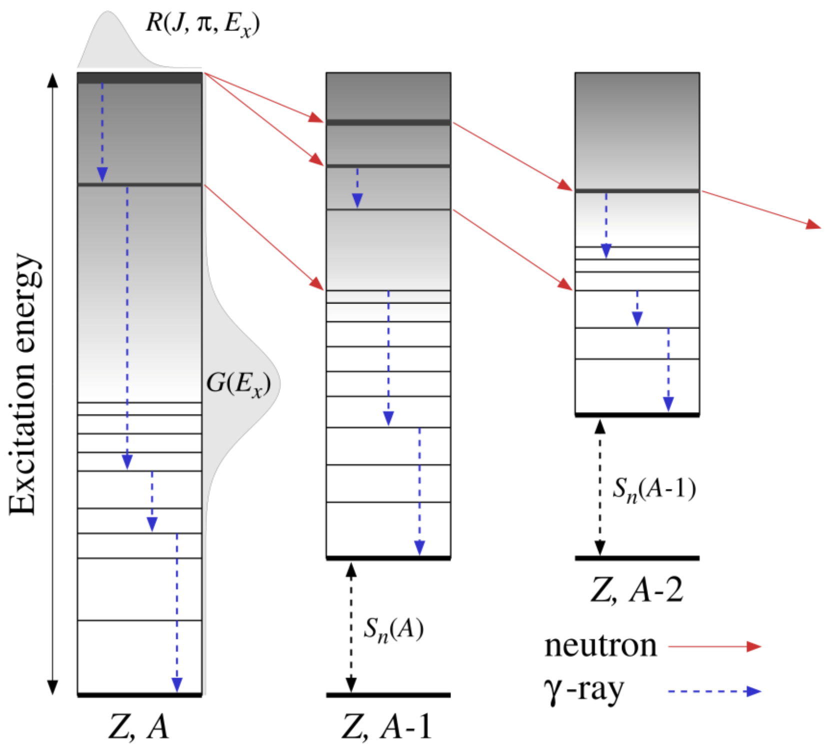
σ_{E_x} : width of the excitation energy distribution

Spin-parity distribution

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

$\sigma^2(E_x)$: spin-cut off parameter

f^2 : scaling factor



Sensitivity study of fission observables

Tokyo Tech

Spin-parity distribution

$$R(J,\pi,E_x) = \frac{1}{2}\cdot\frac{2J+1}{2X\sigma^2(E_x)}\exp\left\{-\frac{(J+1/2)^2}{2X\sigma^2(E_x)}\right\}$$

X : scaling factor

For primary fission fragments → $X = f^2$

For fission products → $X = f_s$

to assure a reasonable agreement with experimental data.

The number of continuum states N

$$\Delta_{\mathrm{bins}}(Z,A) = (E_x^{\mathrm{max}} - E_x^{\mathrm{level}})/N$$

$\Delta_{\mathrm{bins}}(Z,A)$: energy width of discretized continuum state

E_x^{max} : maximum excitation energy

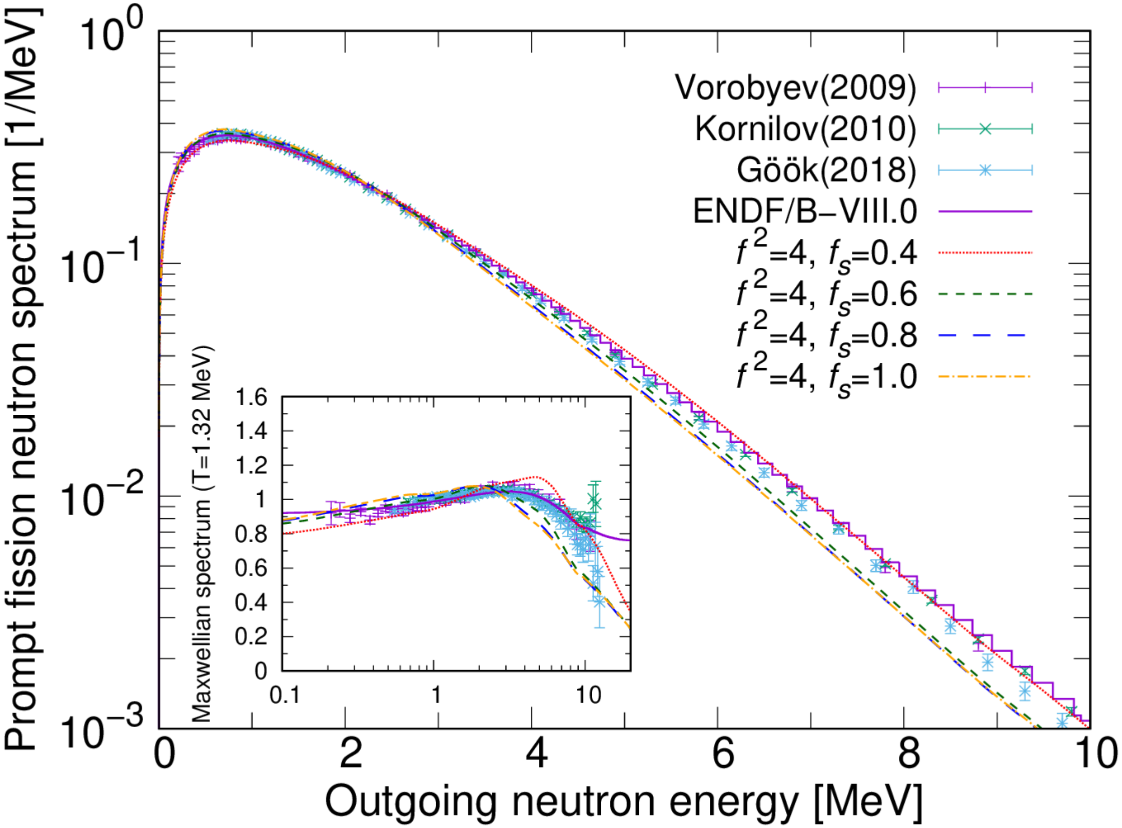
E_x^{level} : excitation energy at the last discrete level

Sensitivity on scaling parameters

Tokyo Tech

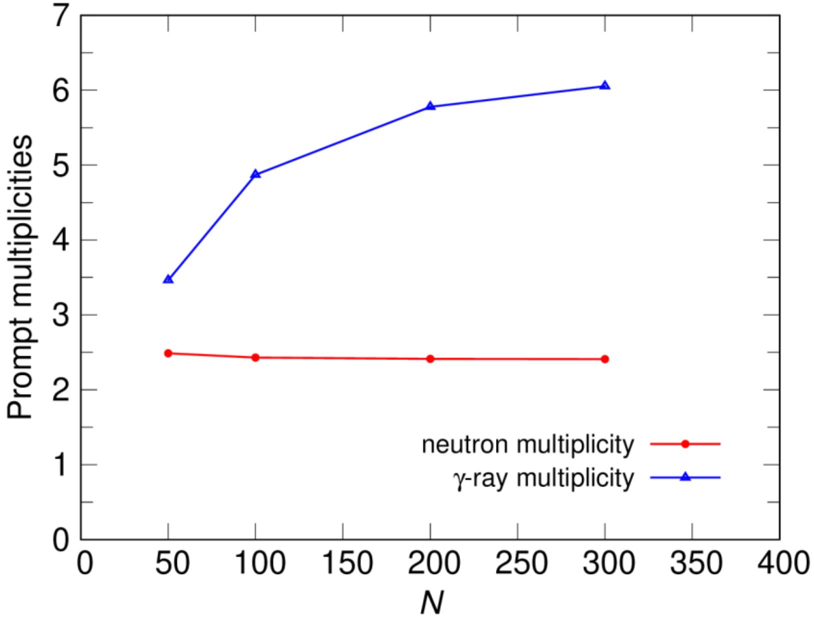
- Sensitivity study using $(Y_{\mathrm{ff}}(Z,A), \mathrm{TKE}, \bar{E}_x, \sigma_{E_x})$ obtained from HF³D
- Prioritize to reproduce the neutron multiplicity $\bar{\nu}_n$ and the shape of PFNS
- Run parameter sensitivity analysis 3 < f^2 < 6 and 0.4 < f_s < 1.0

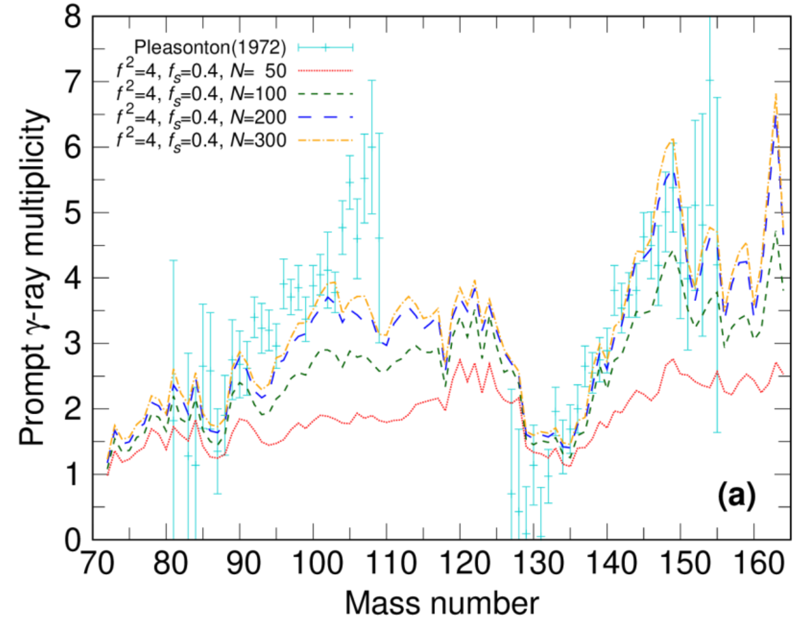
f^2	f_s	$\bar{\nu}_n$
3	0.4	2.49
3	0.6	2.47
3	0.8	2.45
3	1.0	2.44
4	0.4	2.41
4	0.6	2.40
4	0.8	2.39
4	1.0	2.38
5	0.4	2.35
5	0.6	2.34
5	0.8	2.33
5	1.0	2.33
6	0.4	2.30
6	0.6	2.29
6	0.8	2.29
6	1.0	2.29
ENDF-B/VIII.0		2.41
JEFF-3.3		2.41

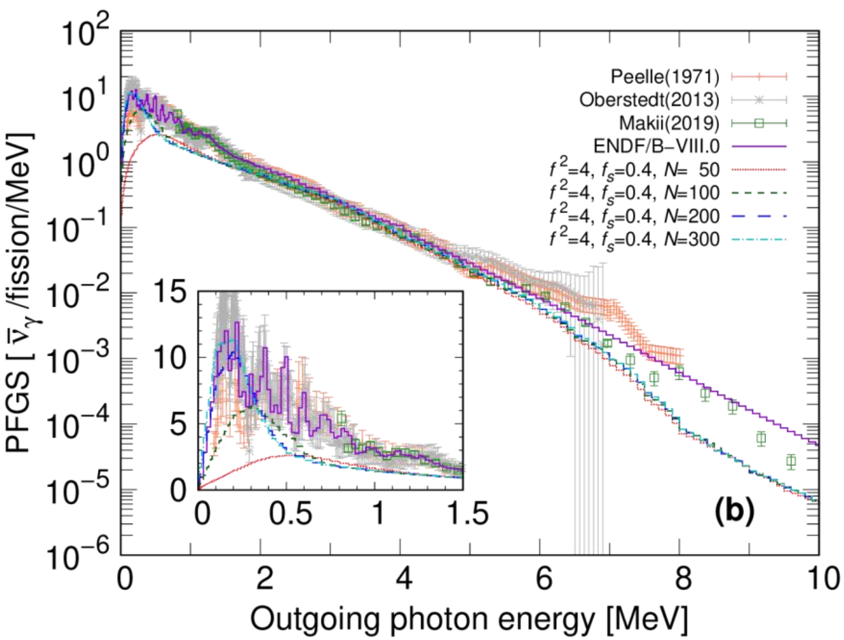


- **By comparing with evaluated data, we conclude $f^2 = 4$ and $f_s = 0.4$ are the optimal values.**
- Our result is consistent with another recent study ($f_s = 0.4 - 0.5$).
  A. Rodrigo, et al., arXiv:2303.09595 (2023)

Sensitivity on the number of continuum states





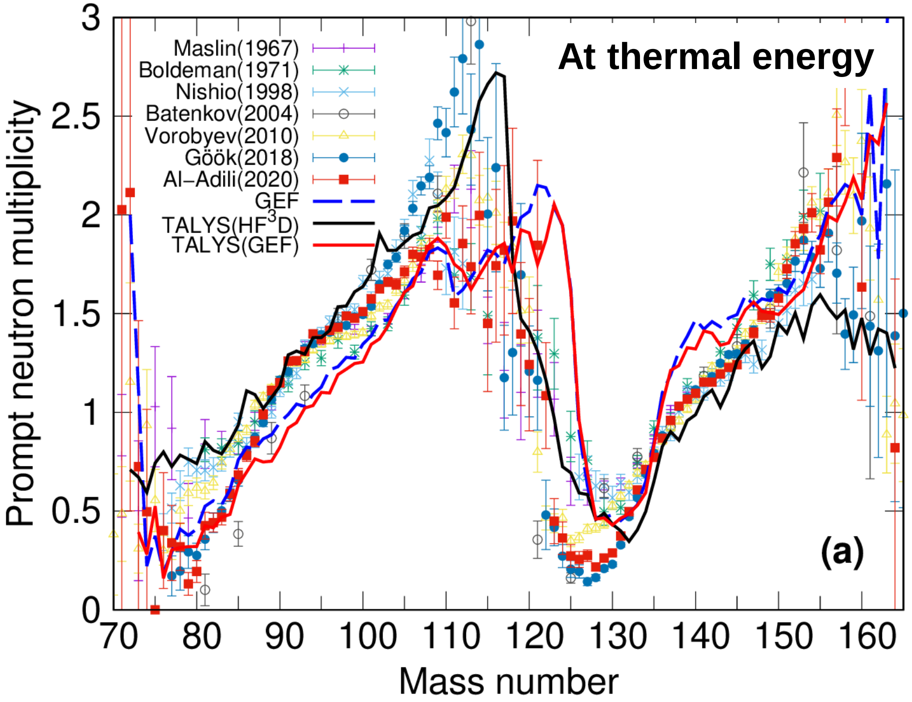


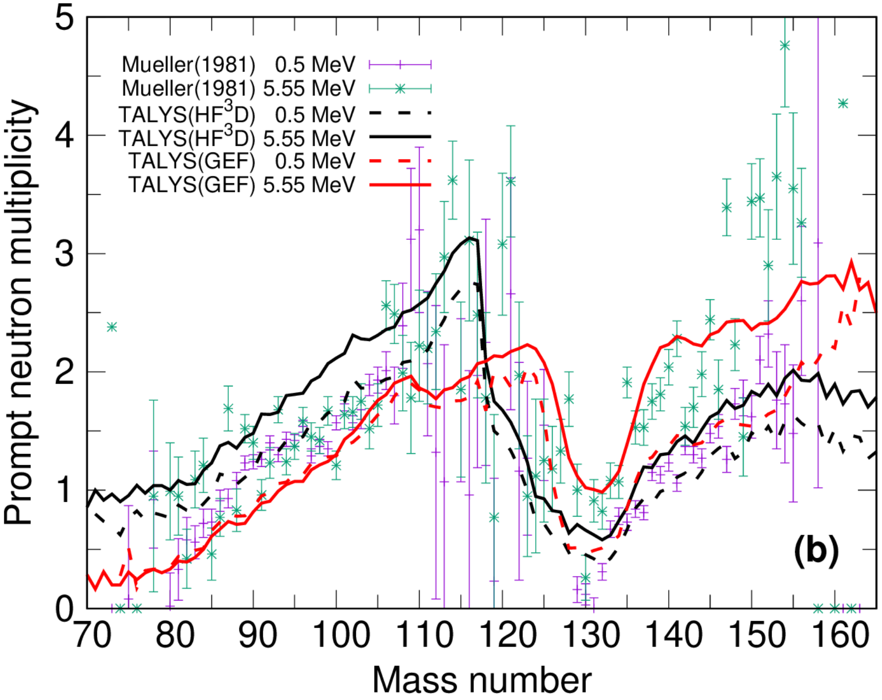
- The γ-ray multiplicity $\bar{\nu}_\gamma$ increases with increasing N.
- A prominent peak appears in PFGS.

  ∵ Transitions between small energy levels increase as N increases.
- **We chose $N = 300$ as the optimal value for improved consistency with experimental and evaluated data.**

Application to ^{235}U(n,f)

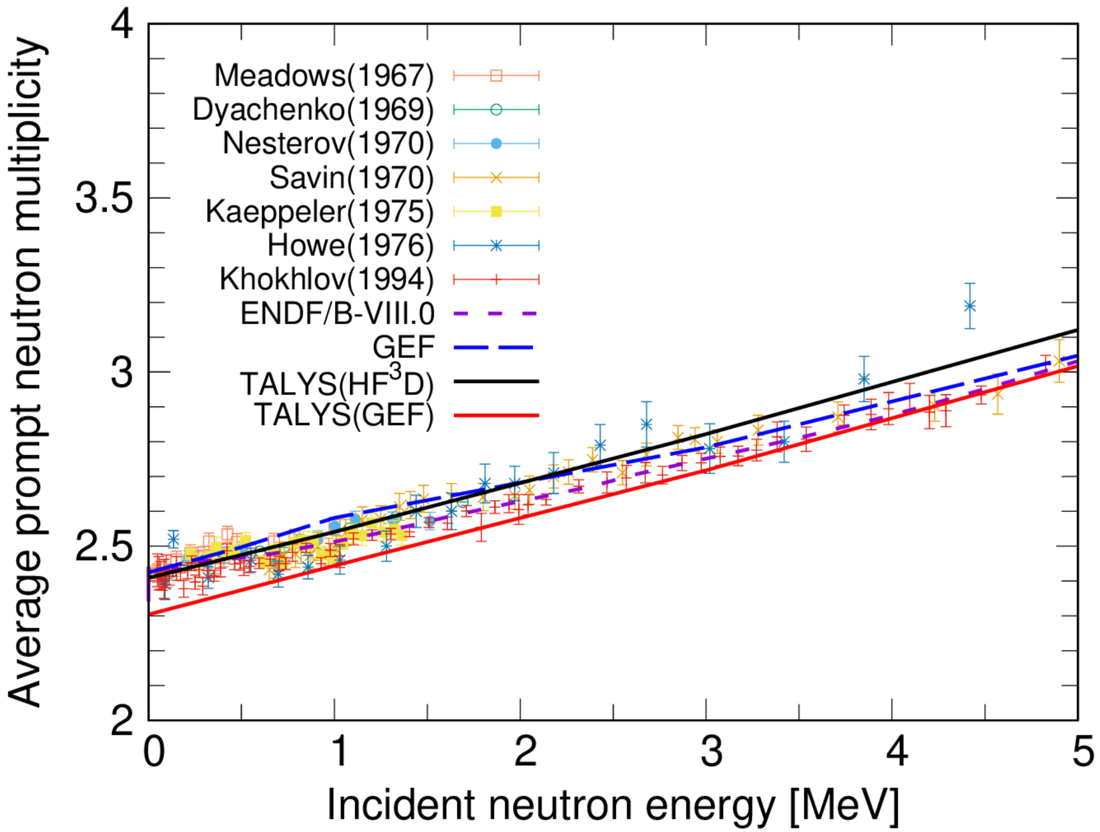
- The optimal values: $f^2 = 4$, $f_s = 0.4$, and $N = 300$
- Comparison between TALYS(GEF), TALYS(HF^{3}D), experimental, and evaluated data





- TALYS results show the saw-tooth shape that is consistent with experimental data.
- TALYS(GEF) reproduces that the $\bar{\nu}_n$ increases from heavy fragments.
- TALYS(HF^{3}D) does not exhibit the trend.
  →TALYS reflects the difference in the energy-sorting mechanism from GEF and HF^{3}D

$^{235}U(n,f)$: neutron multiplicity



	$\bar{\nu}_n$
TALYS(GEF)	2.30
TALYS(HF³D)	2.41
GEF	2.42
ENDF-B/VIII.0	2.41
JEFF-3.3	2.41

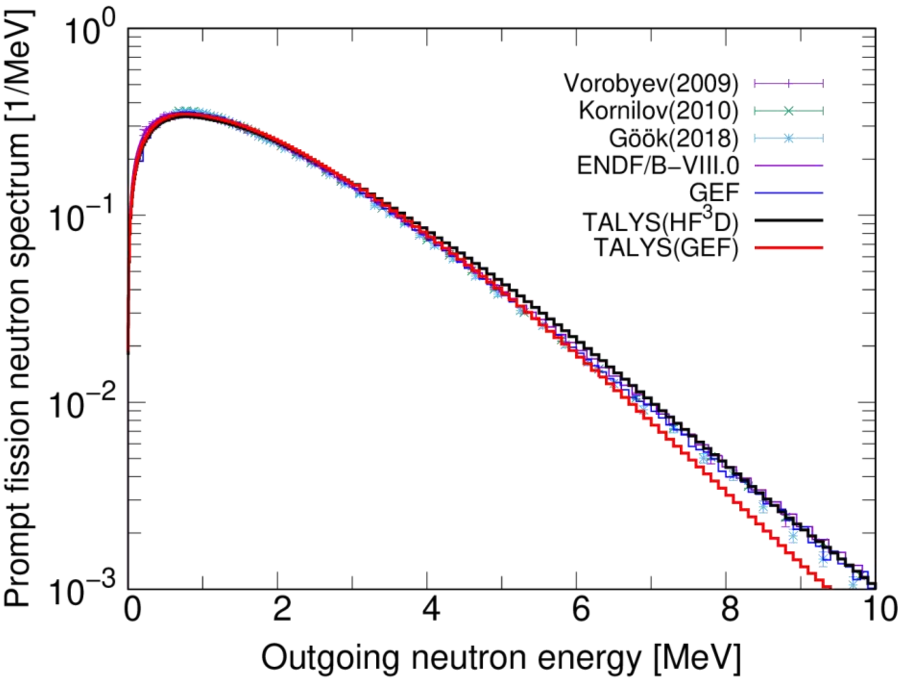
- TALYS(HF³D) successfully reproduces the evaluated value at thermal energy as original HF³D model.

  S. Okumura, T. Kawano, P. Jaffke, P. Talou, and S. Chiba, JNST, 55(9), 1009-1023 (2018).

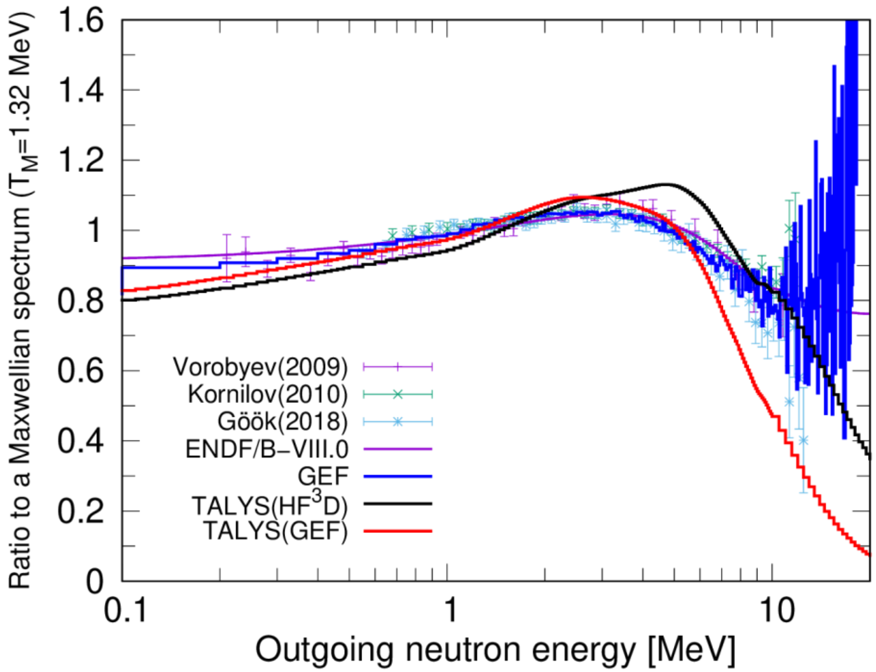
- TALYS(GEF) underestimates the evaluated data at thermal energy by about 0.1, but it agrees with the data as the incident energy increases.

^{235}U(n,f): PFNS

PFNS in the laboratory frame

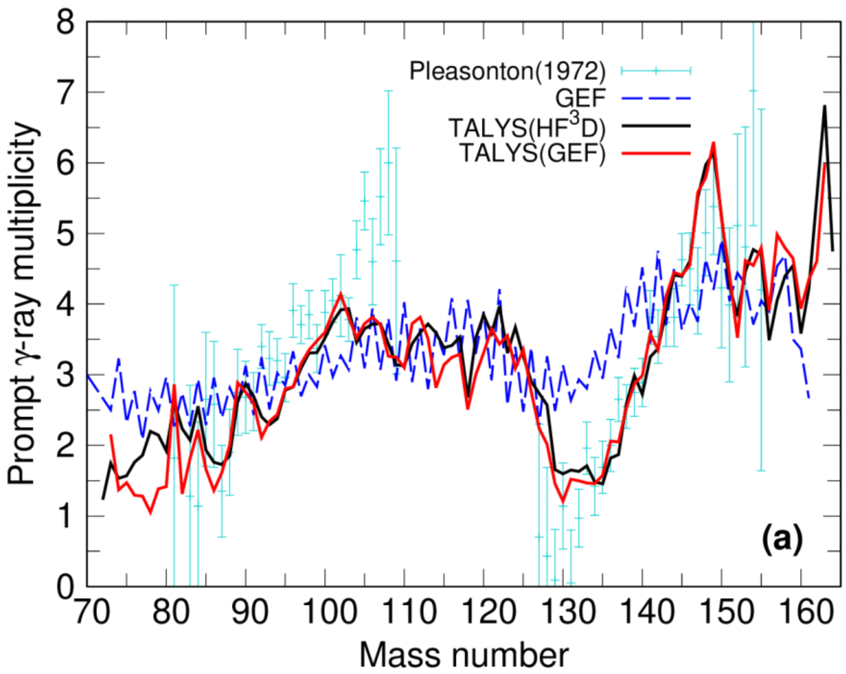


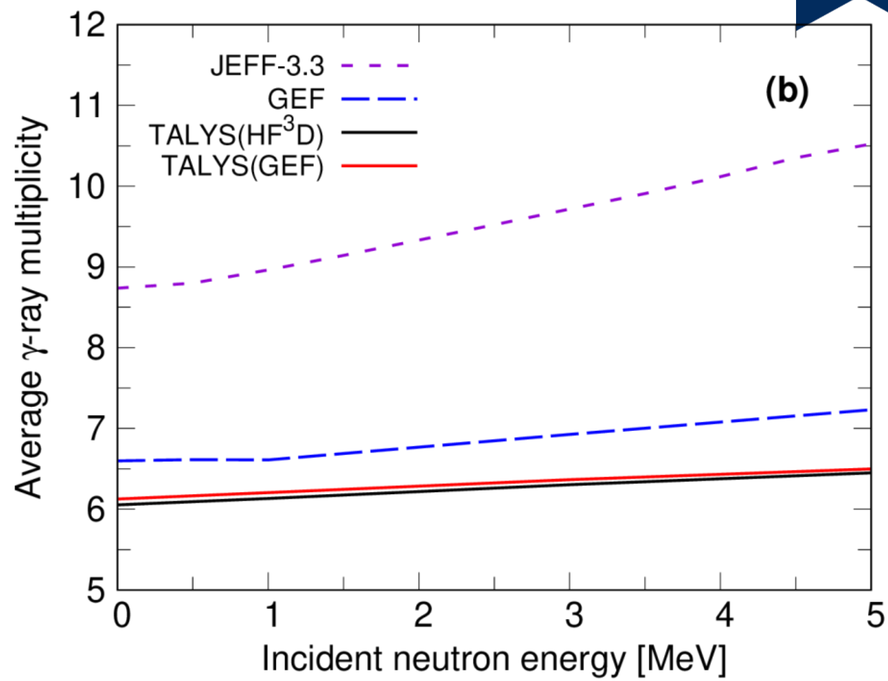
PFNS as ratio to a Maxwellian spectrum



- TALYS(GEF) is underestimated at higher energies.
- The pronounced peak in the TALYS(HF^{3}D) around 6 – 7 MeV is well above the experimental data.

^{235}U(n,f): γ-ray multiplicity

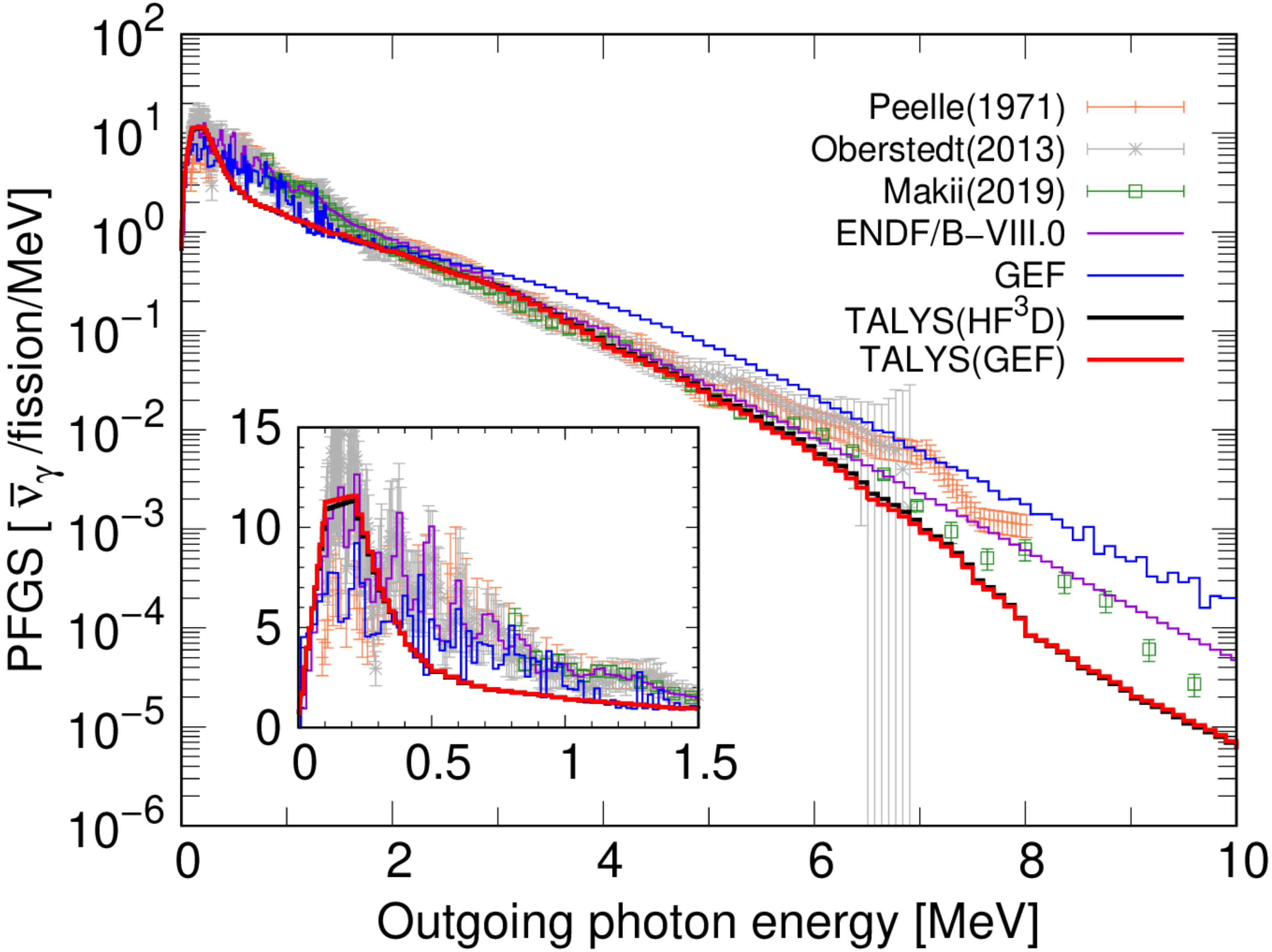




	$\bar{\nu}_\gamma$
TALYS(GEF)	6.13
TALYS(HF³D)	6.05
GEF	6.61
Oberstedt (2013)	8.19 ± 0.11
Verbinski (1973)	6.70 ± 0.30
Pleasonton (1972)	6.51 ± 0.30
Peelle (1971)	7.45 ± 0.35
ENDF-B/VIII.0	8.58
JEFF-3.3	8.74

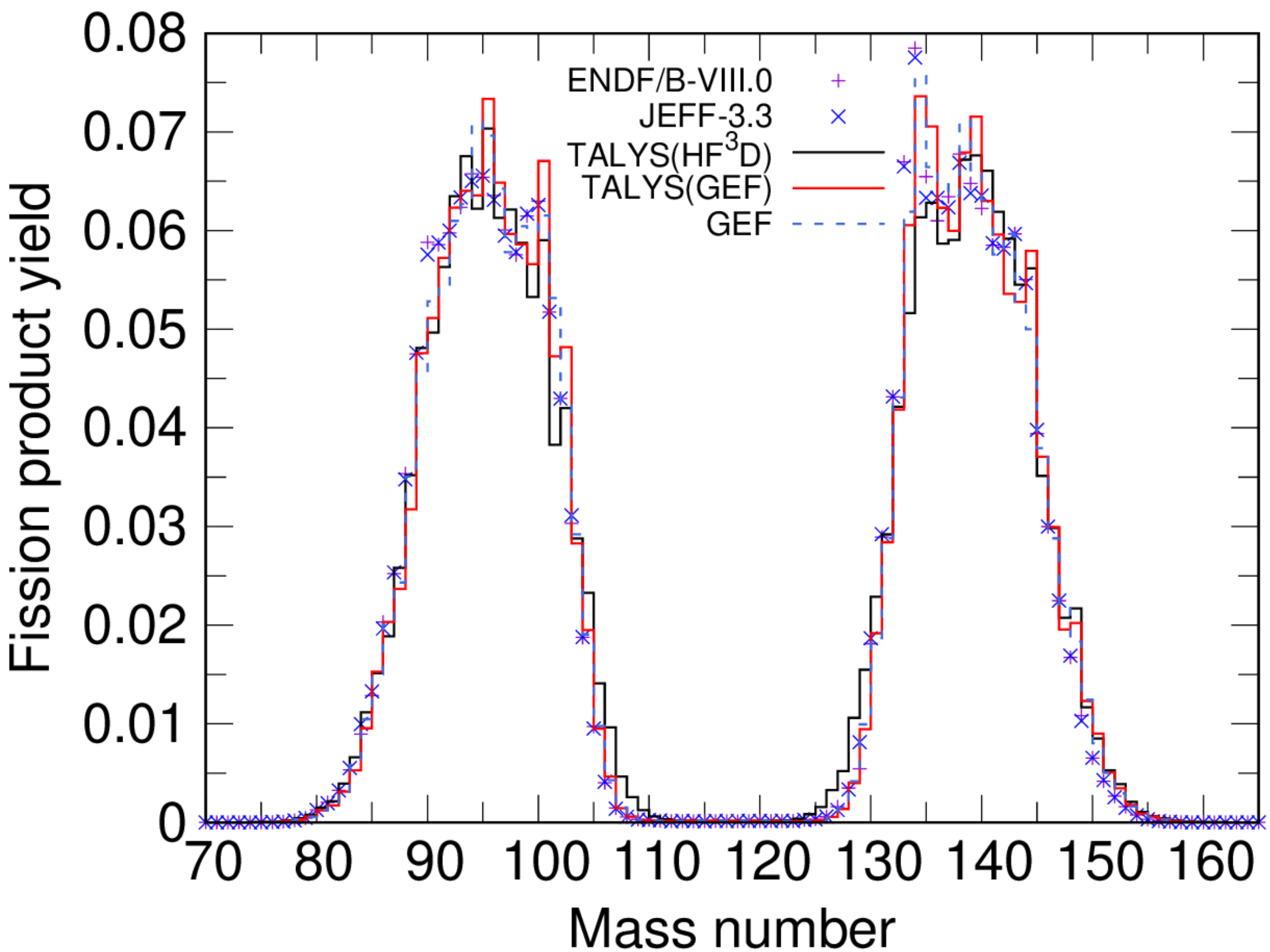
- While stand-alone GEF has a flatter $\bar{\nu}_\gamma$, TALYS results exhibit the saw-tooth shape.
- TALYS' $\bar{\nu}_\gamma$ are smaller around fragment mass number A=100 to 110.
- TALYS underestimates $\bar{\nu}_\gamma$ compared to experimental and evaluated data.

$^{235}U(n,f)$: PFGS



- A pronounced peak is observed around 0.2 MeV in both TALYS(GEF) and TALYS(HF^3D).

$^{235}U(n,f)$: fission product yield

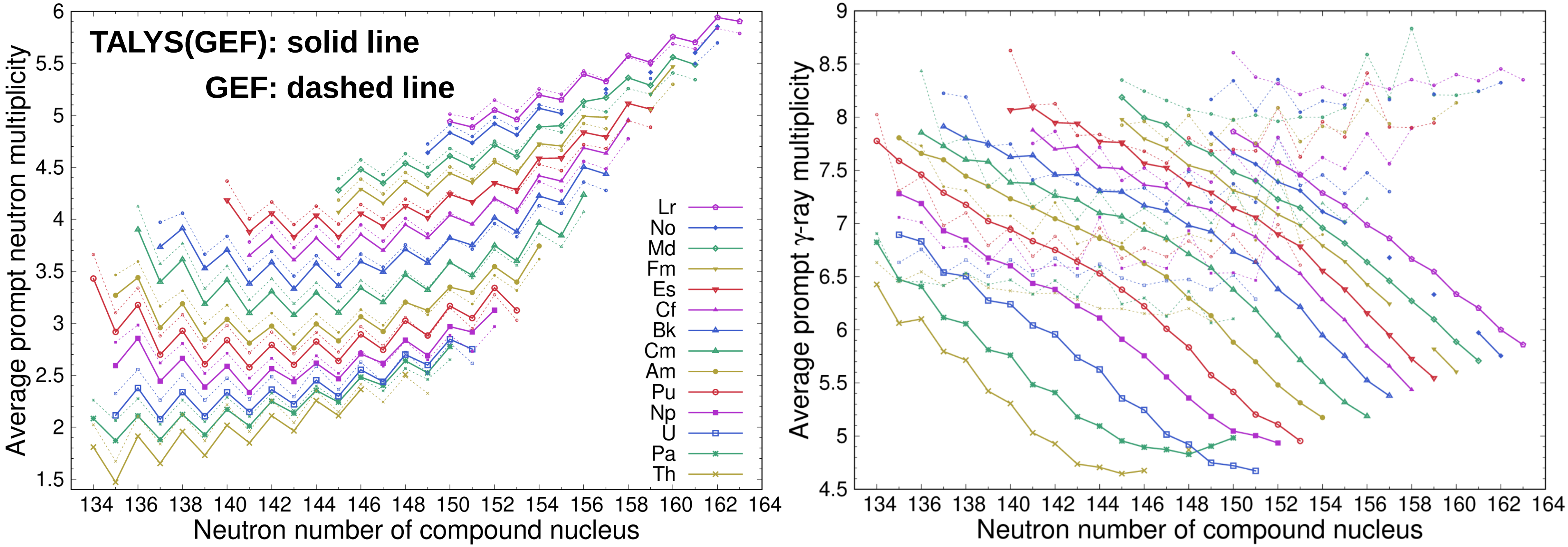


- Both TALYS results reproduce the prominent peak at A = 138 for heavy fragments and at A = 94, 100 for light ones.
- The prominent peak at A = 134 appears only in TALYS(GEF).

Global study on actinides

Tokyo Tech

We examined 243 selected actinide isotopes with 1 MeV incident neutron energy using: $f^2 = 4$, $f_s = 0.4$, and $N = 150$.



TALYS is now able to perform this kind of global calculation of statistical decay of primary fission fragments, ranging from very neutron deficient to neutron-rich nuclei.

- $\bar{\nu}_n$ calculated by stand-alone GEF and TALYS(GEF) coincides with each other quite well including the zigzag pattern caused by the pairing effects.

- $\bar{\nu}_\gamma$ for the neutron-rich nuclei differs much between TALYS(GEF) and GEF, which reflect difference of the statistical decay calculation in these codes.

Conclusions

- TALYS recently has been extended to perform Hauser-Feshbach statistical decay calculation with fission fragment distribution database generated by GEF, HF^{3}D, SPY, and user's own data.

- TALYS has a limitation within the energy range up to first-chance fission. In the future, TALYS will be responsible for multi-chance fission.

- The optimal parameters are decided to prioritize to reproduce $\bar{\nu}_n$ and the shape of PFNS.

- TALYS shows a decent agreement with the experimental and evaluated data of prompt neutron observables and independent fission product yield, especially.

- TALYS is now able to perform this kind of global calculation of statistical decay of primary fission fragments, ranging from very neutron deficient to neutron-rich nuclei.

Acknowledgements

- Authors thank T. Kawano (Los Alamos National Laboratory) and K.-H. Schmidt for valuable discussions.

- The IAEA-NDS acknowledges the internship program "The nuclear Regulation Human Resource Development Program (ANSET: Advanced Nuclear 3S Education and Training)" entrusted to Tokyo Institute of Technology, Tokyo, Japan by the Nuclear Regulation Agency of Japan, for supporting this work.

- A. Al-Adili would like to acknowledge Liljewalch travel scholarships and Ingegerd Berghs stiftelse for their research grants.

- K. Fujio thanks C. Ishizuka and acknowledges her Grant-in-Aid for Scientific Research (B), MEXT, Japan, and by Japan Society for the Promotion of Science (JSPS) KAKENHI Grant Number 21H01856.

Thank you for your kind attention!

Other important parameters

- **Optical model potentials**

  Koning-Delaroche global optical model

- **Level density parameters**

  Constant temperature model using the level density parameters and systematics from:

  A. J. Koning, S. Hilaire, S. Goriely, Nucl. Phys. A810, 13-76 (2008).

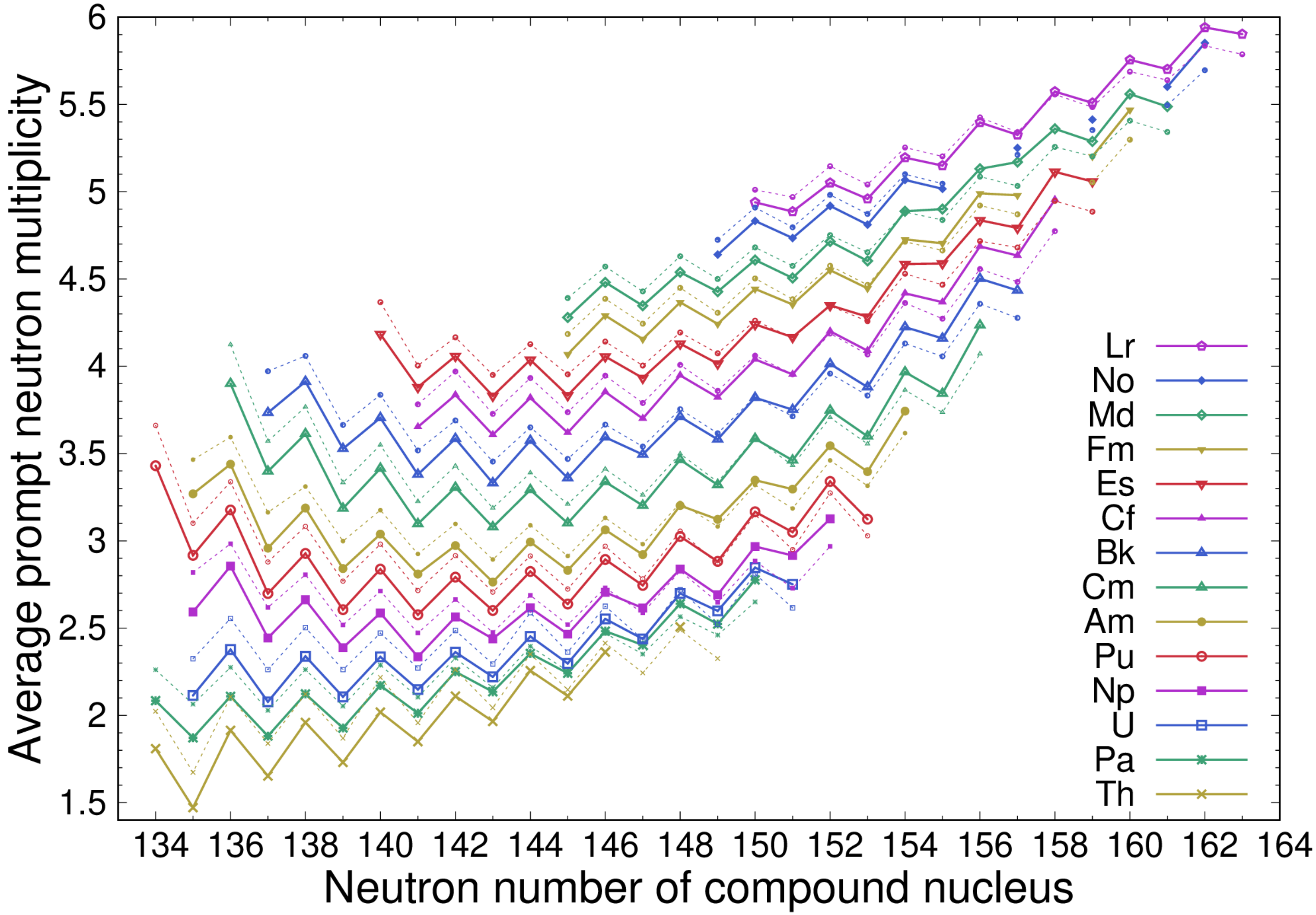
- **E1 and M1 *γ*-ray strength function**

  IAEA-CRP SMLO 2019 tables and IAEA GSF CRP 2018

- **Discrete level properties**

  RIPL-3

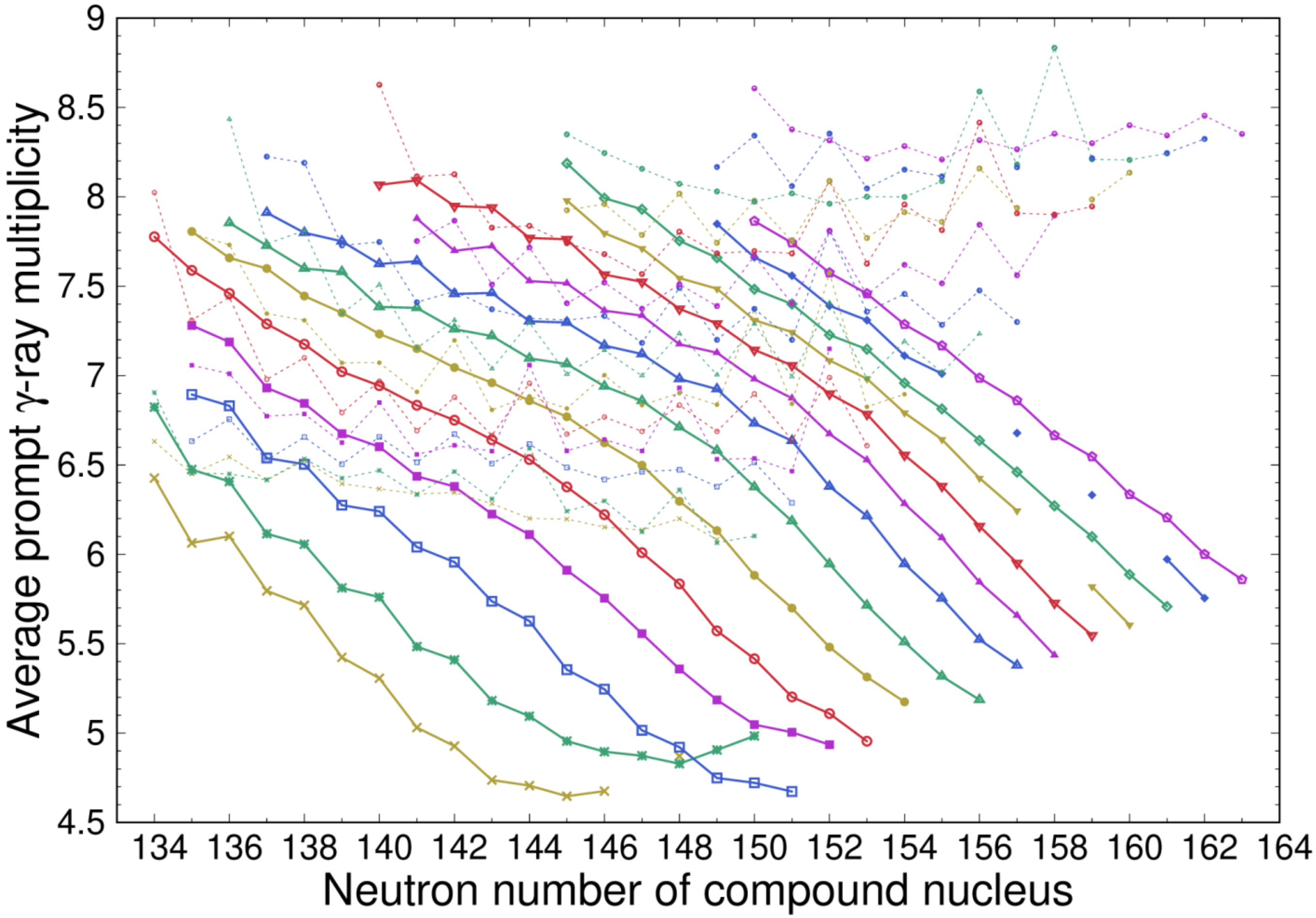
Global study on actinides



・The zigzag pattern is attributed to the difference in neutron separation energy of the compound nucleus.

・The even *N* compound nucleus gains more excitation energy due to the pairing of the captured incident neutron compared to an odd *N* compound nucleus.

Global study on actinides



- $\bar{\nu}_\gamma$ is known to be sensitive to the angular momentum population in the fragments.

→ Different treatments of the fragment angular momenta in GEF and TALYS could be one reason for such discrepancies.

Sensitivity on scaling parameters

TALYS(HF^{3}D)						
# of N	f^2	f_s	$\overline{\nu}_\gamma$	$\overline{\nu}_n$	$\langle\epsilon_\gamma\rangle$[MeV]	$\langle\epsilon_n\rangle$[MeV]
300	3	0.4	5.06	2.49	0.869	2.049
	3	0.6	5.76	2.47	0.818	1.945
	3	0.8	6.21	2.45	0.786	1.915
	3	1.0	6.50	2.44	0.764	1.907
	4	0.4	6.05	2.41	0.772	2.079
	4	0.6	6.92	2.40	0.728	1.941
	4	0.8	7.48	2.39	0.699	1.899
	4	1.0	7.85	2.38	0.677	1.887
	5	0.4	6.85	2.35	0.714	2.107
	5	0.6	7.90	2.34	0.675	1.938
	5	0.8	8.55	2.33	0.646	1.886
	5	1.0	8.96	2.33	0.625	1.869
	6	0.4	7.45	2.30	0.681	2.132
	6	0.6	8.66	2.29	0.646	1.935
	6	0.8	9.36	2.29	0.617	1.876
	6	1.0	9.85	2.29	0.593	1.855
ENDF-B/VIII.0			8.58	2.41	0.85	2.00
JEFF-3.3			8.74	2.41	0.81	

Sensitivity on *N*

TALYS(HF^{3}D)						
# of N	f^2	f_s	$\overline{\nu}_\gamma$	$\overline{\nu}_n$	$\langle\epsilon_\gamma\rangle$[MeV]	$\langle\epsilon_n\rangle$[MeV]
50	4	0.4	3.46	2.49	1.192	1.990
100	4	0.4	4.87	2.43	0.923	2.045
200	4	0.4	5.78	2.41	0.804	2.072
300	4	0.4	6.05	2.41	0.772	2.079
ENDF-B/VIII.0			8.58	2.41	0.85	2.00
JEFF-3.3			8.74	2.41	0.81	

^{235}U(n,f): multiplicities and average energy

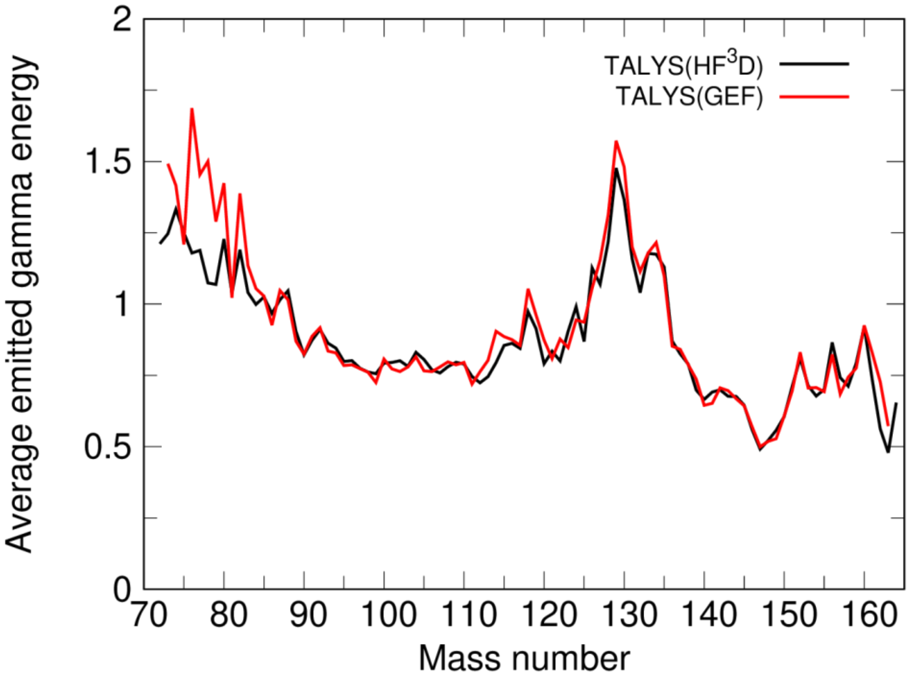
Tokyo Tech

- The optimal values: $f^2 = 4,\ f_s = 0.4$, and $N = 300$

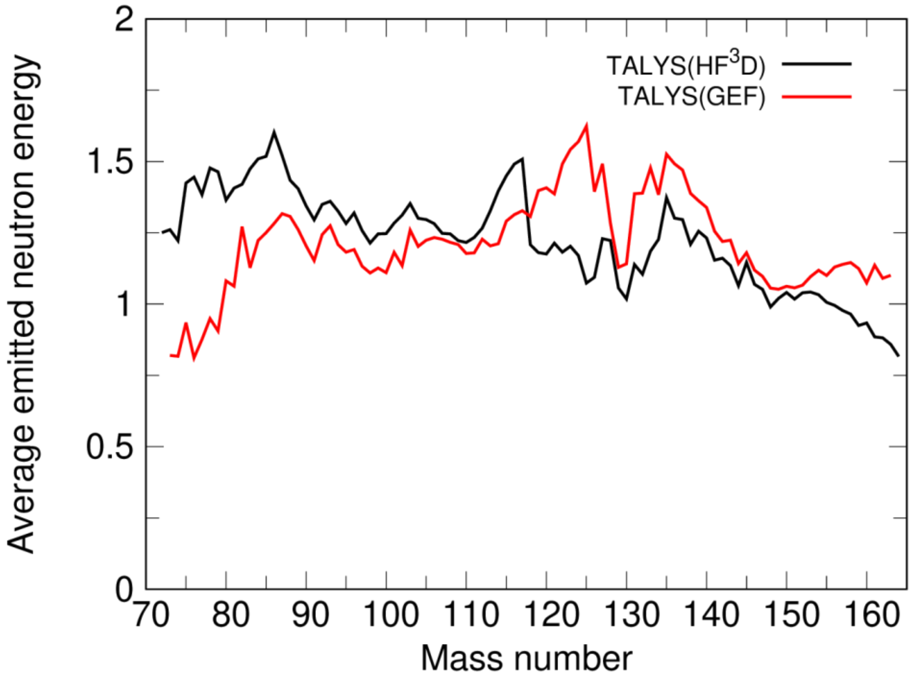
	$\overline{\nu}_\gamma$	$\overline{\nu}_n$	$\langle\epsilon_\gamma\rangle$[MeV]	$\langle\epsilon_n\rangle$[MeV]
TALYS(GEF)	6.13	2.30	0.761	1.991
TALYS(HF^{3}D)	6.05	2.41	0.772	2.079
GEF	6.61	2.42	0.962	1.997
Oberstedt et al.(2013)	8.19±0.11		0.85±0.02	
Verbinski et al.(1973)	6.70±0.30		0.97±0.05	
Pleasonton et al.(1972)	6.51±0.30		0.99±0.07	
Peelle et al.(1971)	7.45±0.35		0.96±0.05	
ENDF-B/VIII.0	8.58	2.41	0.85	2.00
JEFF-3.3	8.74	2.41	0.81	

$^{235}U(n,f)$: average energies

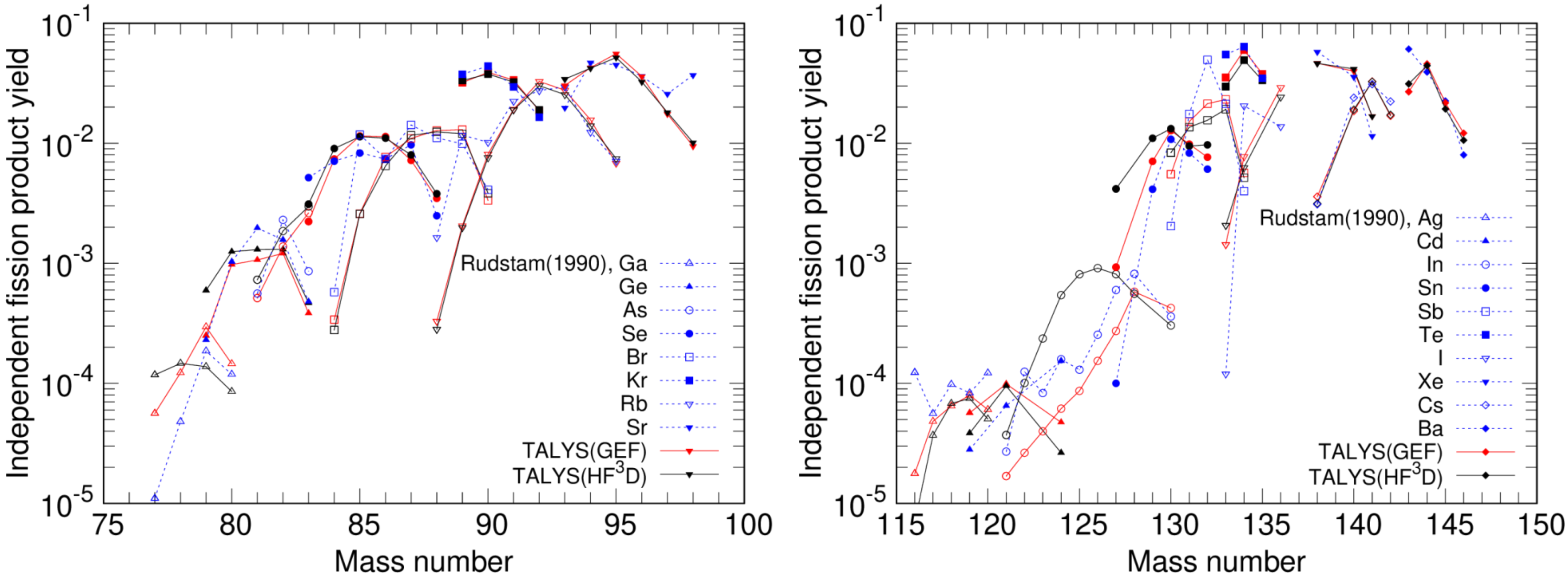
Average emitted γ-ray energy



Average emitted neutron energy

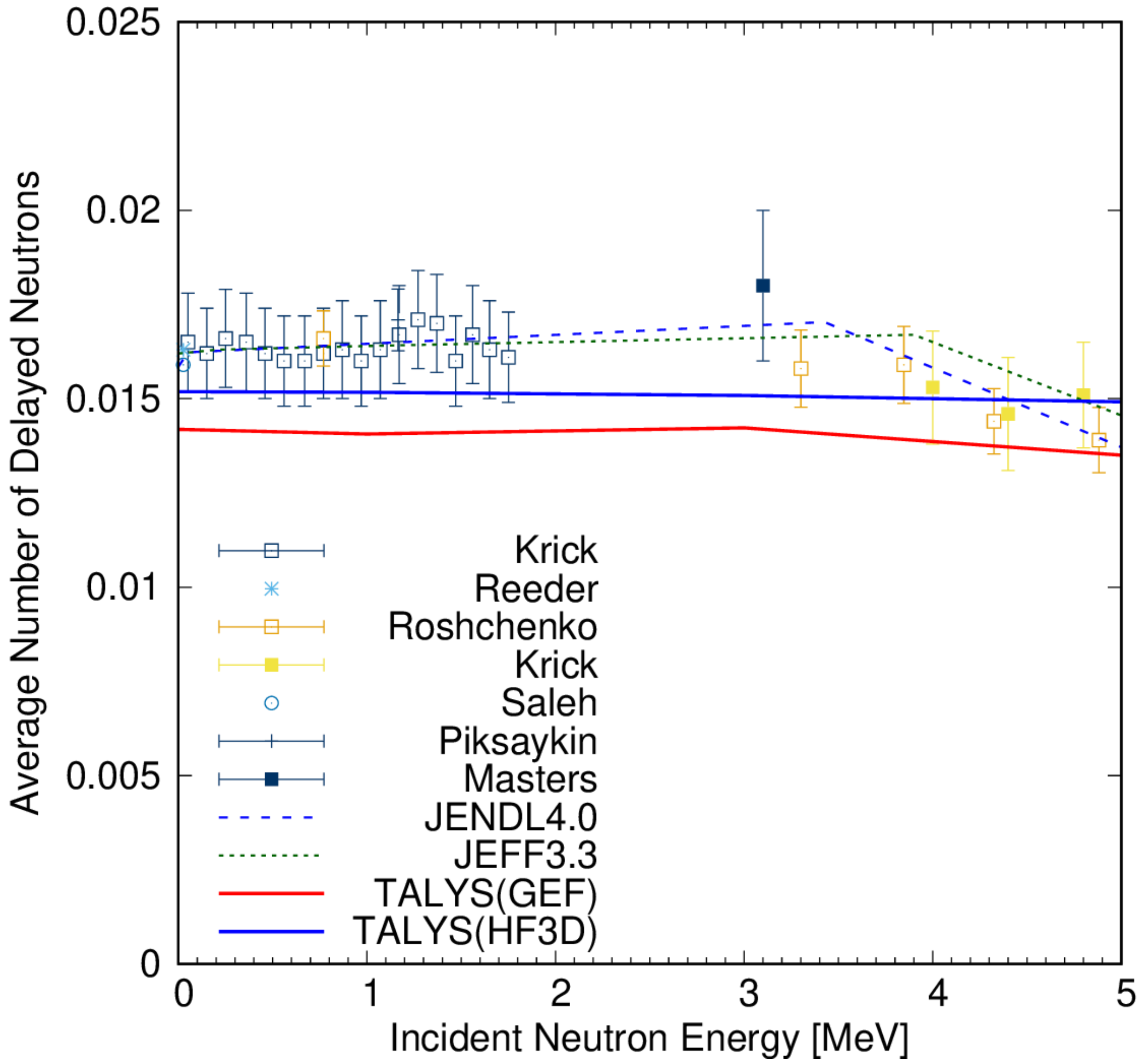


$^{235}U(n,f)$: fission product yield



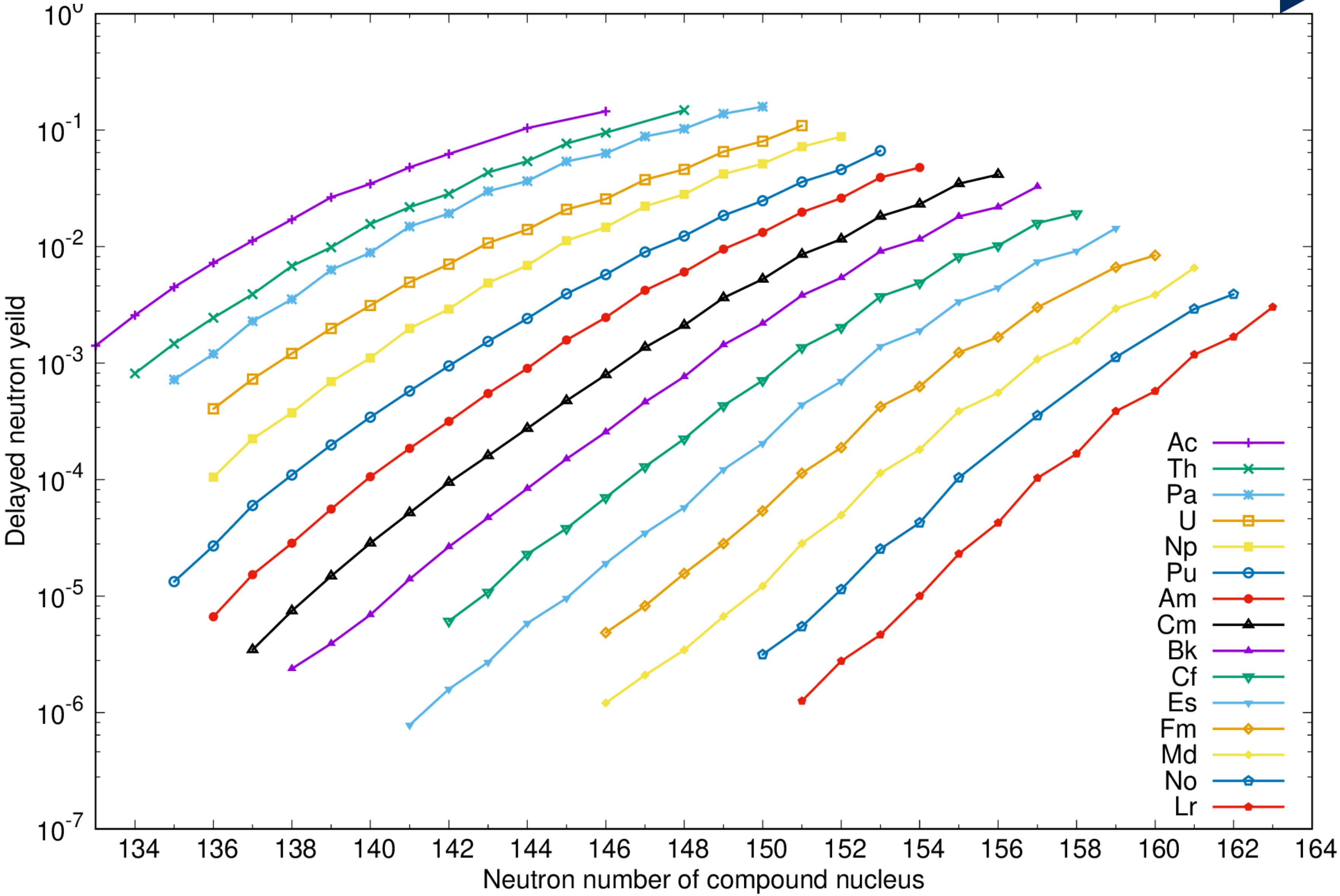
- TALYS results are roughly consistent with the tendency shown in the experimental data.

$^{235}U(n,f)$: average number of delayed neutron



Calculated by S. Okumura

Global study of delayed neutron yield



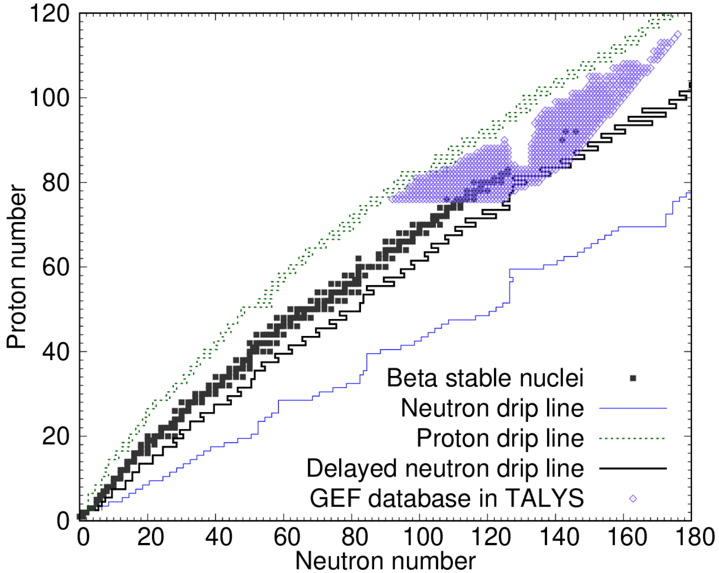
Calculated by S. Okumura

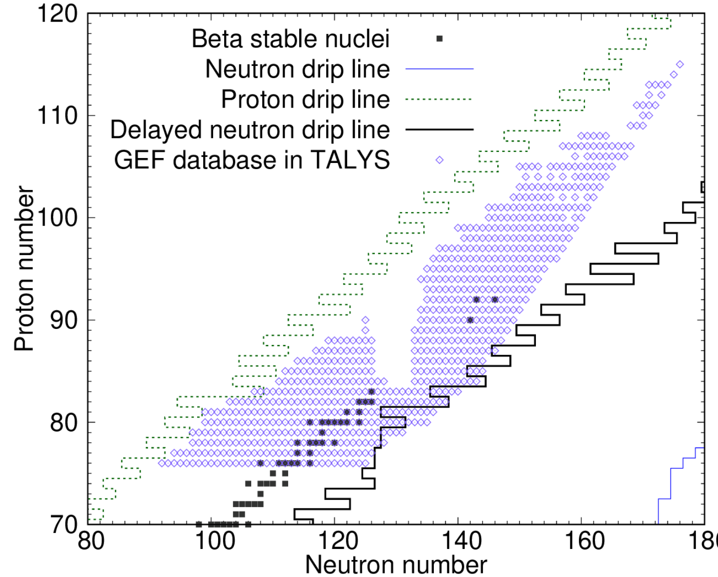
Fission fragment database in TALYS

GEF Monte Carlo-based phenomenological fission model

K. –H. Schmidt, B. Jurado, C. Amouroux, C. Schimitt, Nuclear Data Sheets, 131, 107-221 (2016).

・For 737 fissioning nuclei ranging from $_{76}$Os to $_{115}$Mc





HF³D Designed with a fully deterministic technique with fitting functions

S. Okumura, T. Kawano, P. Jaffke, P. Talou, and S. Chiba, JNST, 55(9), 1009-1023 (2018).

・For neutron-induced fission of ^{235}U, ^{238}U, and ^{239}Pu

SPY Obtained from a statistical scission point model using microscopic calculation

J. –F. Lemaître, S. Goriely, S. Hilaire, and J.-L. Sida, Phys. Rev. C99, 034612 (2019).

Arbitrary fission fragment data provided by users