IAEA
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Atoms for Peace and Development

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Toward a consistent calculation of prompt and beta decay observables from fission fragment by TALYS

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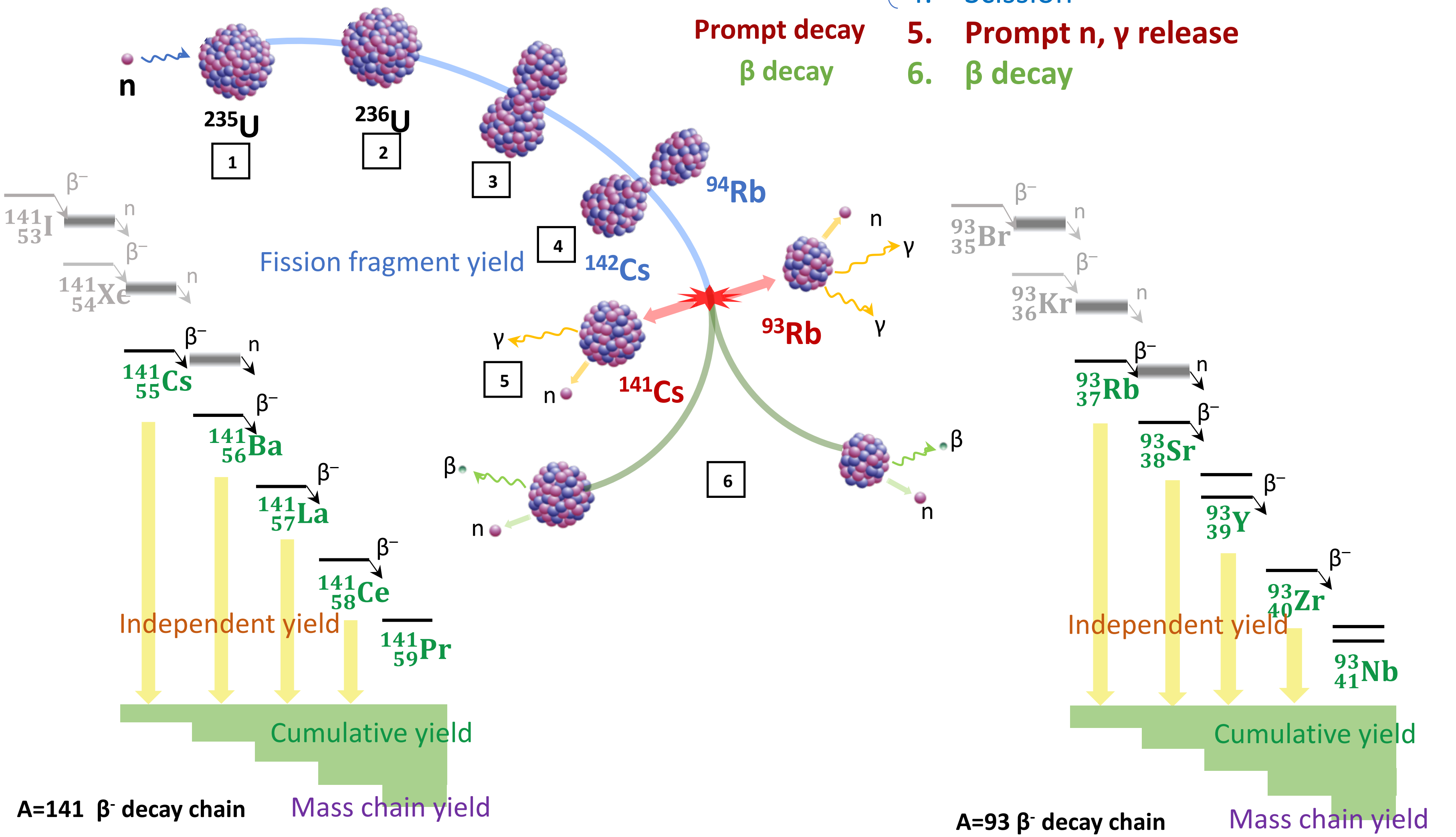
Introduction

Nuclear fission process consists of (at least) 3 different physics

Fission physics
1. Capture neutron by ^{235}U
2. Compound nucleus formation of ^{236}U
3. Deformation and elongation
4. Scission

Prompt decay
5. **Prompt n, γ release**

β decay
6. **β decay**



Required consistencies among fission observables

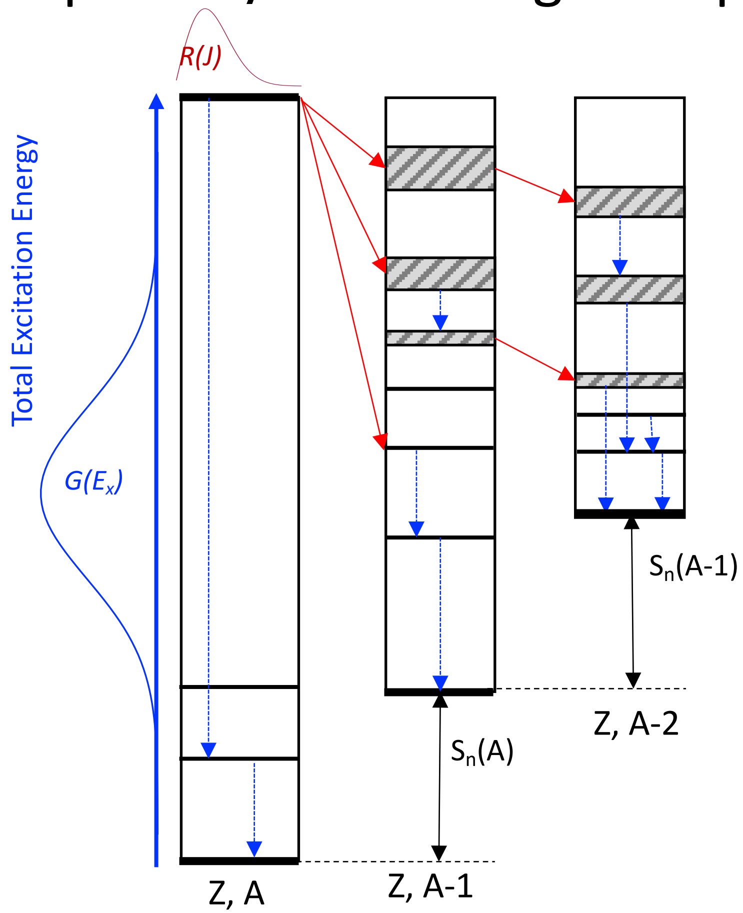
- Number of total neutron emissions (MF1 MT452)
  - Number of prompt neutron emissions (MF1 MT456)
  - Prompt neutron spectrum (MF5 MT18)
  - Number of beta-delayed neutron emissions (MF1 MT455)
    - Beta-delayed neutron emission probabilities (branching ratio) in the decay data
- Independent fission product yield (MF8 MT454)
  - Number of beta-delayed neutron emissions (MF1 MT455) via Decay data
  - Cumulative fission product yield via Decay data
  - Decay heat via Decay data
- Cumulative fission product yield(MF8 MT459)
  - Decay data
  - Independent fission product yield (MF8 MT454)
  - Number of beta-delayed neutron emissions (MF1 MT455)

In order to ensure consistencies among fission observables, it is important to calculate from fission fragment to beta decay in one flow.

Identifying Inconsistencies in Fission Product Yield Evaluations with Prompt Neutron Emission
P. Jaffke, *J. Nucl. Sci. Eng.*,190,258-270 (2018) .

Hauser-Feshbach statistical decay for fission fragments

- To treat a primary fission fragment as a compound nucleus
- Distributions of primary fission fragment characterized by Y(Z, A, E_{ex}, J^{Π}) are generated and integrated deterministically for all primary fission fragment pairs (no MonteCarlo sampling).



Neutron emission multiplicity

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

- Distribution of excitation energy, *G(E)*

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

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

- Probability of nucleus having the state of spin *J* and parity *Π, R(J, Π)*

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

σ²(U): spin cut-off parameter
U: Excitation energy
f: scaling factor

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

Inputs for Hauser-Feshbach calculation in TALYS

Prompt decay

1. Read fission fragment distribution from file:

$$Y_{ff}(Z, A, E_{ex}, J, \Pi)$$

Y_{ff}: fragment yield
Z: fragment charge
A: framgment mass
E_{ex}: Excitation energy
J: spin
Π : parity

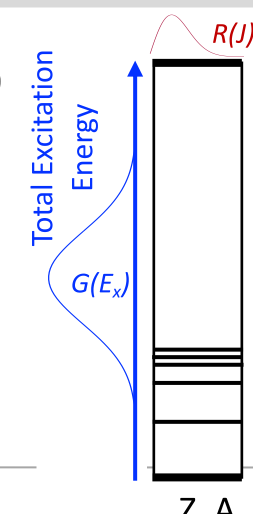
```
# Z          =   92
# A          =  236
# Ex (MeV)  = 6.55e+00
# Ntotal     =  195
```

} Information of compound system

# Zl	Al	Zh	Ah	Yield	TKE[MeV]	TXE[MeV]	El[MeV]	Wl[MeV]	Eh[MeV]	Wh[MeV]
30	74	62	162	3.0000e-06	1.4373e+02	2.5550e+01	9.7733e+00	1.7875e+00	1.5777e+01	5.7377e+00
30	75	62	161	1.1000e-05	1.4544e+02	2.2786e+01	5.7400e+00	3.1184e+00	1.7046e+01	6.9337e+00
31	75	61	161	2.0000e-06	1.4076e+02	2.6930e+01	5.7300e+00	5.5013e+00	2.1200e+01	2.4042e+00
30	76	62	160	5.0000e-05	1.4532e+02	2.6206e+01	6.1234e+00	2.4469e+00	2.0082e+01	6.5358e+00
				(omission of a middle part)						
46	117	46	119	9.0000e-05	1.6262e+02	3.4208e+01	1.7155e+01	8.5389e+00	1.7053e+01	7.6726e+00
47	117	45	119	7.0000e-06	1.6130e+02	3.2700e+01	1.9750e+01	7.0597e+00	1.2950e+01	4.2823e+00
45	118	47	118	7.0000e-06	1.6167e+02	3.1759e+01	1.4299e+01	1.0776e+01	1.7460e+01	8.7686e+00
46	118	46	118	9.0000e-05	1.6435e+02	3.5416e+01	1.7522e+01	6.7362e+00	1.7893e+01	7.0032e+00
47	118	45	118	1.1000e-05	1.6072e+02	3.2713e+01	1.6269e+01	5.4600e+00	1.6444e+01	7.6689e+00

2. Reconstruct fission fragment distributions (*$G(E_x)$ and $R(J^\Pi)$*)

3. Run Hauser-Feshbach statistical decay calculation
   - neutron(s) and gamma(s) emission from the fragment



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

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

Fission fragment yield models stored in TALYS (1.96)

Prompt decay

GEF (ffmodel 1)

Designed with global fitting parameters based on experimental data

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

From $_{76}$Os to $_{115}$Mc, 737 nuclides

HF³D (ffmodel 2)

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.

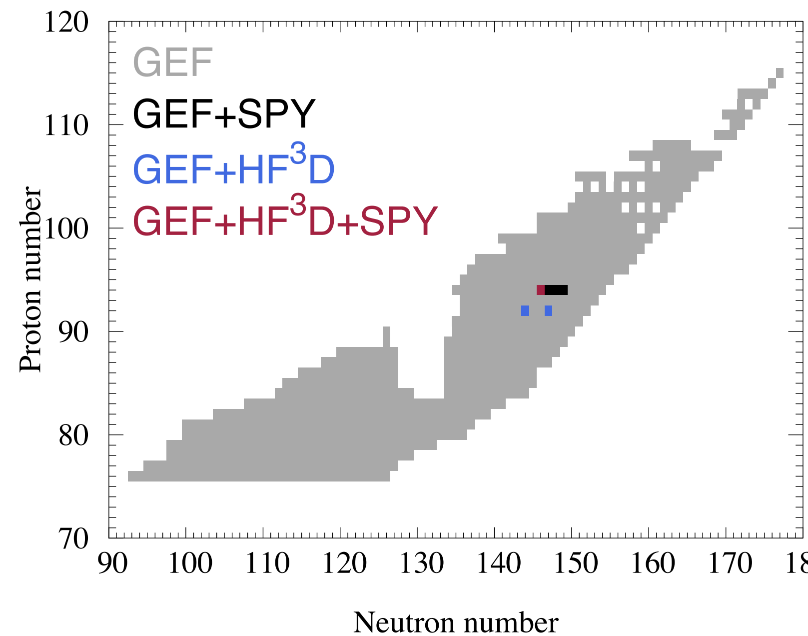
^{236}U, ^{239}U, and ^{240}Pu, 3 nuclides

SPY (ffmodel 3)

Designed with a statistical scission point model using microscopic calculation

J.-F. Lemaître, S. Goriely, S. Hilaire, and J.-L. Sida, PRC99, 034612, 2019.

^{240}Pu, ^{241}Pu, ^{242}Pu, and ^{243}Pu, 4 nuclides



… more and updated fission fragment distributions are expected for GEF and SPY model

Local (ffmodel 0)

Arbitrary fission fragment data provided by users. (will be implemented in next update of TALYS)

Please see details in the IAEA NDS report https://nds.iaea.org/publications/nds/iaea-nds-0239/

Calculatable physical quantities

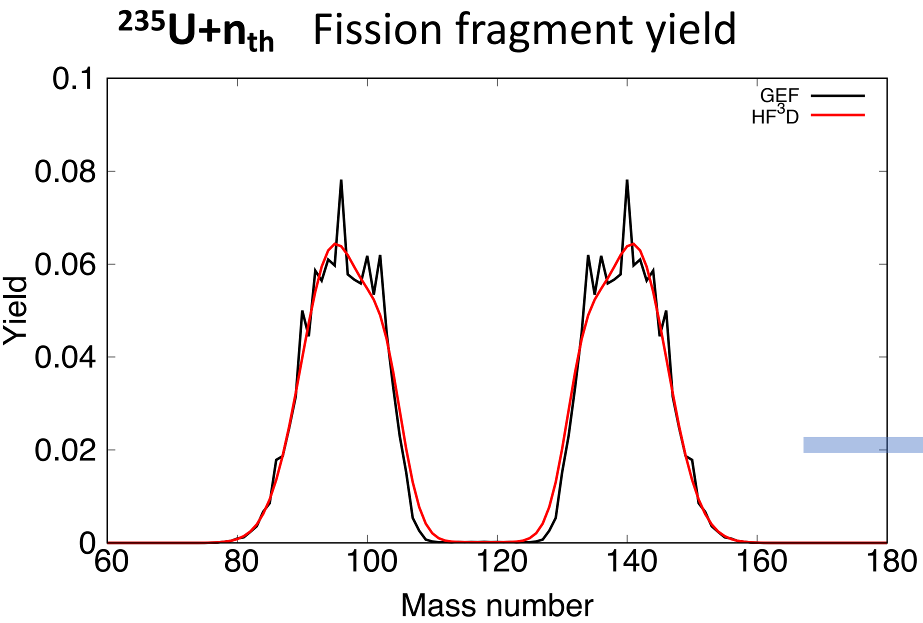
Table 1: Representative fission quantities comparable to experimental data.

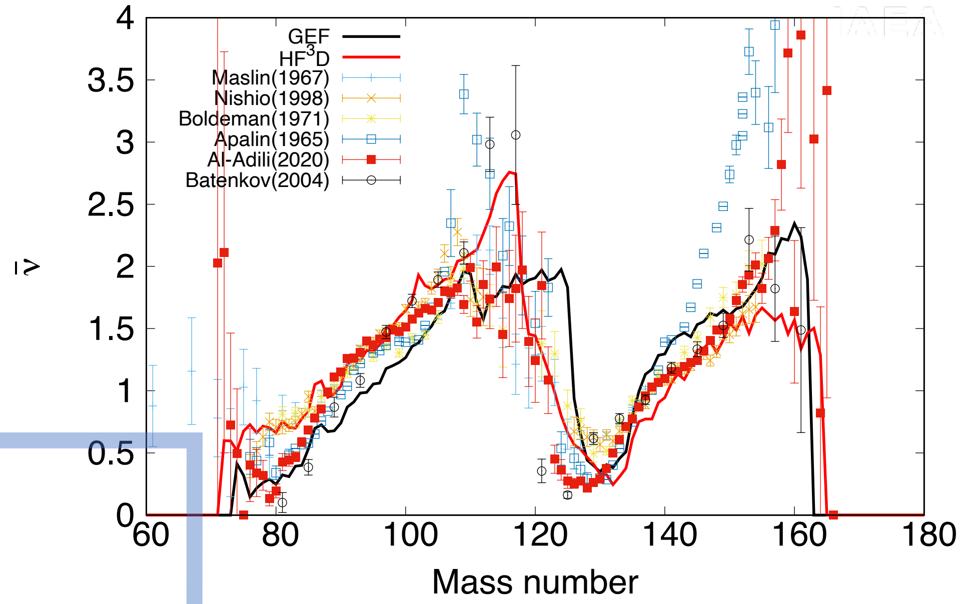
Type	Description
$Y_i(A)$	Independent fission yield as a function of mass number
$Y_i(Z, A, M)$	Independent fission yield of all isotopes including meta-stable state
$\overline{\nu}$	Average number of neutrons per fission
$\overline{\gamma}$	Average number of γ-rays per fission
$\overline{\nu}(A)$	Average neutron multiplicity as a function of fission product mass
$\overline{\gamma}(A)$	Average γ-ray multiplicity as a function of fission product mass
$\langle E_n \rangle$	Average prompt neutron energy
$\langle E_\gamma \rangle$	Average prompt γ-ray energy
$\langle E_n \rangle(A)$	Average neutron energy as a function of product mass
$\langle E_\gamma \rangle(A)$	Average γ-ray energy as a function of product mass
$\mathrm{P}(\nu)$	Neutron multiplicity distribution
$\chi(\nu)$	Prompt fission neutron energy spectrum (PFNS)
$\phi(\gamma)$	γ-ray energy spectrum

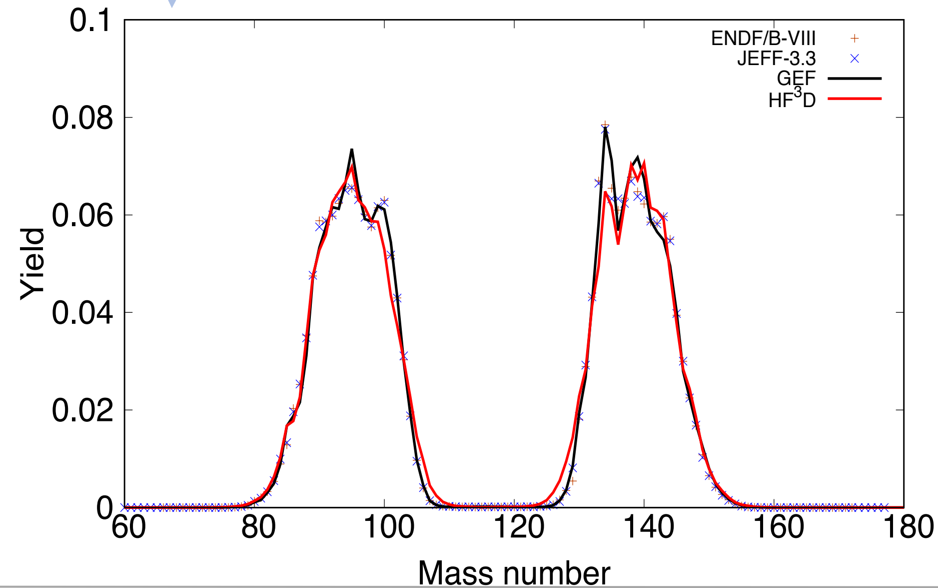
Calculated neutron observables for $^{235}U+n_{th}$

Prompt decay

Work from K. Fujio in IAEA-NDS-0239

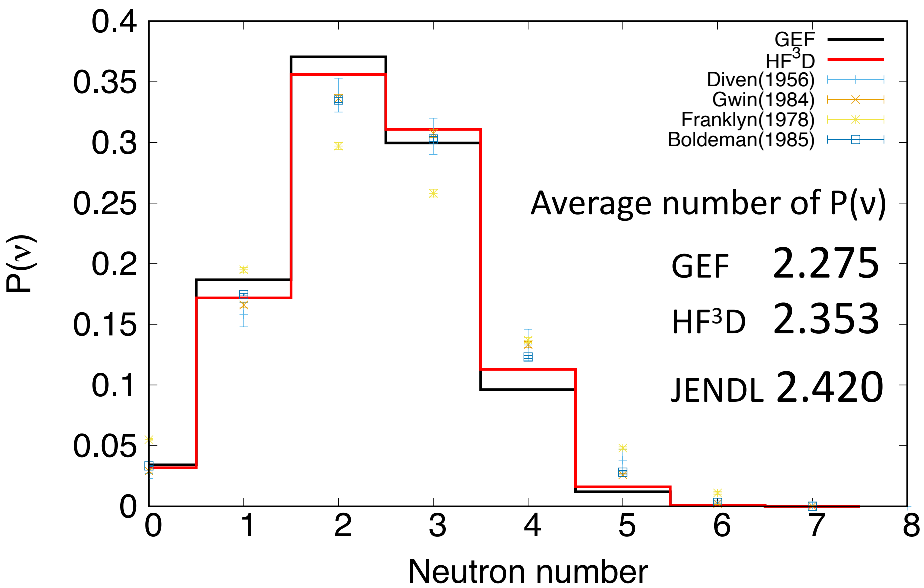


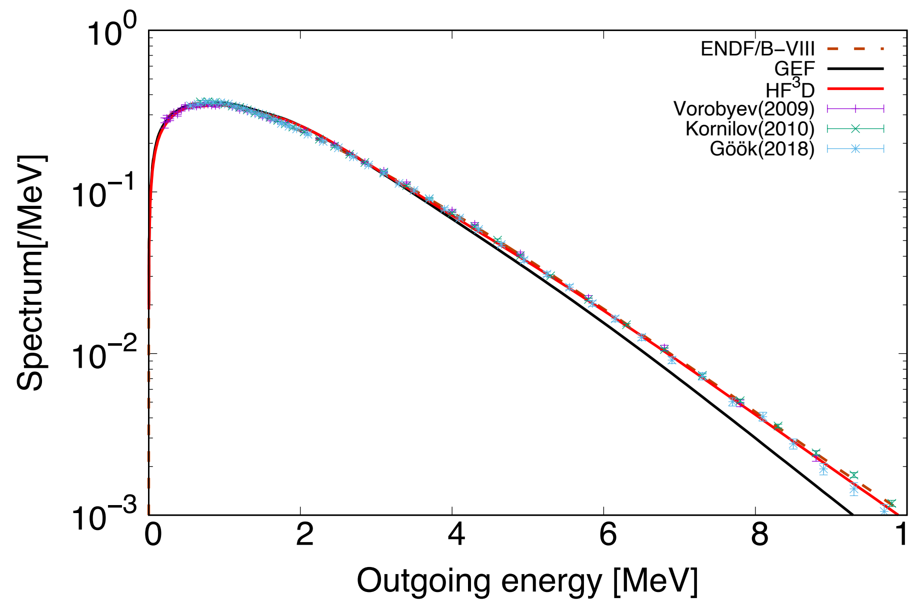


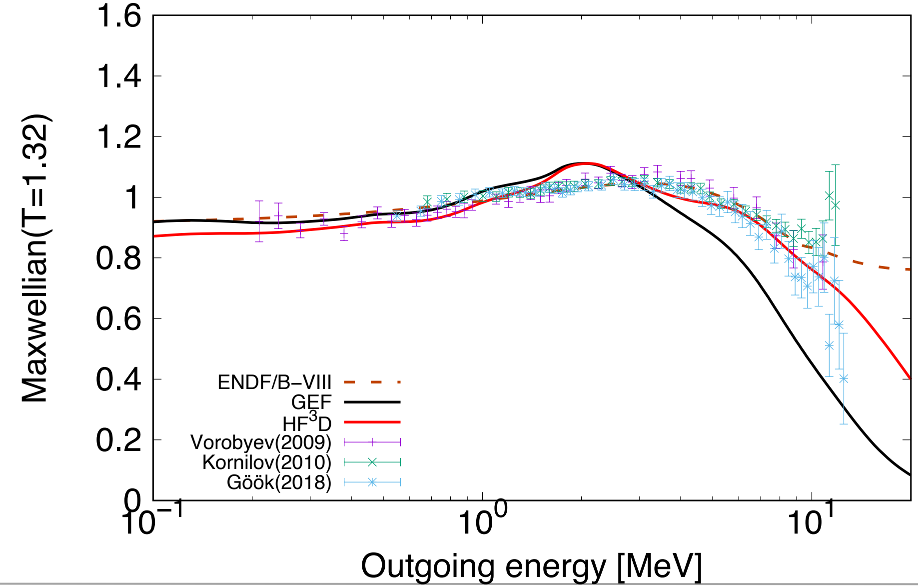


Calculated neutron observables for $^{235}U+n_{th}$

Work from K. Fujio in IAEA-NDS-0239

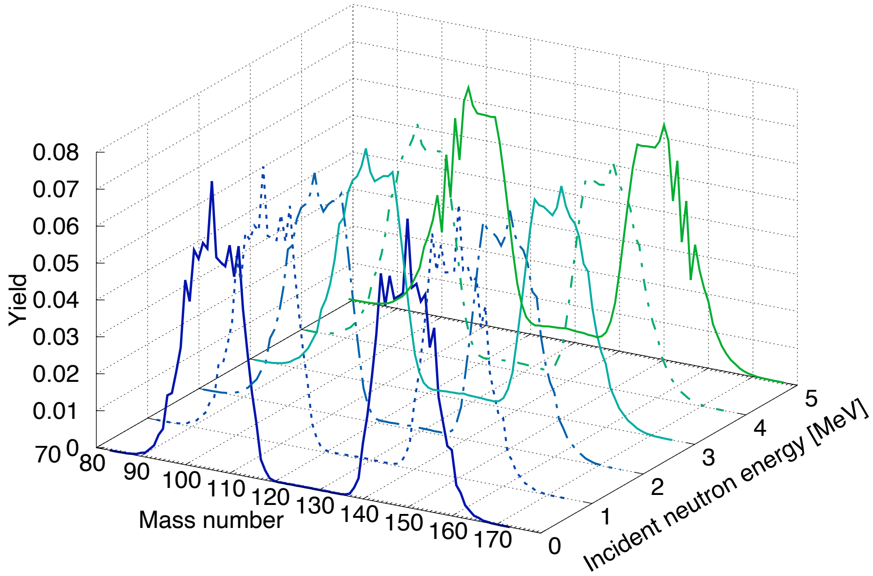


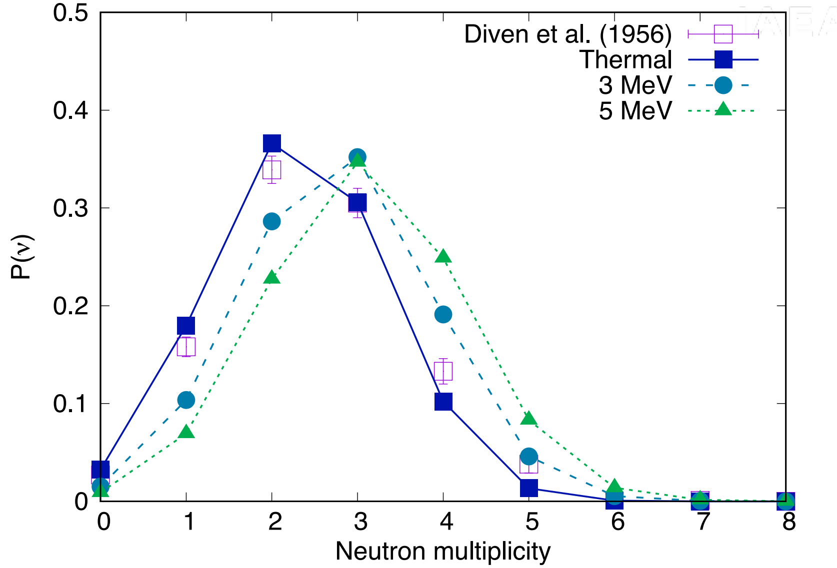


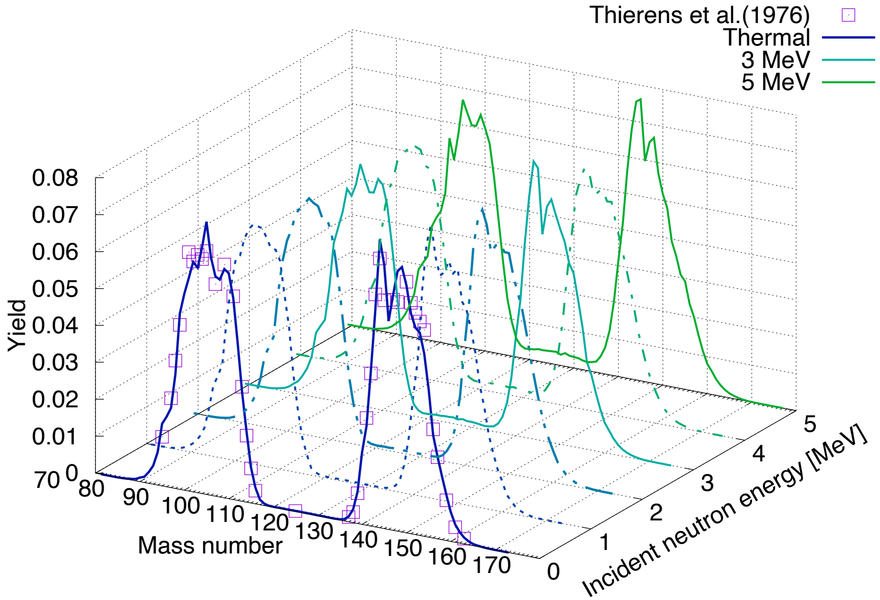


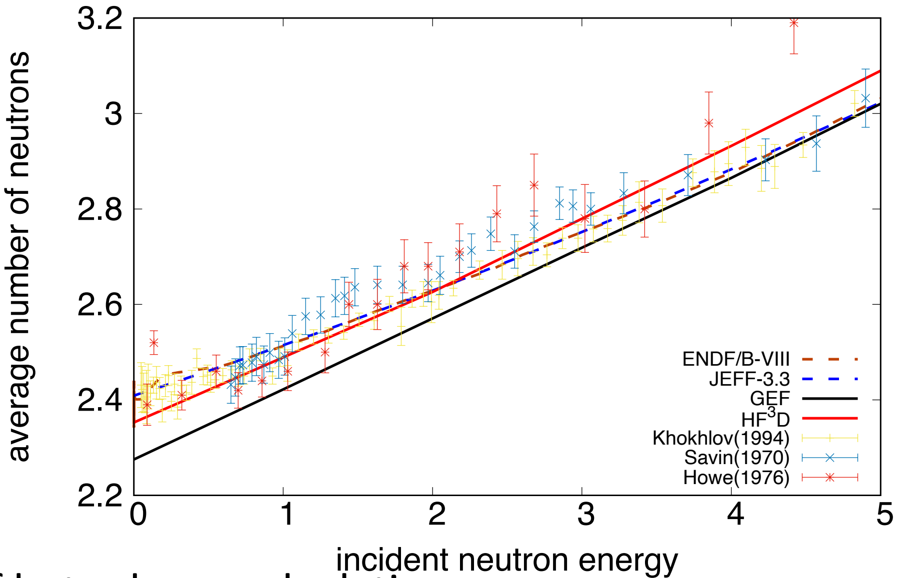
Energy dependent fission observables for ^{235}U+n

Work from K. Fujio in IAEA-NDS-0239









Independent fission product yield → input of beta-decay calculation

Standalone beta decay program

- Python

1. Convert ENDF format decay data library files to
   - (1) Simplified format (inspired by the Oyak code)

```
   55   141    0  2.4910000E+01  6.0000000E-02  1.3970950E+02    2    5 1920
1.5473620E+06  1.8786310E+05  1.7248140E+06  5.7510480E+03  7.5359650E+01  3.0848980E+00
1.0000000E+00  0.0000000E+00  5.2560000E+06  1.0000000E+04  9.9965800E-01  2.6533000E-05
1.5000000E+00  0.0000000E+00  7.2100000E+05  1.2000000E+04  3.4200000E-04  1.4000000E-05
```

   - (2) JSON format
2. Generate β-decay chains from decay data library
3. Import independent fission product yield file (TALYS output format)

```
#   Z    A iso      FP yield       FF yield        FP xs          FF xs
   30   74 -1     5.3961E-06     3.0000E-06     1.9191E+00     1.0670E+00
   30   75 -1     1.4014E-05     1.1000E-05     4.9841E+00     3.9123E+00
   31   75 -1     2.7919E-06     2.0000E-06     9.9294E-01     7.1132E-01
```

4. Solve the Bateman equations
5. Calculate beta-decay observables from independent yield
   - Cumulative fission product yield (at 1000 years time period)
   - Decay heat from β and γ rays (time dependent)
   - Delayed neutron yield (at 1000 years time period and time dependent)
   - Spectrum (Under development)

- Preview decay-chain
- Open source in Github
  - Test version: https://github.com/shinokumura/FPY_betadecay
  - Will be moved to Github/IAEA-NDS near future

Features

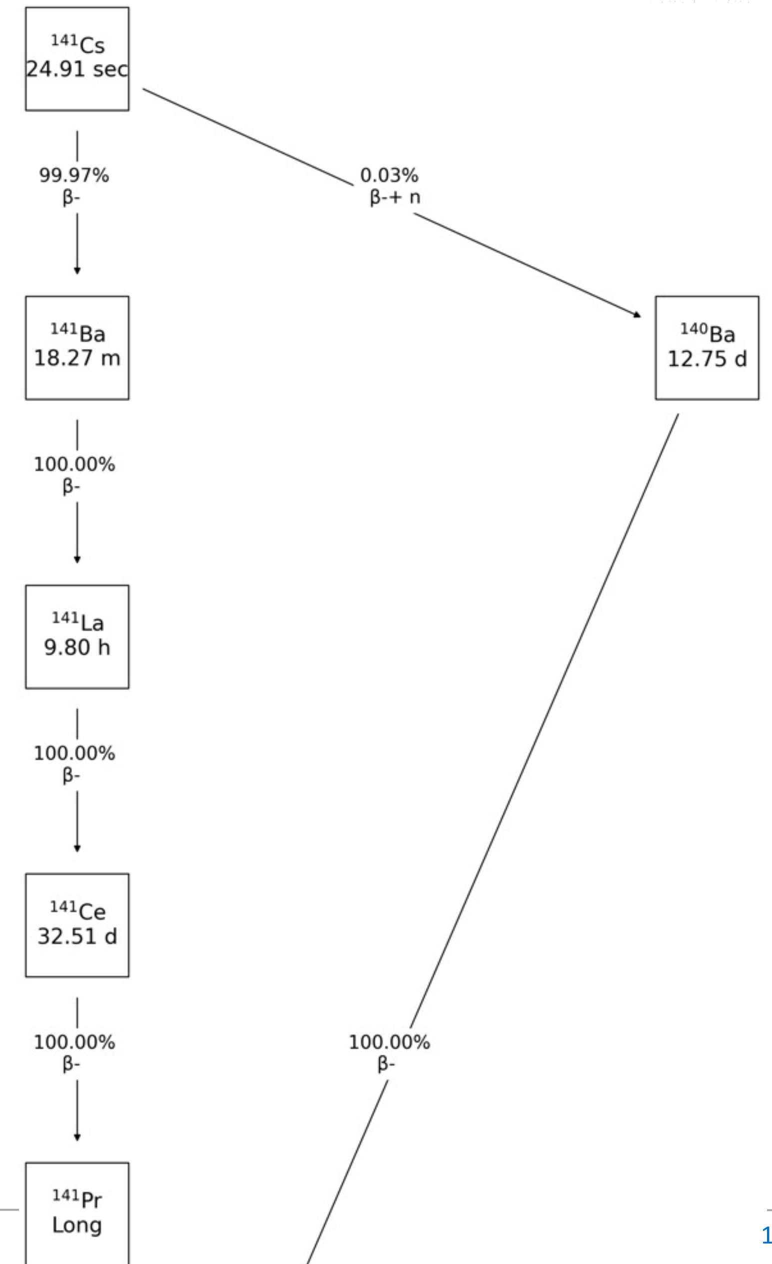
Decay data


```
"55-Cs-141-00": {
   "Z": "55",
   "ELM": "Cs",
   "MASS": "141",
   "LIS": "00",
   "HL": "2.4910000E+01",
   "LAMBDA": 0.027826,
   "En_beta": "1.5473620E+06",
   "En_gamm": "1.7248140E+06",
   "En_alpha": "7.5359650E+01",
   "DecayInfo": {
     "0": {
       "RTYP": "1.0000000E+00",
       "RFS": "0.0000000E+00",
       "Q": "5.2560000E+06",
       "BR": "9.9965800E-01",
       "DAUGHTER": "56-Ba-141-00"
     },
     "1": {
       "RTYP": "1.5000000E+00",
       "RFS": "0.0000000E+00",
       "Q": "7.2100000E+05",
       "BR": "3.4200000E-04",
       "DAUGHTER": "56-Ba-140-00"
     }
   },
   "daughters": [
     "56-Ba-141-00",
     "56-Ba-140-00"
   ]
 },
```


Decay chain (linearized)


```
"55-Cs-141-00": {
   "1": {
       "chain": [
       "56-Ba-141-00",
       "57-La-141-00",
       "58-Ce-141-00",
       "59-Pr-141-00"
       ],
       "branching": [
       0.999658,
       1.0,
       1.0,
       1.0
       ],
       "rtyp": [
       1.0,
       1.0,
       1.0,
       1.0
       ],
       "lmbds": [
       0.027826,
       0.00063232,
       4.9118e-05,
       2.4676e-07,
       6.9315e-51
       ],
       "en_betas": [
       "1.5473620E+06",
       "9.6628250E+05",
       "9.8713460E+05",
       "1.9438810E+05",
       0.0
       ],
       "en_gamms": [
       "1.7248140E+06",
       "9.0968270E+05",
       "2.6780420E+04",
       "7.6901970E+04",
       0.0
       ]
       },
   "2": {
       "chain": [
       "56-Ba-140-00",
       "57-La-140-00",
       "58-Ce-140-00"
       ],…
```


Decay chain (network diagram plot)



Method

1. Import calculated independent fission product yield, $Y_{IND}(Z, A, M)$ by TALYS

yieldZA1.00E-06.fis

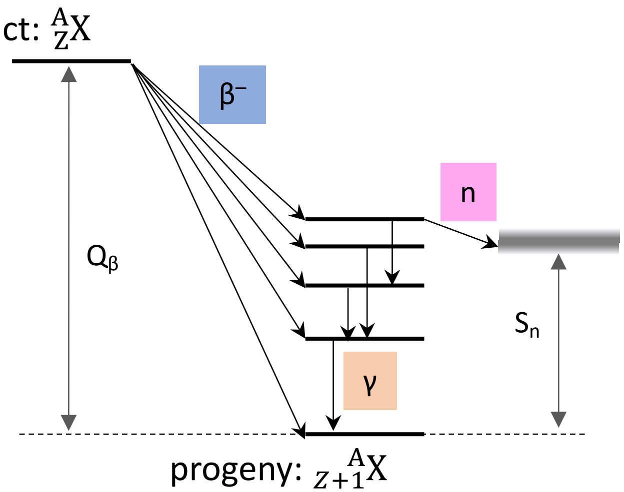
```
# n + 235U : Z, A Fission yields
# E-incident =  1.00000E-06
#
#
#   Z    A iso      FP yield      FF yield         FP xs         FF xs    Isom. Ratio
   30   74 -1     5.3961E-06    3.0000E-06    1.9191E+00    1.0670E+00
   30   75 -1     1.4014E-05    1.1000E-05    4.9841E+00    3.9123E+00
   31   75 -1     2.7919E-06    2.0000E-06    9.9294E-01    7.1132E-01
   30   76 -1     5.7899E-05    5.0001E-05    2.0592E+01    1.7783E+01
   31   76 -1     5.5761E-06    3.0000E-06    1.9832E+00    1.0670E+00
   32   76 -1     1.9258E-06    2.0000E-06    6.8493E-01    7.1132E-01
   30   77 -1     7.2165E-05    4.0001E-05    2.5666E+01    1.4226E+01
   30   77  0     5.3674E-05                  1.9090E+01                    7.4378E-01
   30   77  1     1.8490E-05                  6.5761E+00                    2.5622E-01
   31   77 -1     5.7907E-05    4.6001E-05    2.0595E+01    1.6360E+01
   29   78 -1     2.1861E-06    3.0000E-06    7.7751E-01    1.0670E+00
```

- ^{235}U + n (E_n= thermal – 5 MeV)
- Note: Implementation of multi-chance fission energy range is underway

2. Import decay data library (any decay data library in ENDF format)

Decay heat and delayed neutron yield at E_n= thermal

β decay



Decay heat:

Sum of average energies of β and γ rays from fission products as a function of time following a single fission event.

$$DH_{\gamma,\beta}(t) = \sum \langle E_{\gamma,\beta} \rangle \lambda_{\gamma,\beta} N_i(t)$$

$N_i(t)$: FP Yield at time *t*

Delayed neutron:

Sum of the number of delayed neutron emissions.

$$\nu_d(t) = \sum P_n \lambda_i N_i(t)$$

$N_i(t)$: FP Yield at time *t*

$$\overline{\nu_d} = \sum P_n N_i$$

N_i: Cumulative yield

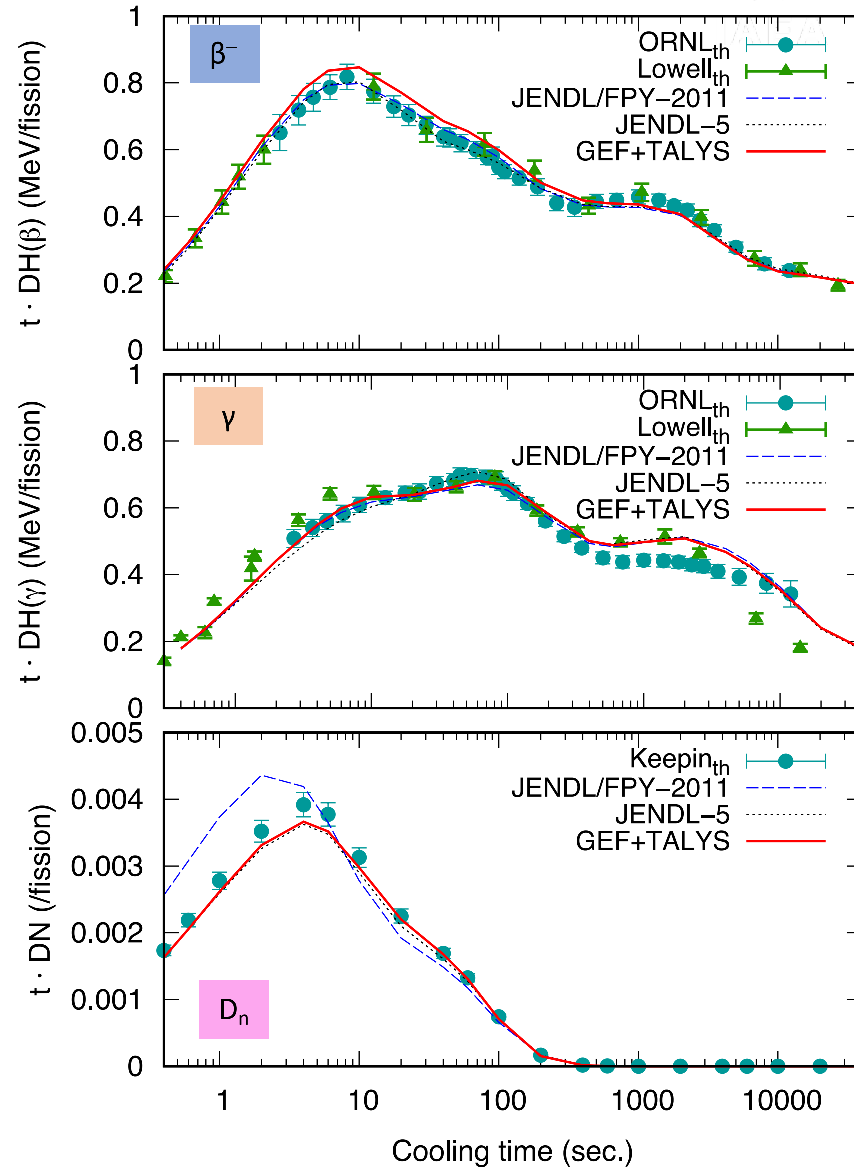


Fig 2. β and γ decay heat and delayed neutron yield burst functions of ^{235}U

Energy dependent cumulative yield

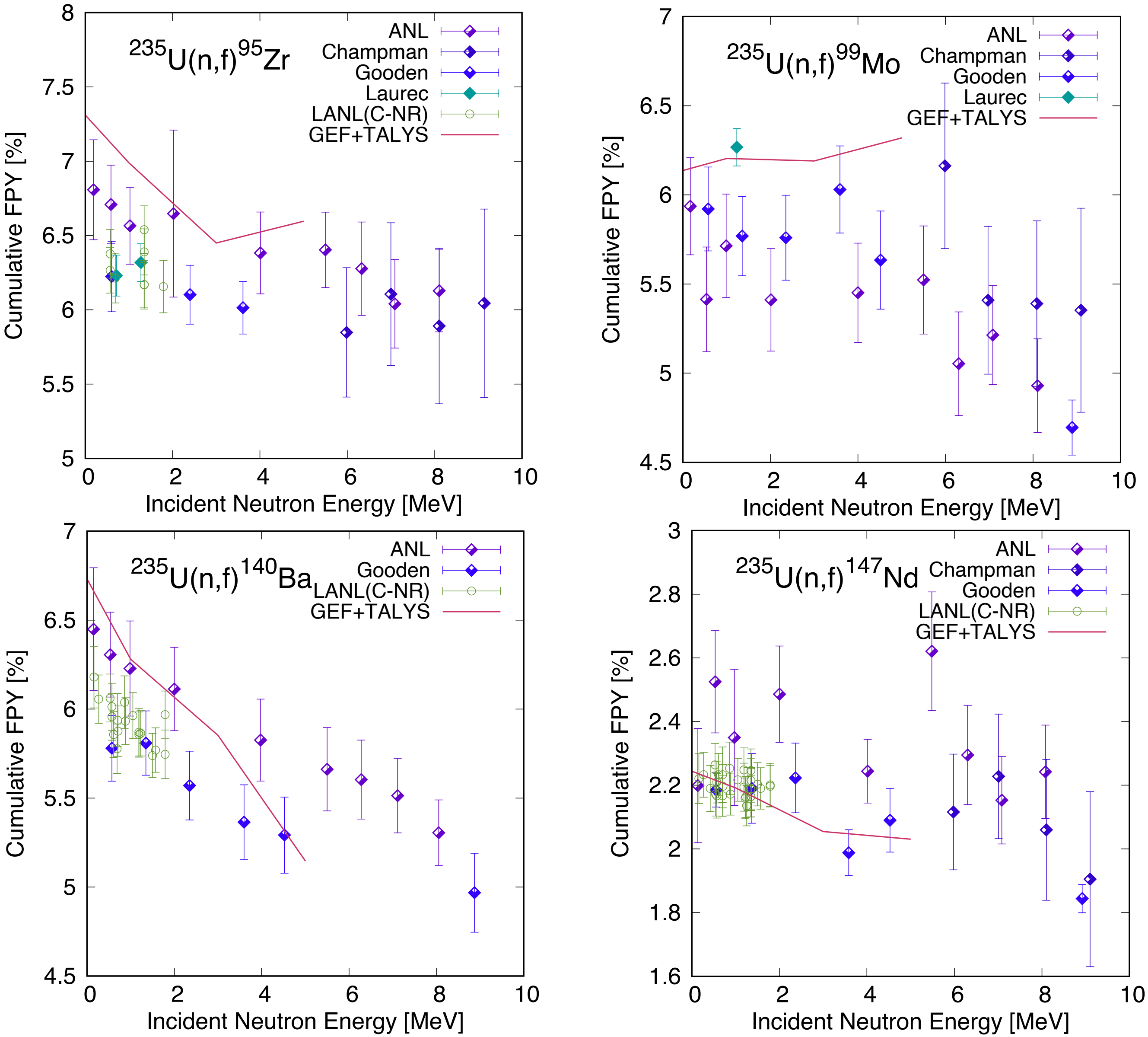


Fig 1. Comparison of cumulative yield of selected fission products showing as function neutron energy

Energy dependent decay heat and delayed neutron

β decay

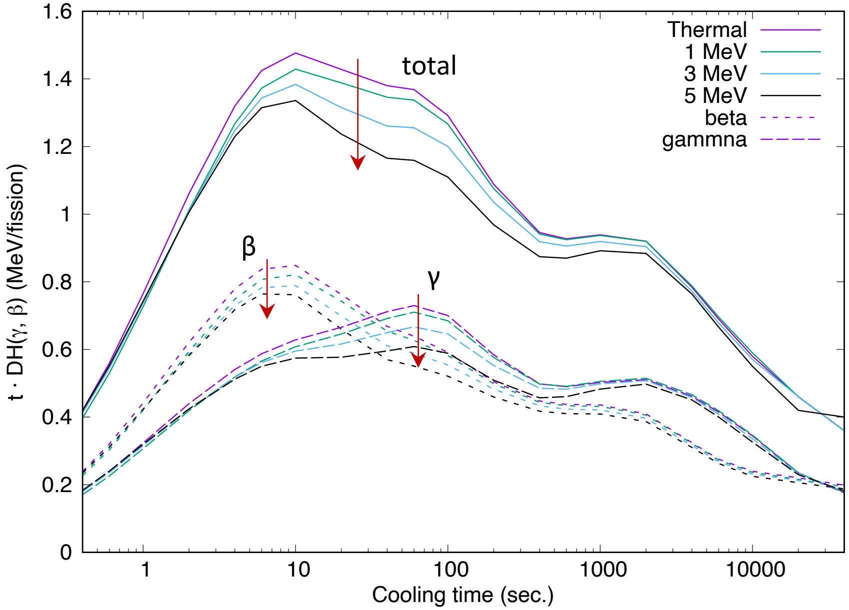
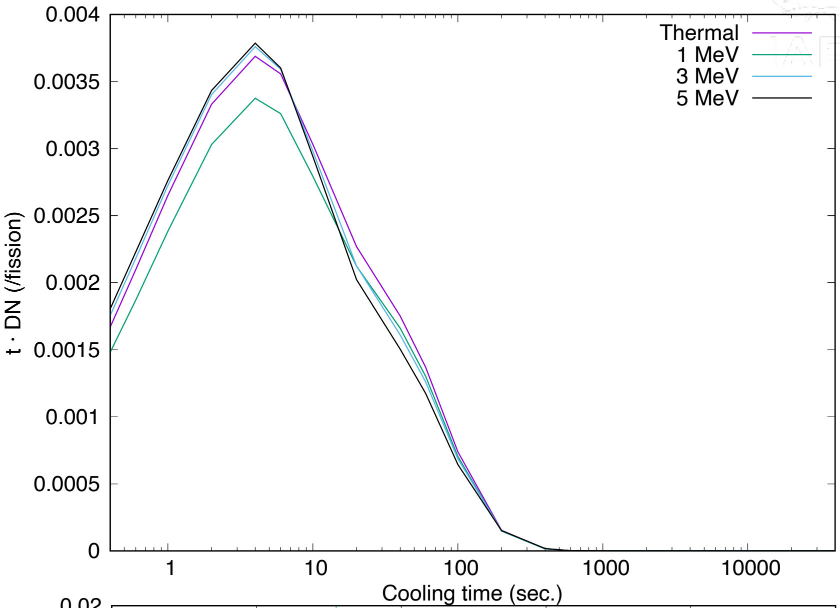


Fig 3. Comparison of total decay heat (–:total, dashed: β and γ) burst functions of ^{235}U for various neutron energies



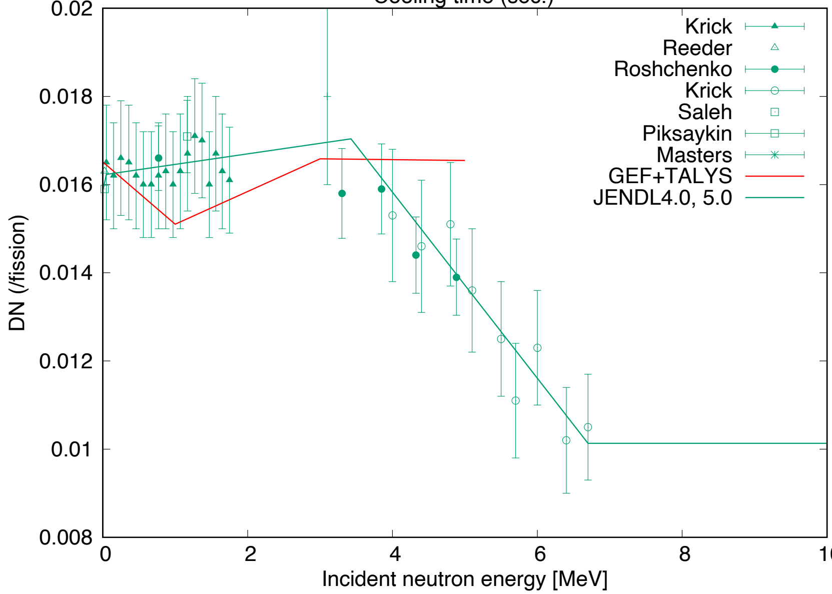


Fig 4. Incident neutron energy dependence of average delayed neutron yield

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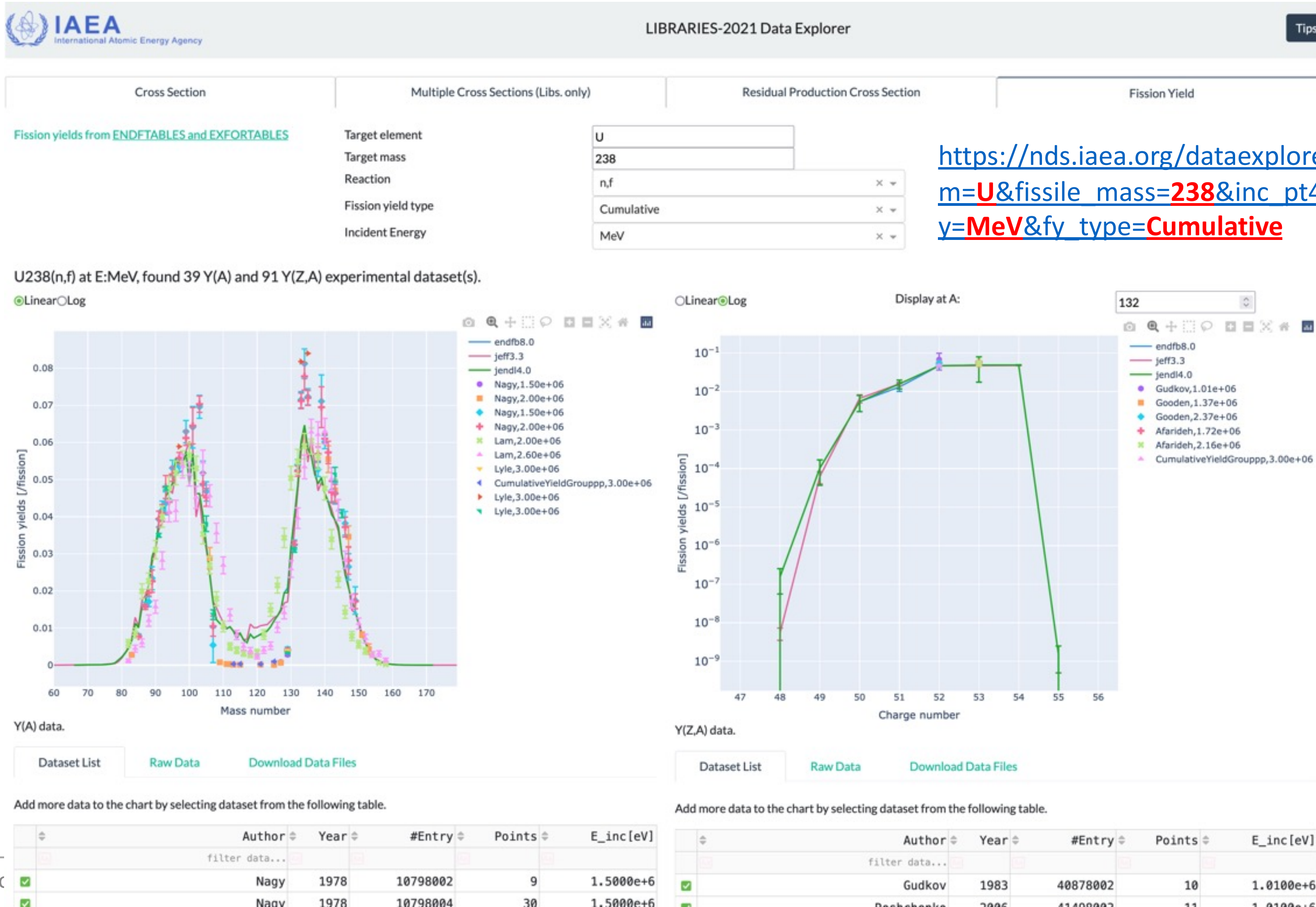
- Easy-to-use nuclear data plotter
  - Evaluated cross section with experimental data: https://nds.iaea.org/dataexplorer/xs
  - Evaluated cross section for comparison: https://nds.iaea.org/dataexplorer/libs
  - Residual production with experimental data: https://nds.iaea.org/dataexplorer/rp
  - Fission yields https://nds.iaea.org/dataexplorer/**fy**
- Data table view and tabulated data download



https://nds.iaea.org/dataexplorer/**fy**?fissile_elem=**U**&fissile_mass=**238**&inc_pt4=**n**&inc_energy=**MeV**&fy_type=**Cumulative**

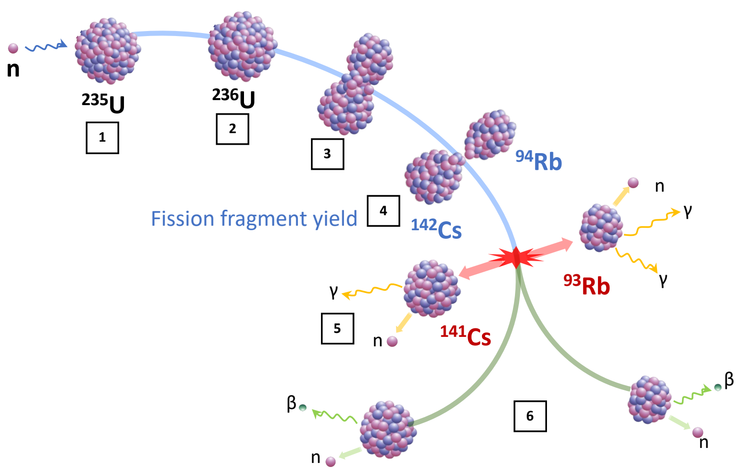
Summary

(1) TALYS[1] fission fragment de-excitation

- Fission fragment distributions by GEF[2], HF^{3}D[3], SPY[4], and user's own model
  - Z_P model fission fragment generator
- Application of the Hauser-Feshbach theory to the fission fragment de-excitation process (currently up to 5 MeV)
- Calculate independent fission product yield, as well as prompt neutron and gamma observables

(2) Beta-decay observables from beta-decay of fission products

- Cumulative fission product yield
- Decay heat from β and γ rays
- Delayed neutron yield



Details will be published in the IAEA NDS report
https://nds.iaea.org/publications/nds/iaea-nds-0239/
(Ad) Fission yield plotter
https://nds.iaea.org/dataexplorer/fy

[1] Koning AJ, Hilaire S, Duijvestijn MC. AIP Conference Proceedings. 2005;769(1):1154–1159.
[2] Schmidt KH, Jurado B, Amouroux C, Schmitt C. Nuclear Data Sheets. 2016;131:107 – 221.
[3] Okumura S, Kawano T, Jaffke P, Talou P, Chiba S. JNST. 2018;55(9):1009–1023.
[4] Lemaitre JF, Goriely S, Hilaire S, Sida JL. Phys Rev C. 2019 Mar;99:034612.

Acknowledgements

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- S. Goriely (Université Libre de Bruxelles) and J.-F. Lemaitre (CEA) for SPY calculations and data supply.

Thank you for your attention.

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