Prediction and emulation of prompt neutrons/γ with FIFRELIN

ESNT Dynamics of Nuclear Fission, 16-19/12/2024, Saclay

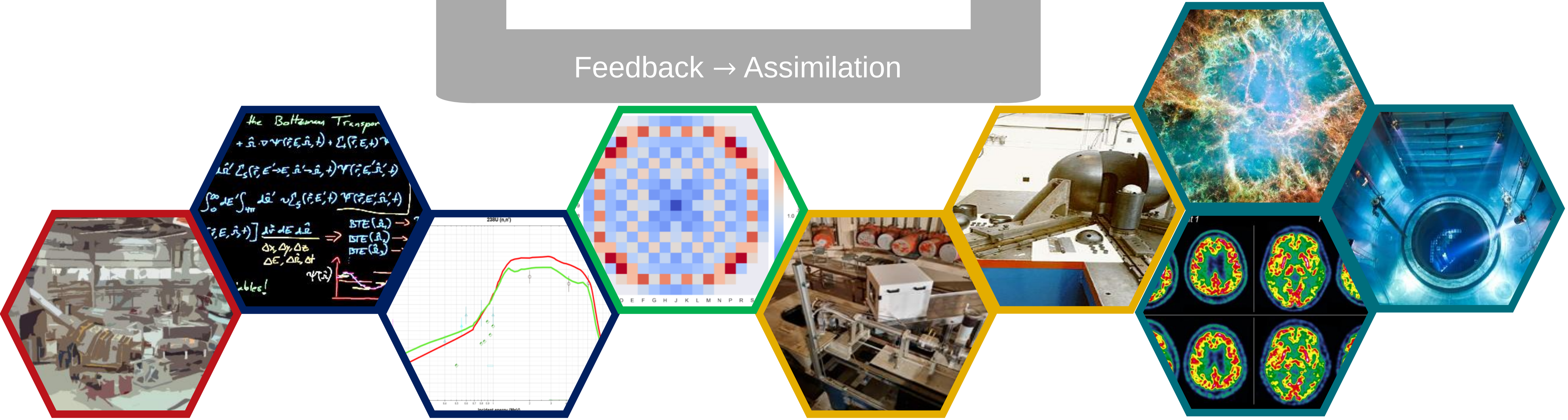
A. Chebboubi, O. Litaize and O. Serot
CEA, DES, IRESNE, DER, SPRC, LEPh, Cadarache, 13108 Saint-Paul-lès-Durance

Nuclear data evaluation pipeline

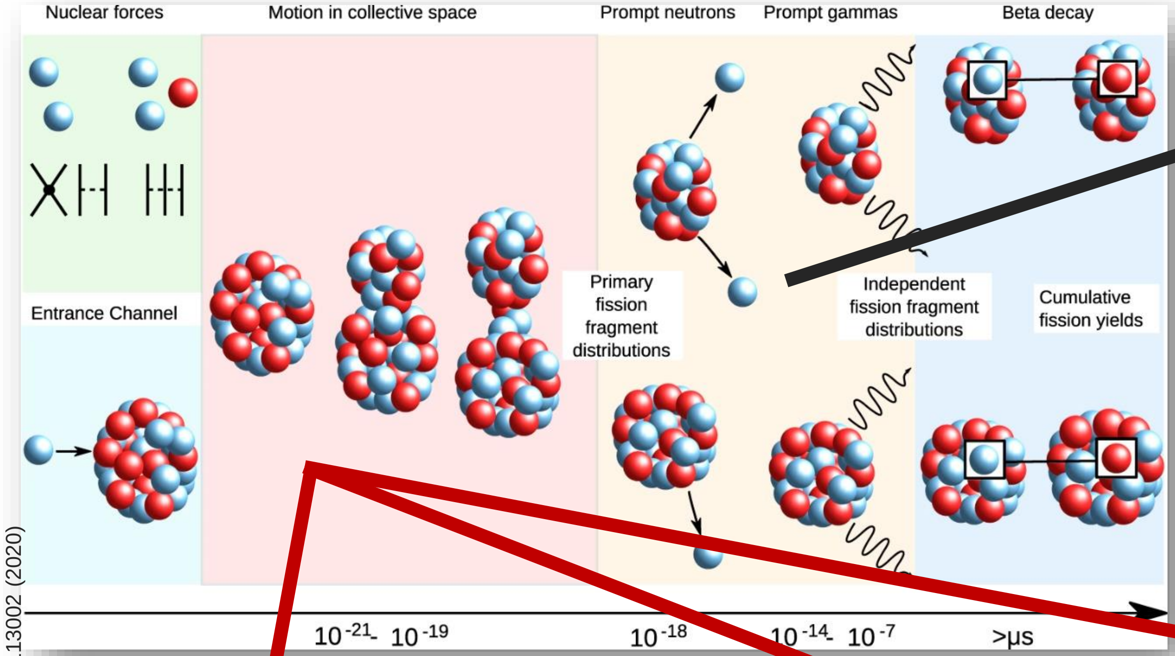
Feedback → Adjusted Library

Measurements → Theory and Evaluation → Processing and transport codes → Benchmarking and Integral measurement → Applications

Feedback → Assimilation



The nuclear fission process



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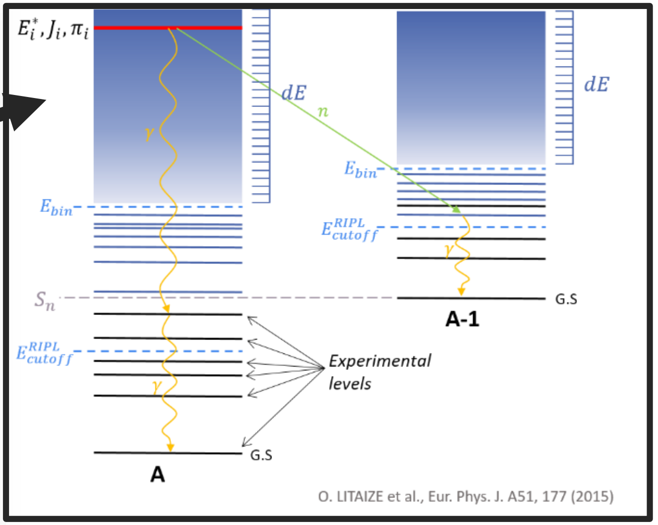
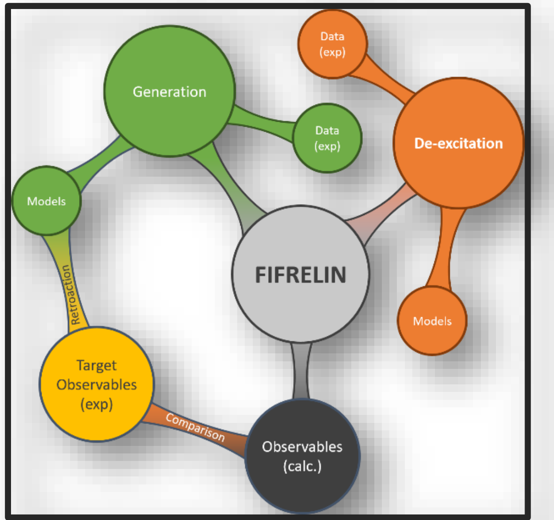
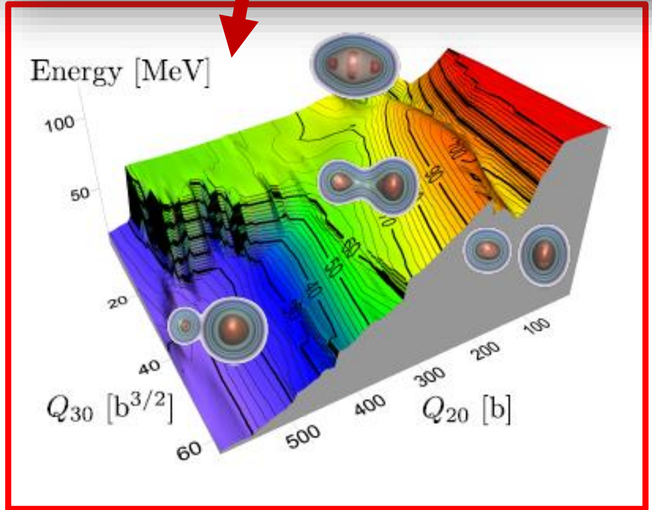




FIFRELIN : generation and de-excitation of fission fragment. Developed by DES/IRESNE



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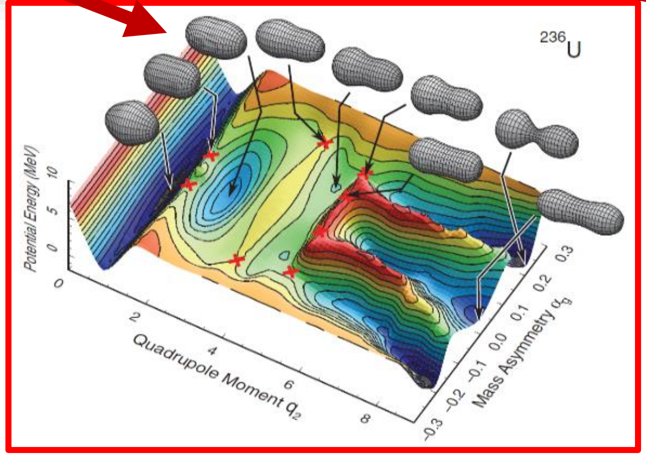
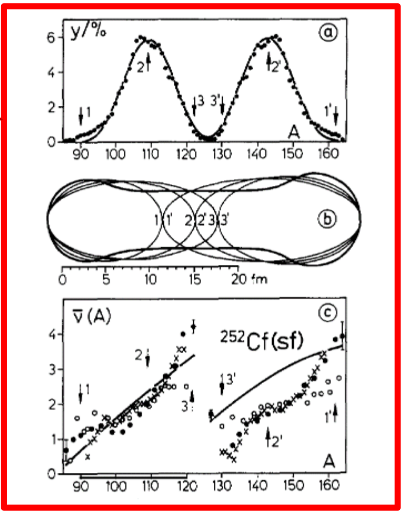


© Ichikawa *et al.*, *Contrasting fission potential energy structure of actinides and mercury isotopes*, Phys. Rev. C 40, 770 (1989)



© U. Brosa *et al.*, *Nuclear scission*, Phys. Reports 197 (4), 167 (1990)

1. Description of FIFRELIN

FIFRELIN : a bridge between experimental and theoretical worlds

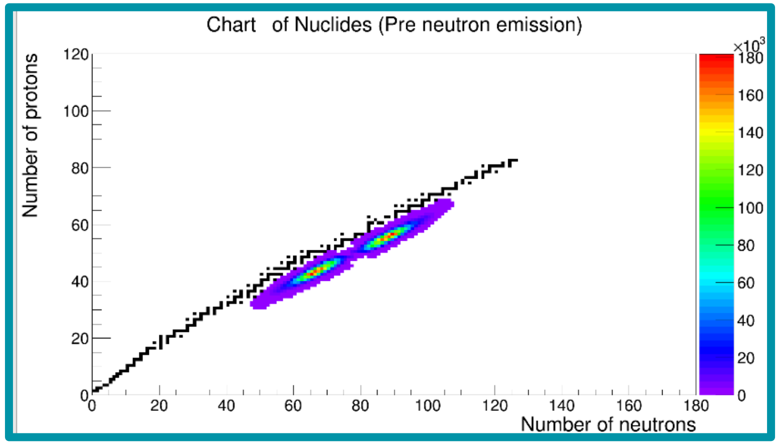
FIFRELIN (FIssion Fragments Evaporation modeLINg)

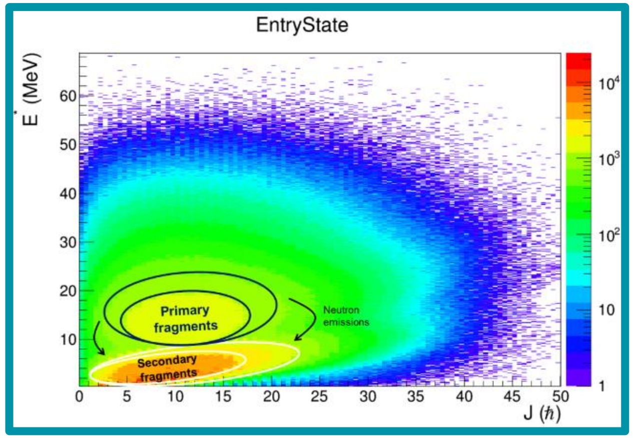
- Goal : characterize fission fragment since its creation (~ scission) until β decay (not included)

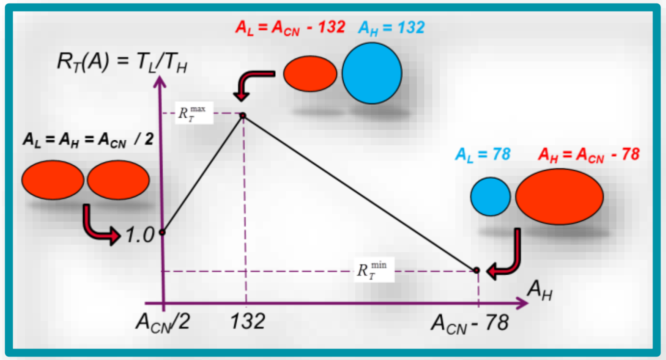
Fission Fragments Generation

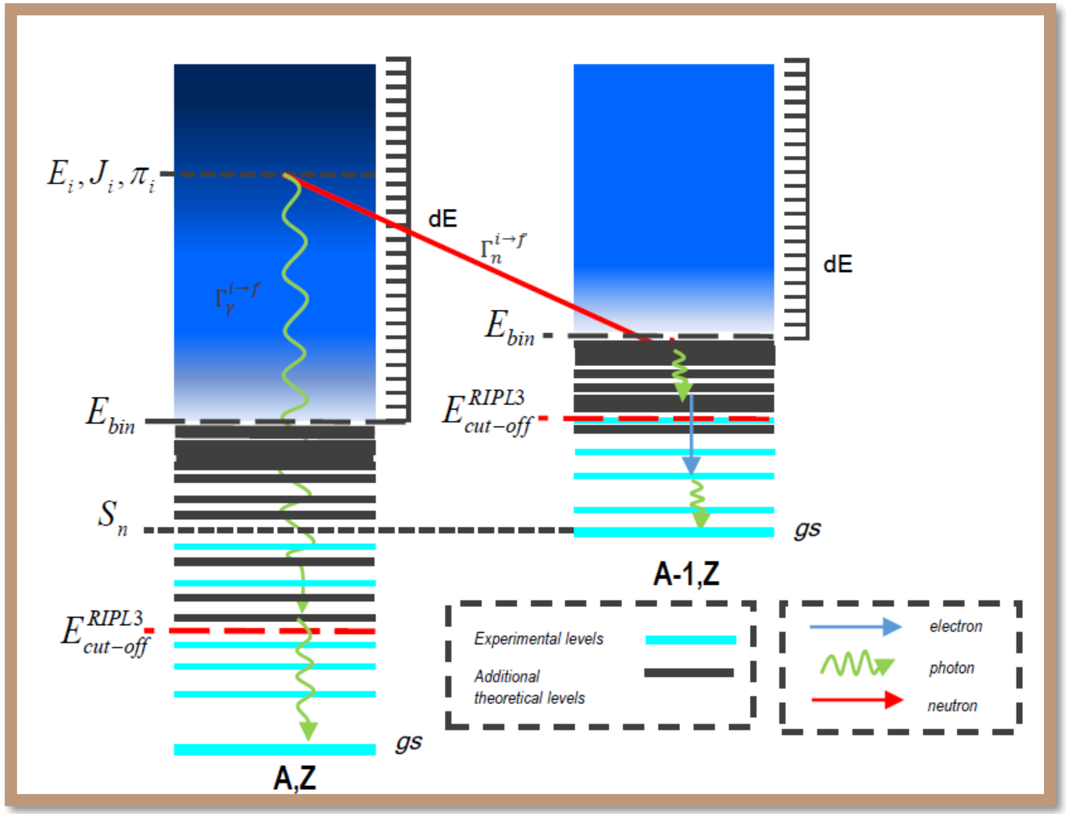
2 steps code

Creation of nuclear levels for given fission fragments and daughters









Fission fragment generation

Ingredient (input files/models) :

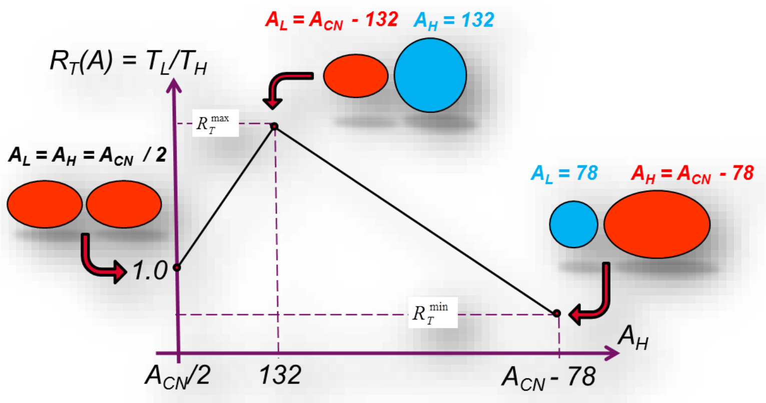
- Pre-neutron mass yields: A (usually obtained from experimental data)
- Nuclear charge calculation: Z (Wahl)
- Pre-neutron emission kinetic energy distributions : KE (usually obtained from experimental data)
- Excitation energy sharing E^* : Temperature Ratio function (2 free parameters)
- Fission fragment angular momentum calculation J^π : 2 models (2 free parameters / 1 free parameter)

Excitation energy after full acceleration

- Instrinsic
- Deformation
- Collective

$$TXE = a_L T_L^2 + a_H T_H^2 + E_{rot}^L + E_{rot}^H$$

At the end, only $TXE - (E_{rot}^L + E_{rot}^H)$ is partitioned through $E_{L,H}^* = a_{L,H} T_{L,H}^2$



Total angular momentum distribution

$$P(J) \propto (2J+1) e^{-\frac{\left(J+\frac{1}{2}\right)^2}{2\sigma_{L,H}^2}}$$

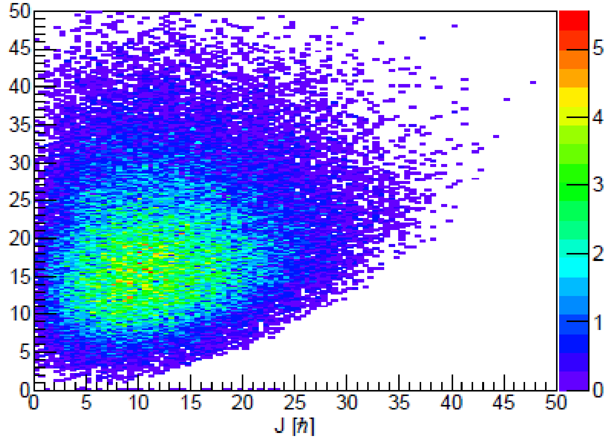
Constant model :

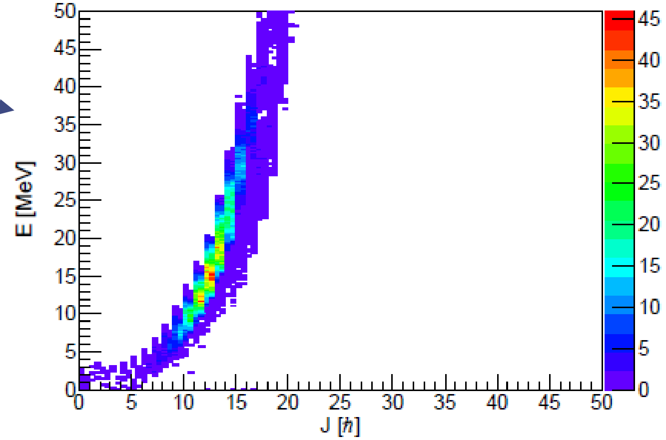
$\sigma_{L,H} = f_{\sigma\,L,H}$ not energy dependant !

Energy dependant model :

$$\sigma_{L,H} = f_{\sigma\,L,H} \times \sigma_{L,H}\left(E_{L,H}^* + E_{rot}^{L,H}\right)$$

$$\sigma_{L,H}^2\left(E_{L,H}^* + E_{rot}^{L,H}\right) = I_{rigid}\left(\frac{a_{L,H}}{\widetilde{a_{L,H}}}\right)\sqrt{\frac{E_{L,H}^* + E_{rot}^{L,H} - \Delta}{a_{L,H}}}$$





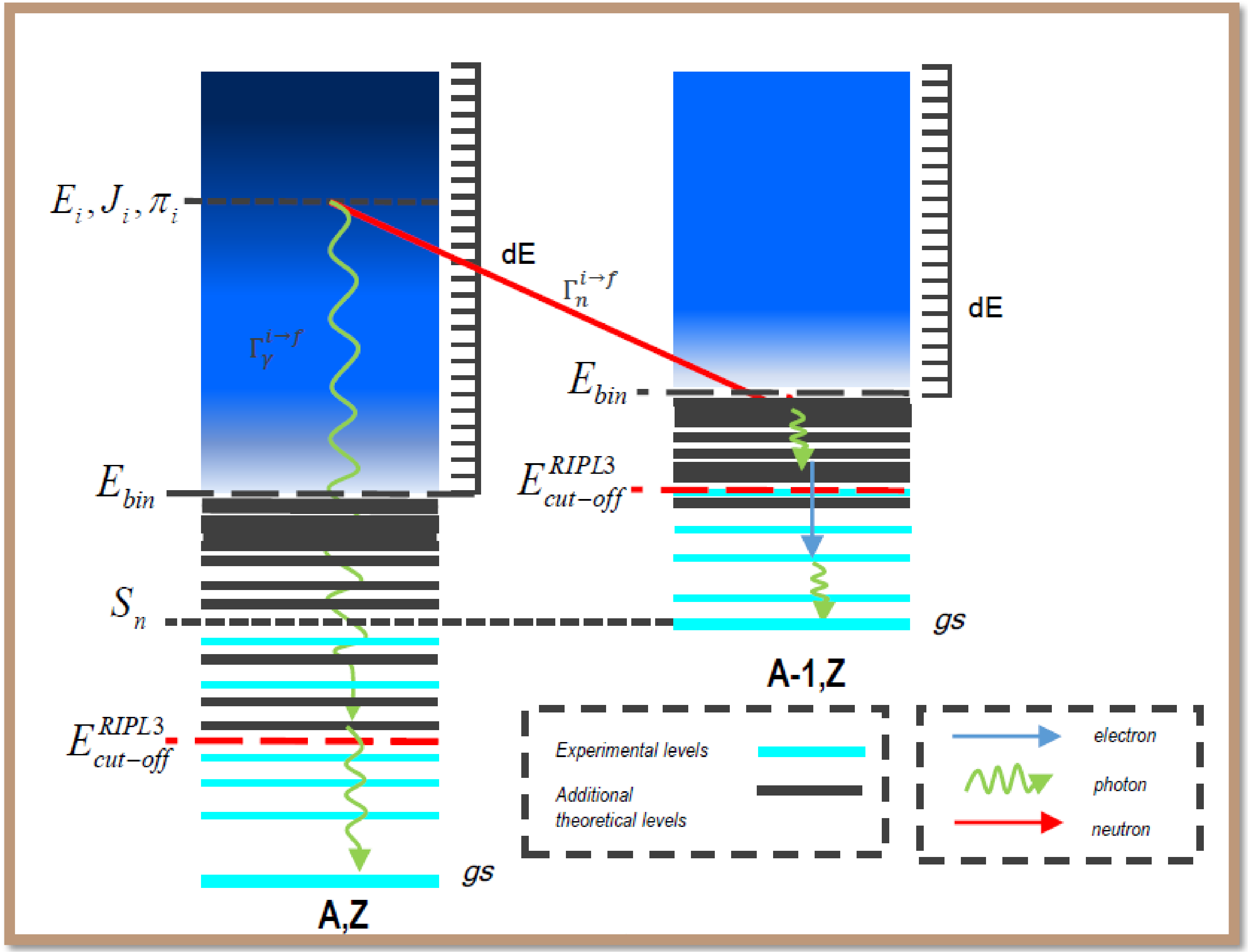
Emission of prompt particles

Ingredient (input files/models) :

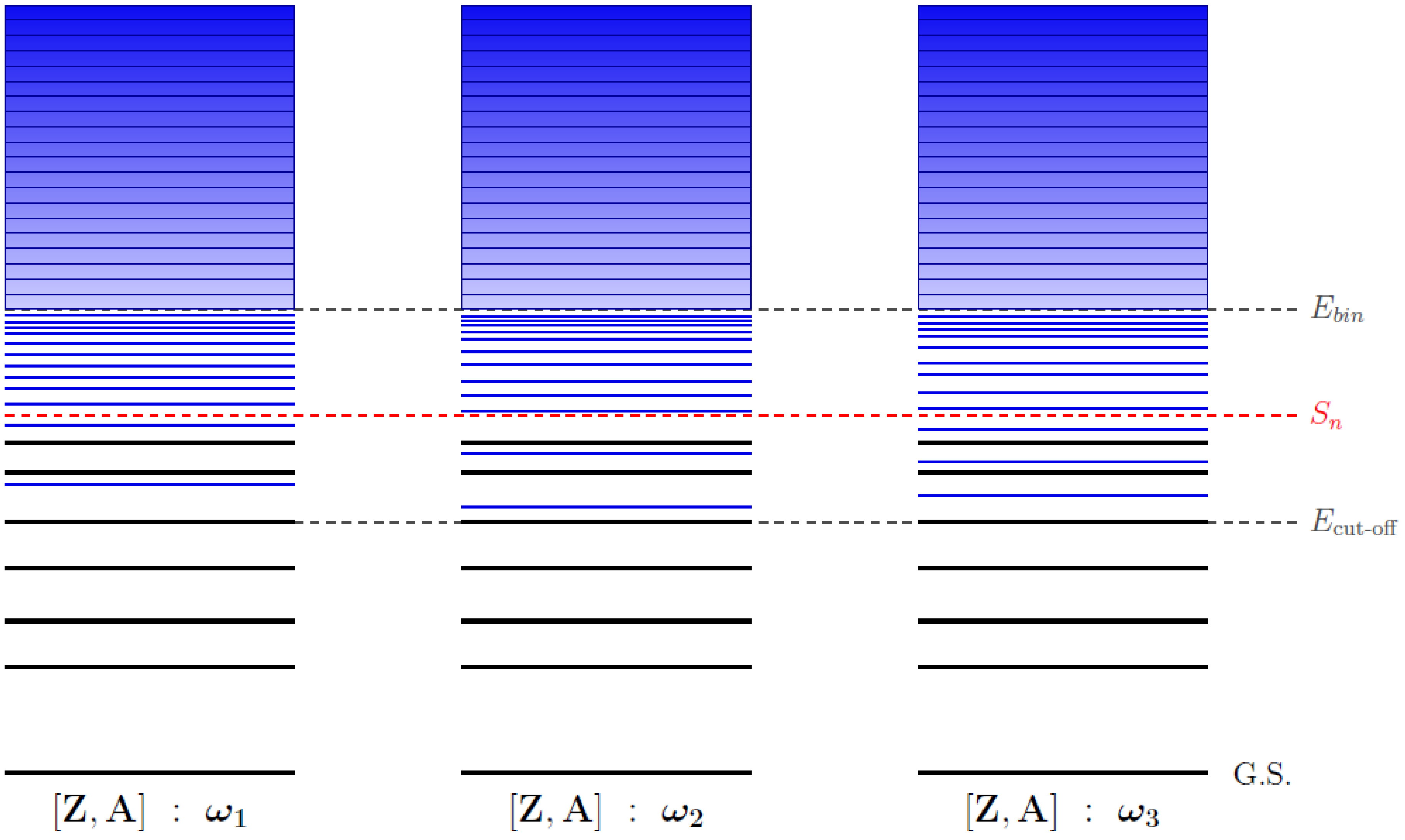
- Experimental nuclear level scheme (RIPL)
- Models of nuclear level density (CGCM, …)
- Models of γ strength function (EGLO, …)
- Neutron transmission coefficients (Koning-Delaroche, …)
- Internal conversion coefficients (BrIcc)

→ complete fission fragment nuclear level scheme up to the entry region

→ determination of de-excitation probability $P\left(E_i^*, J_i^\pi \rightarrow E_f^*, J_f^\pi\right)$ by emitting secondary particles (γ, e^-,neutron)



Multiple level scheme

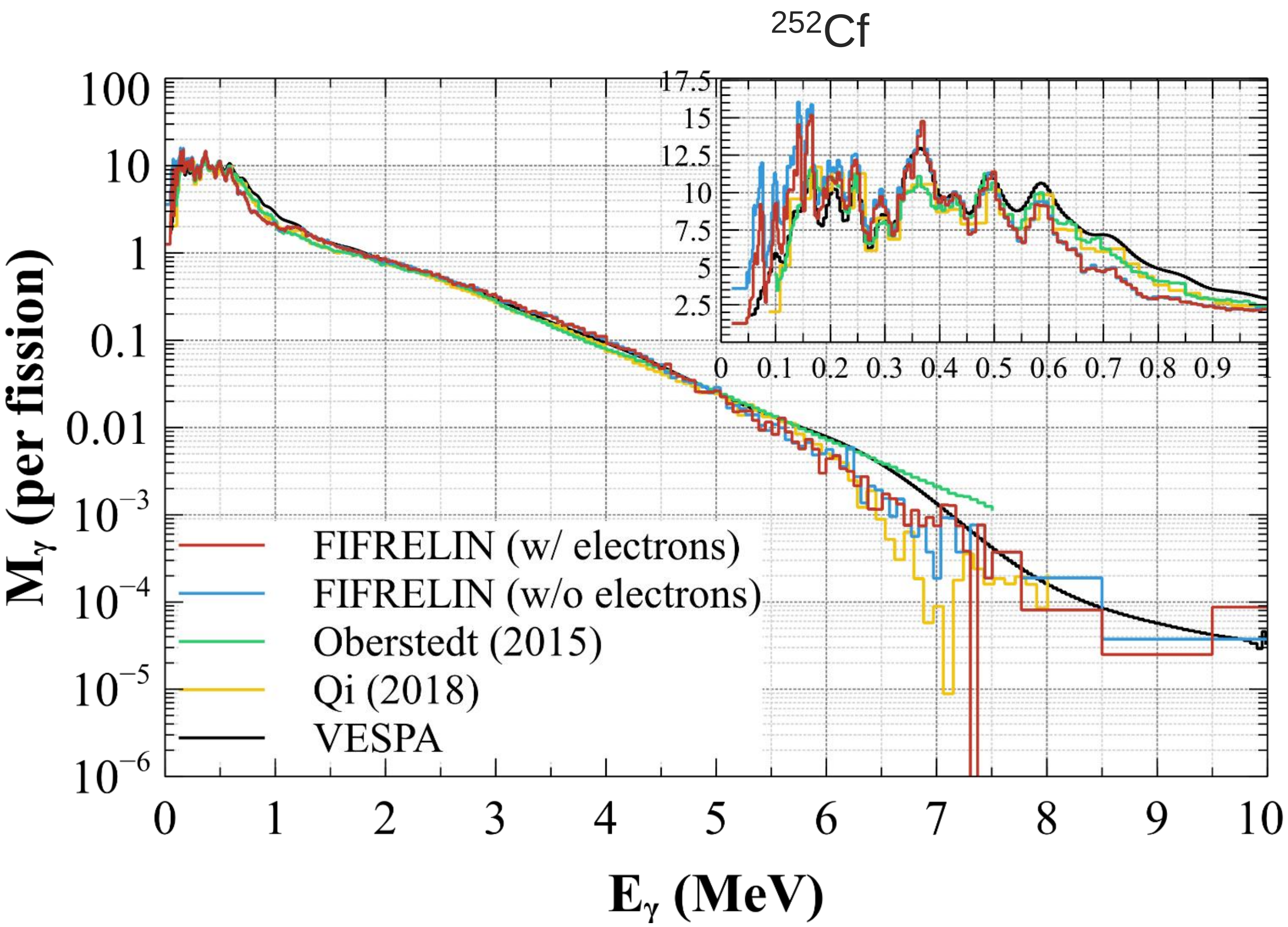


Generalization of electron emission

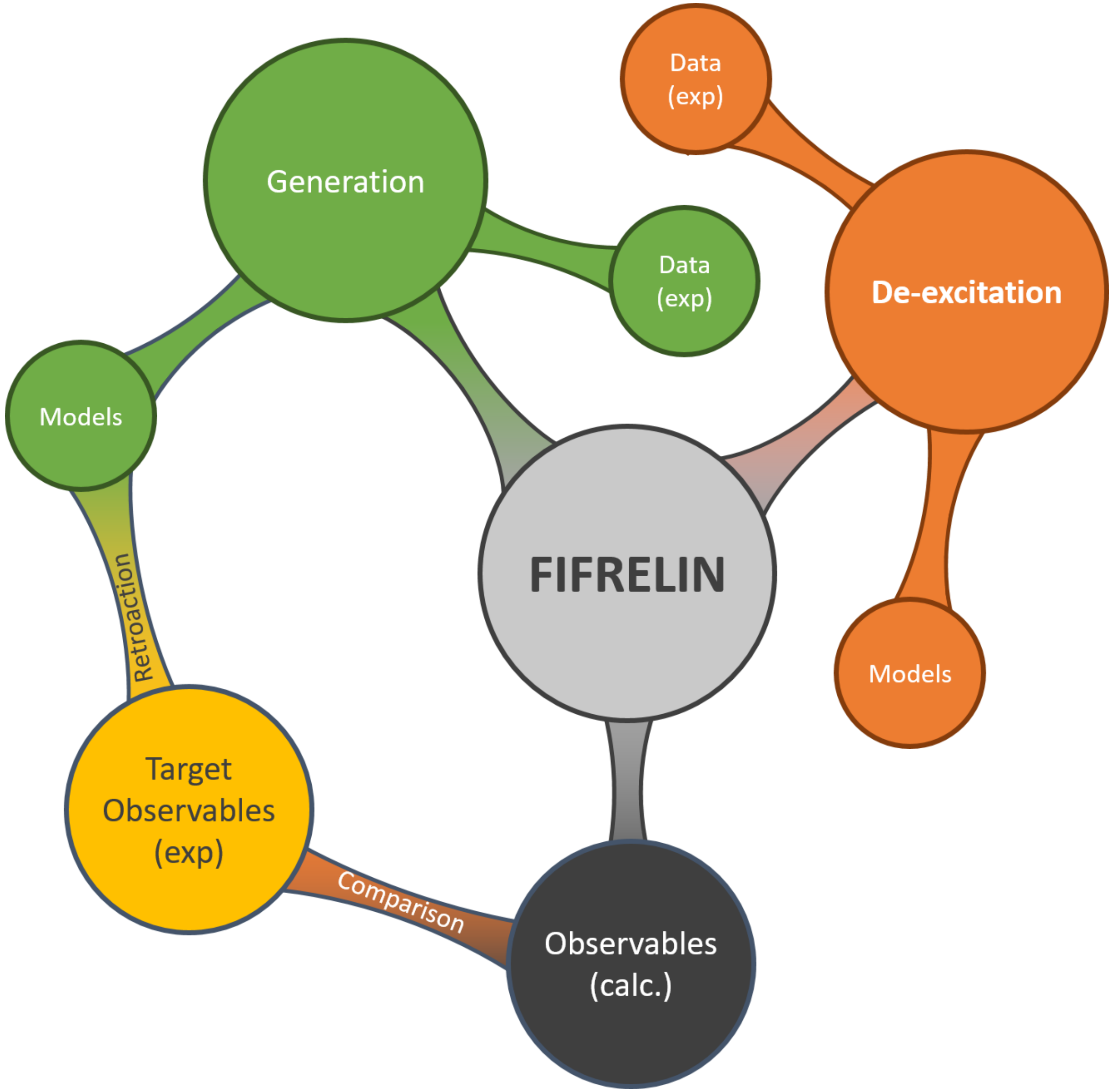
- Before, electrons were coming only from RIPL-3 database : experimental ones

- Now, we have tabulated Internal Conversion Coefficient with BrIcc for
  - $Z = 5 - 110$
  - $E_\gamma = \epsilon_i + 1 - 6000\ keV$ (ϵ_i binding energy of electron on shell i (K,L,M …))
  - $E1 - E6$ and $M1 - M6$
  - Positrons can be emitted !

- Ok but why do we care ?
  - Usefull for some particle physics experiment (detector calibration, background …)
  - Reduce gamma multiplicity (especillay at low-energy)



How FIFRELIN is working?

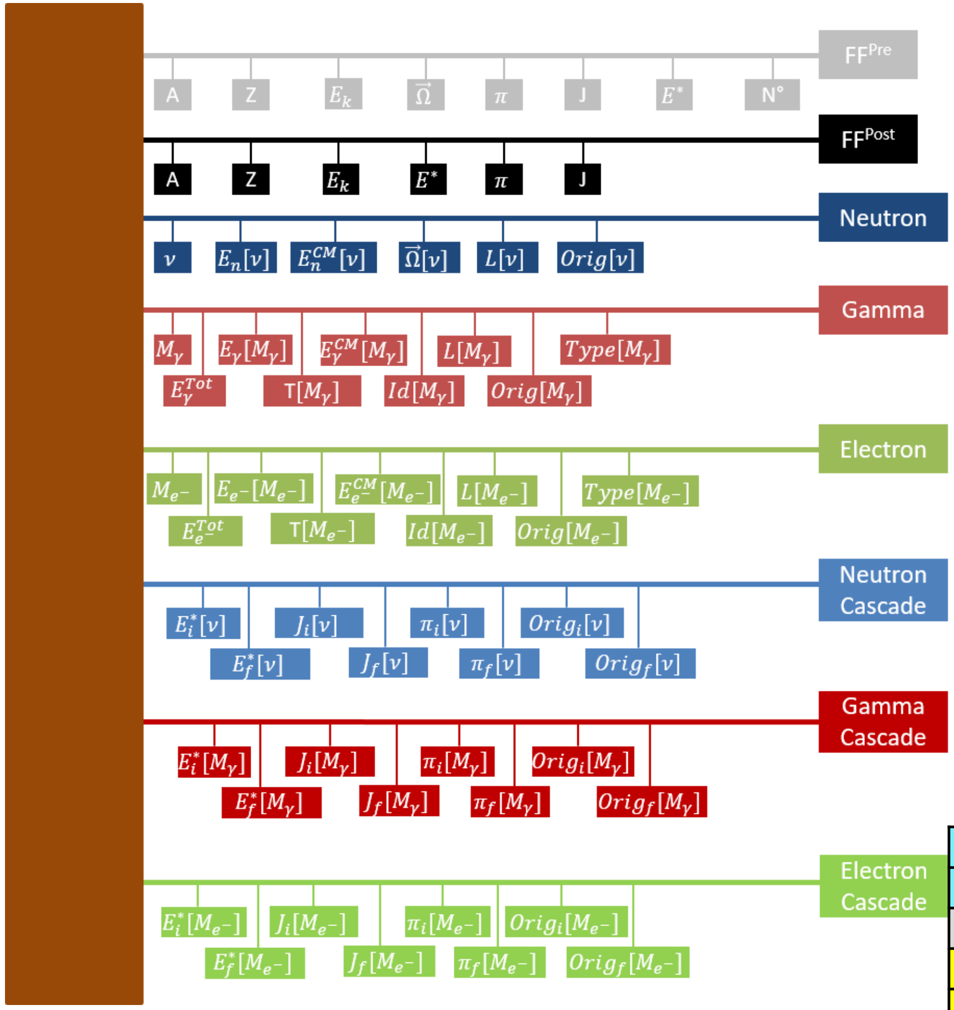


- 4 free parameters to determine excitation energy and angular momentum for each fragment
- Fixed against “target observables” : average neutron multiplicity (light/heavy if existing)

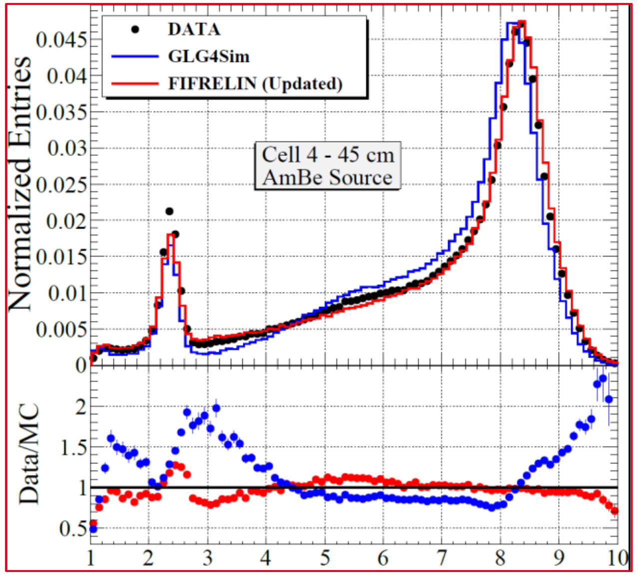
- Limitation : 4D space

Some practical information

- Developed in C++ since 2009
- Highly parallel (OpenMP+MPI)
  - Next step: GPU
- Available through NEA since 13/12/2024: https://www.oecd-nea.org/tools/abstract/detail/nea-1934
- All events are stored in a binary file
  - Convertor to ROOT tree event
  - Convertor to Pandas DataFrame (python) ongoing !
  - Homemade GUI to “play” with all the observables
- Not only for fission: decay for any nuclide (limitation : excitation energy + particle emission)
- A lot of use in neutrino/dark matter community for detector characterization !



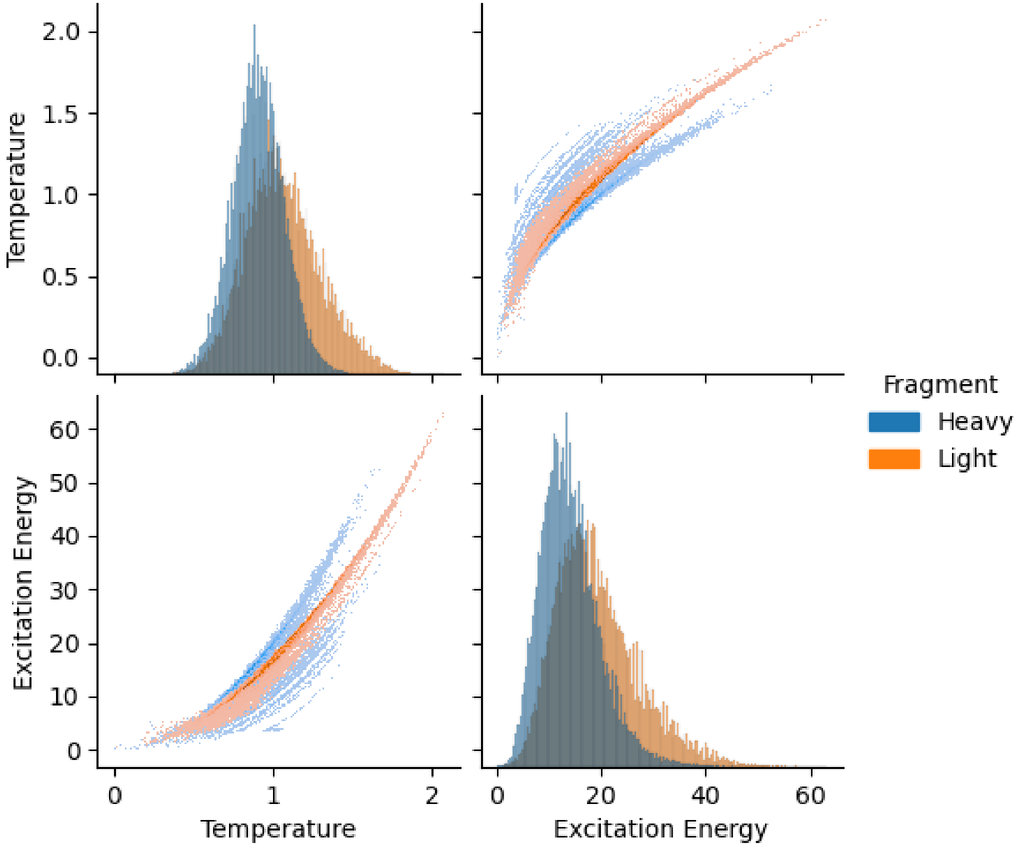
©A. Chalil et al., Improved FIFRELIN de-excitation model for neutrino applications, EPJA, 59, 75 (2023)

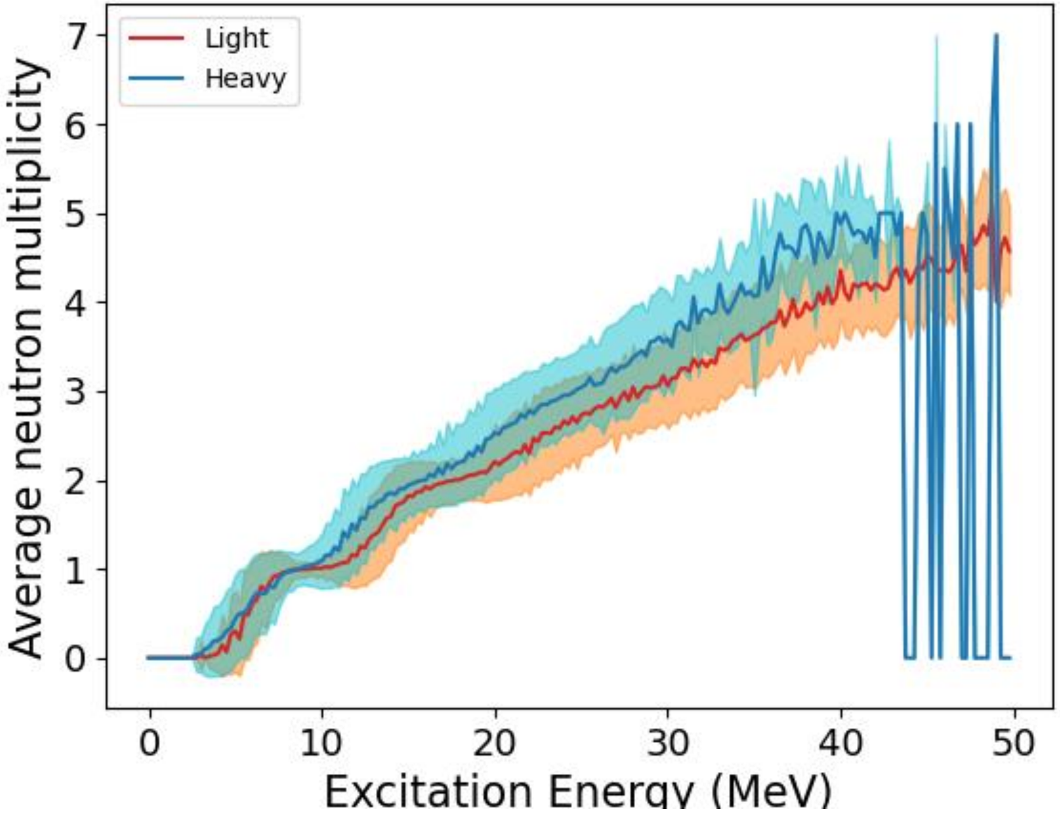


Gd156	(1- , 2-)
Gd158	(1- , 2-)
Al28	(2+, 3+)
Si29	1/2+
Si30	1- (direct)
Si31	1/2+
Na24	(1+, 2+)

Ge71	1/2+
Ge73	1/2+
Ge74	(4+ , 5+)
Ge75	1/2+
Ge77	1/2+
W183	1/2+
W184	(0- , 1-)
W185	1/2+
W187	1/2+

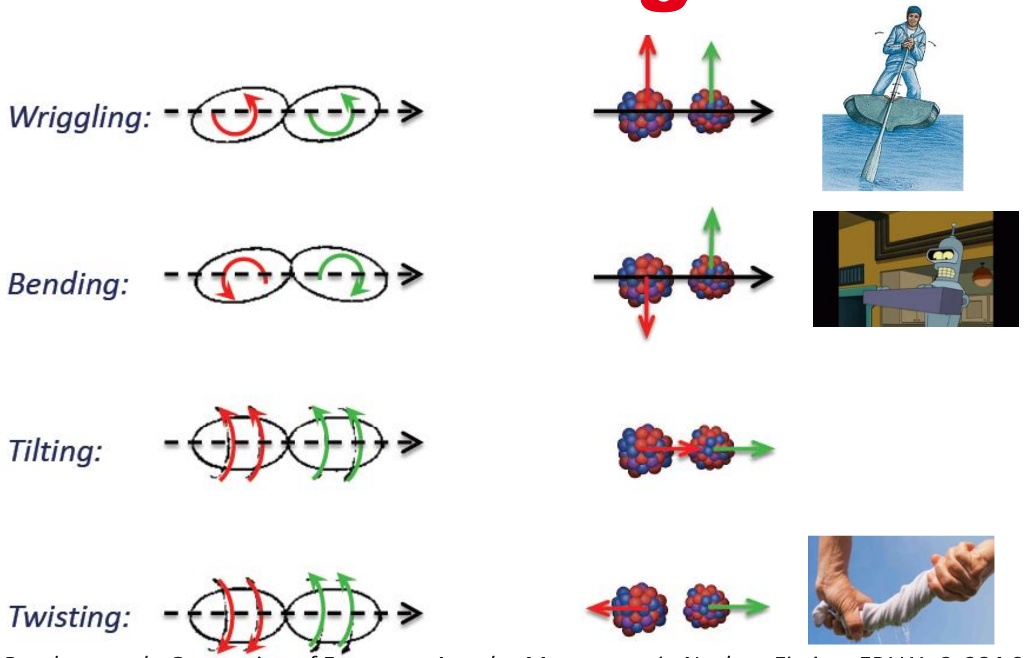
Excitation Energy, Multiplicity, Temperature



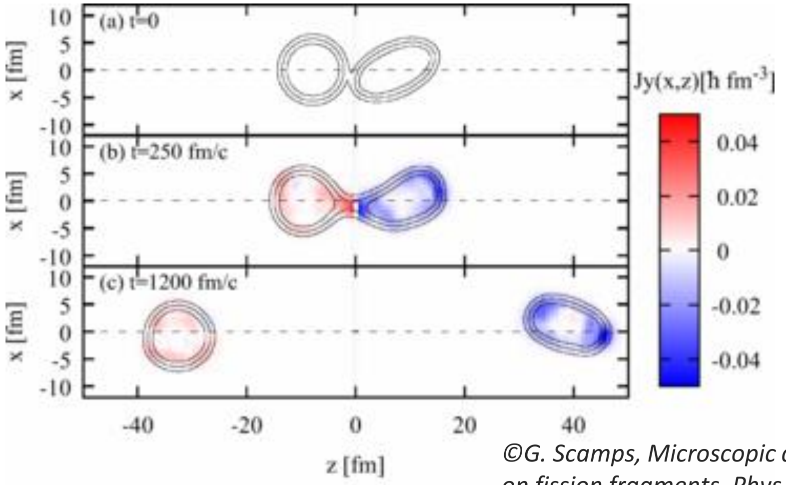


2. Extraction of angular momentum with FIFRELIN

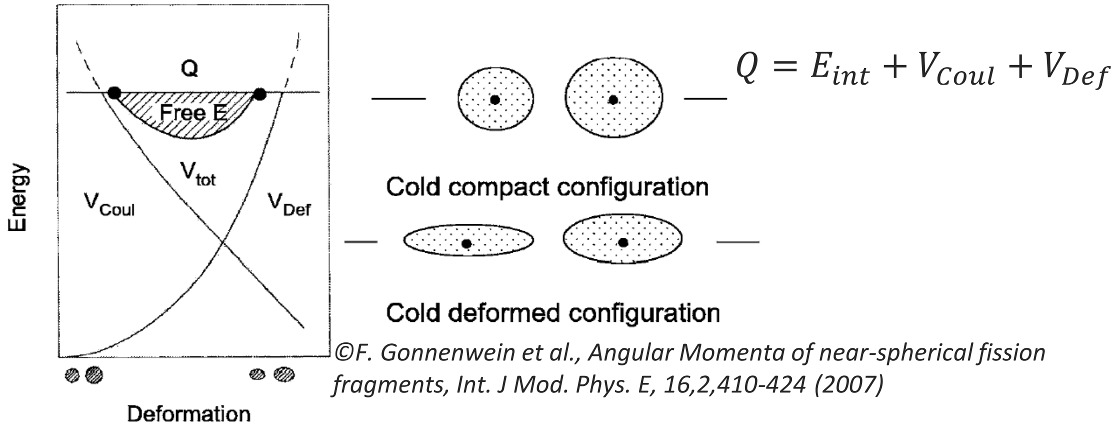
Focus on angular momentum generation



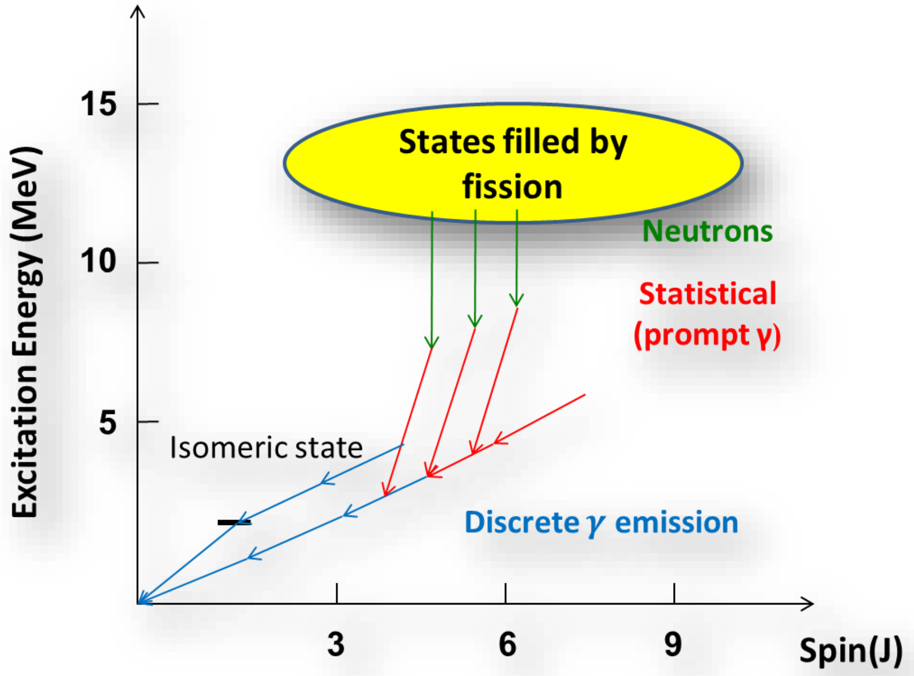
©J. Randrup et al., *Generation of Fragment Angular Momentum in Nuclear Fission, EPJ WoC, 284,04004 (2023)*



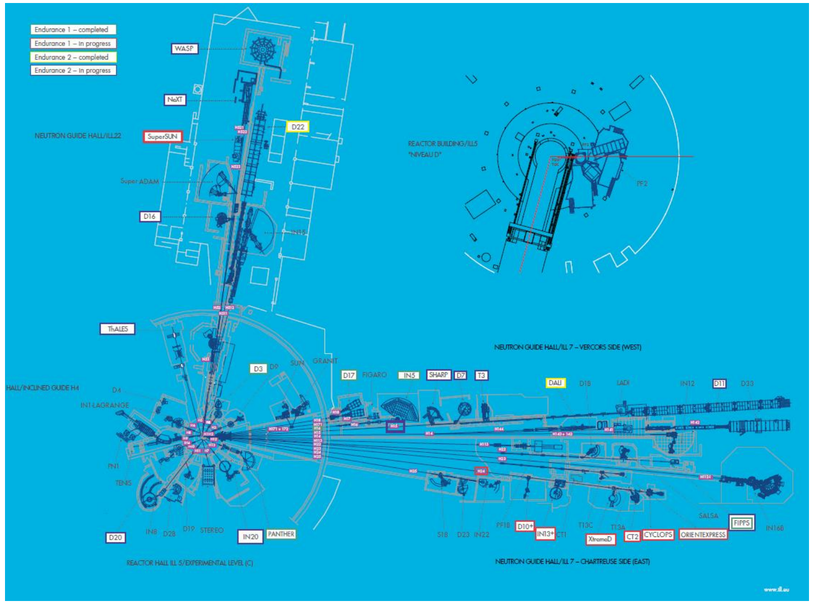
©G. Scamps, *Microscopic description of the torque acting on fission fragments, Phys. Rev. C 106, 054614 (2022)*

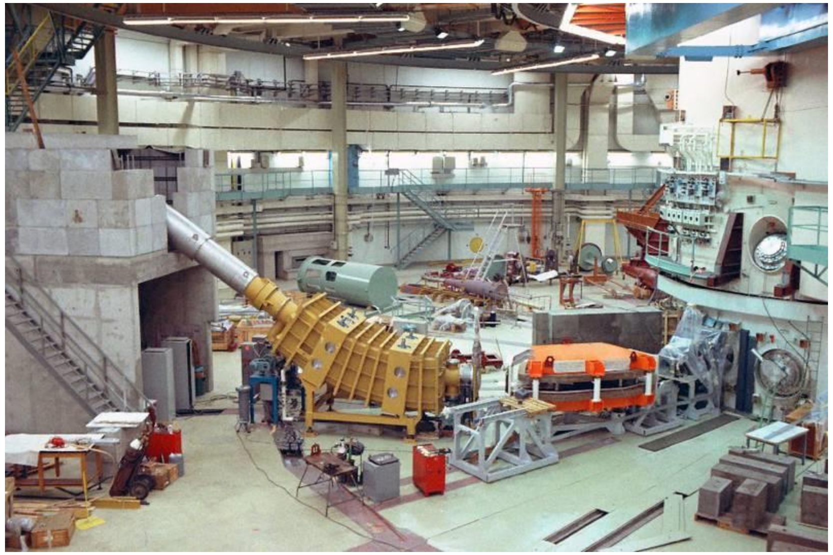


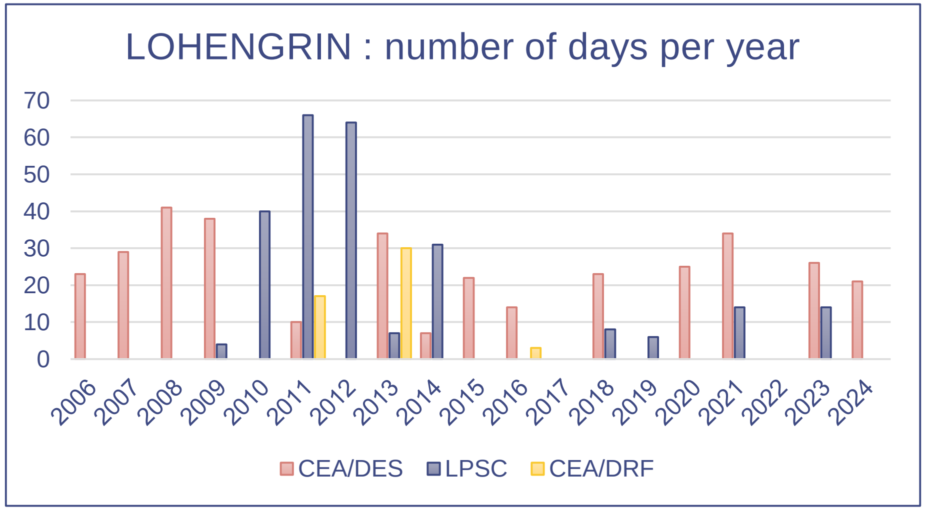
©F. Gonnenwein et al., *Angular Momenta of near-spherical fission fragments, Int. J Mod. Phys. E, 16,2,410-424 (2007)*



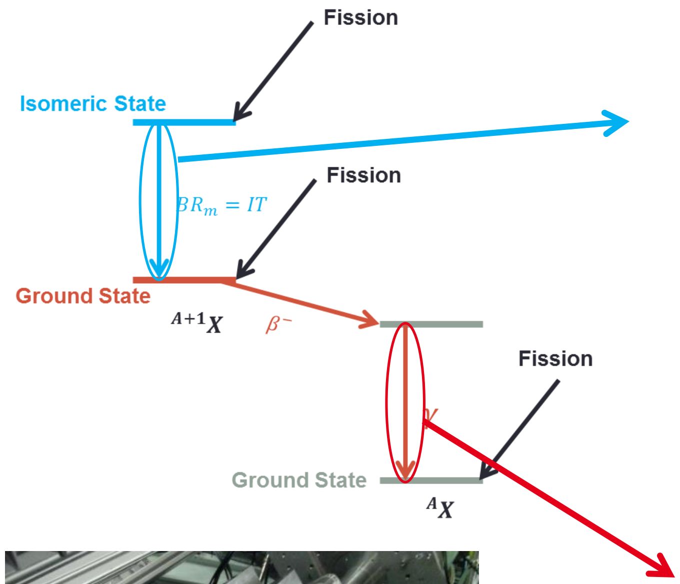
LOHENGRIN spectrometer of ILL

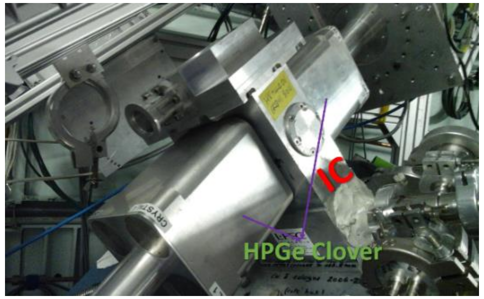


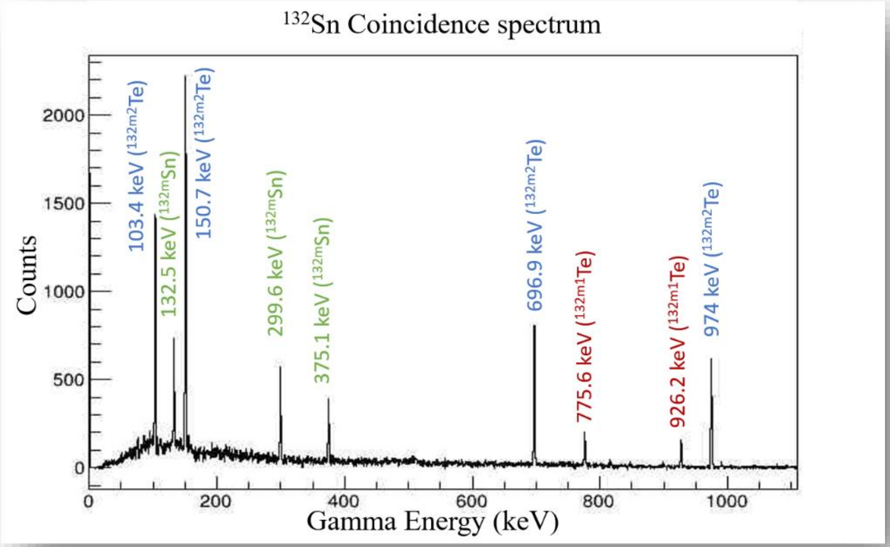


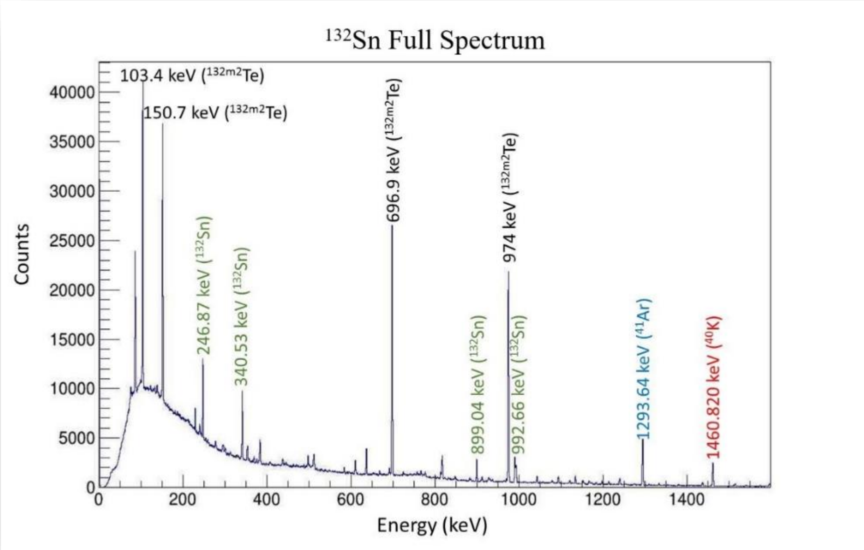


Analysis of µs isomers





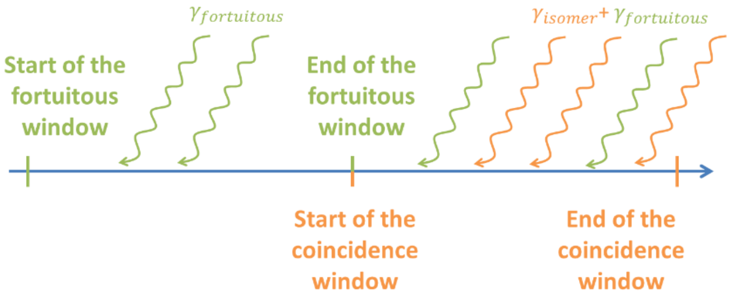


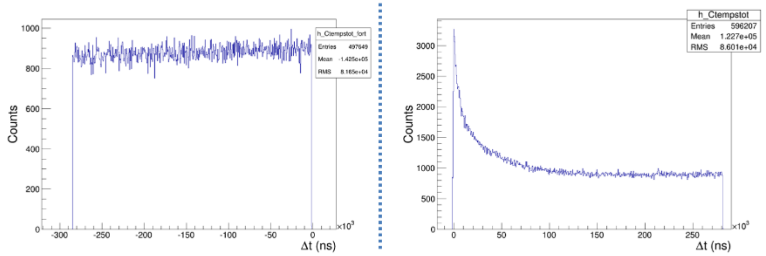


Coincidence between ionization chamber and γ detectors

→ Isomeric state measurement

$\Delta T_{Gate} = 10 T_{1/2}$





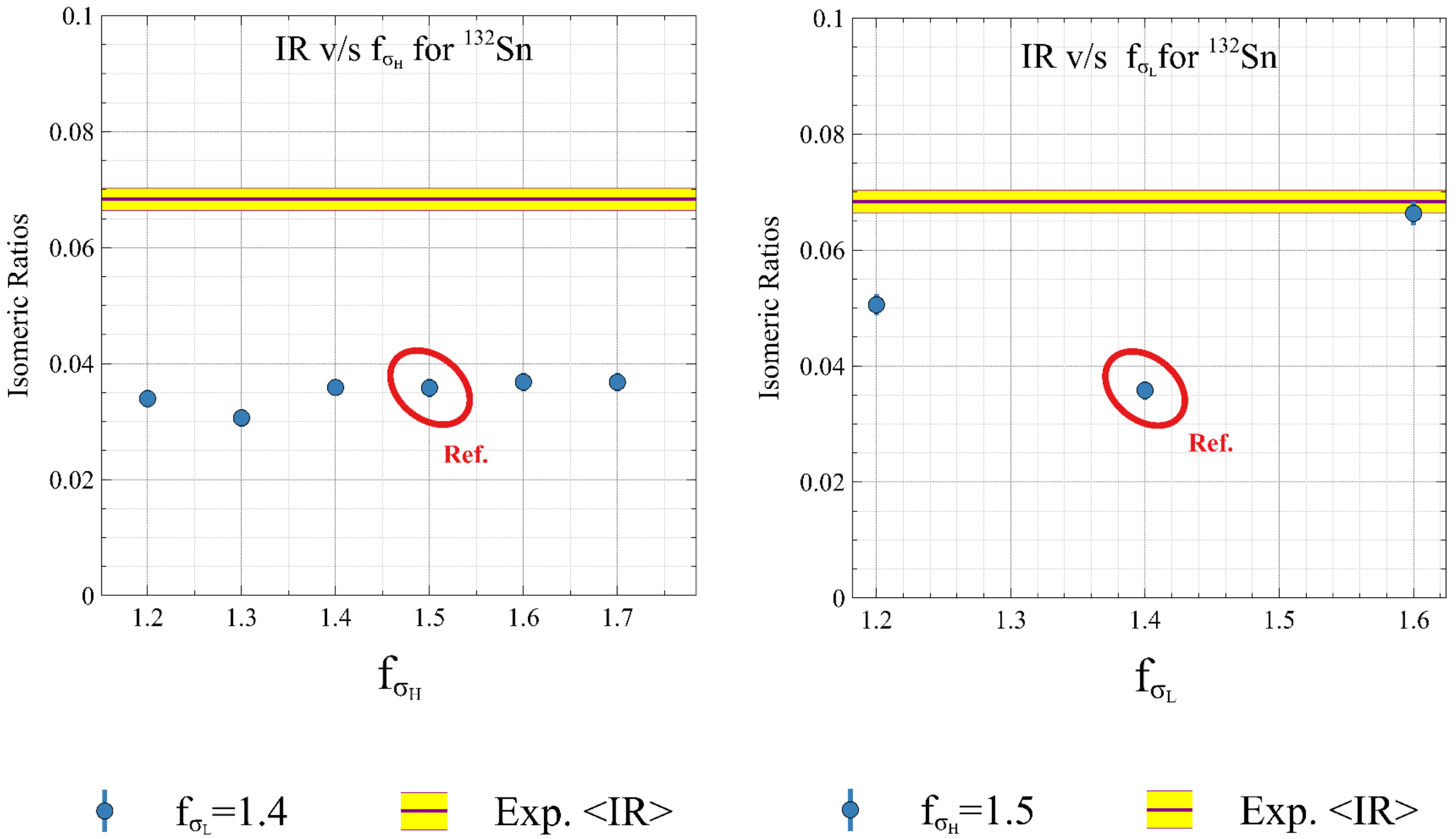
Ungated γ Spectrum i.e. without coincidence

→ Ground state measurement

→ Extraction more difficult because of the S/B ratio

$$IR = \frac{\tau_f(^{132m}Sn)}{\tau_f(^{132m}Sn) + \tau_f(^{132gs}Sn)}$$

Comparison with FIFRELIN calculation



- Level density model : CGCM
- Model of γ strength function (EGLO)
- The impact of f_{σ_L} is more important than f_{σ_H}
- Role of the rotational energy in the total energy excitation sharing ?
- Correlation between both fragments arise naturally !
- Can be explained by nucleons exchange at scission (TDHFB) → role of deformation energy?
- Thermal excitation ?

© J. Nicholson., Determination of fission fragment angular momentum from isomeric ratio measurement, PhD Thesis, UGA, 2021

Direct determination of angular momentum with FIFRELIN decay

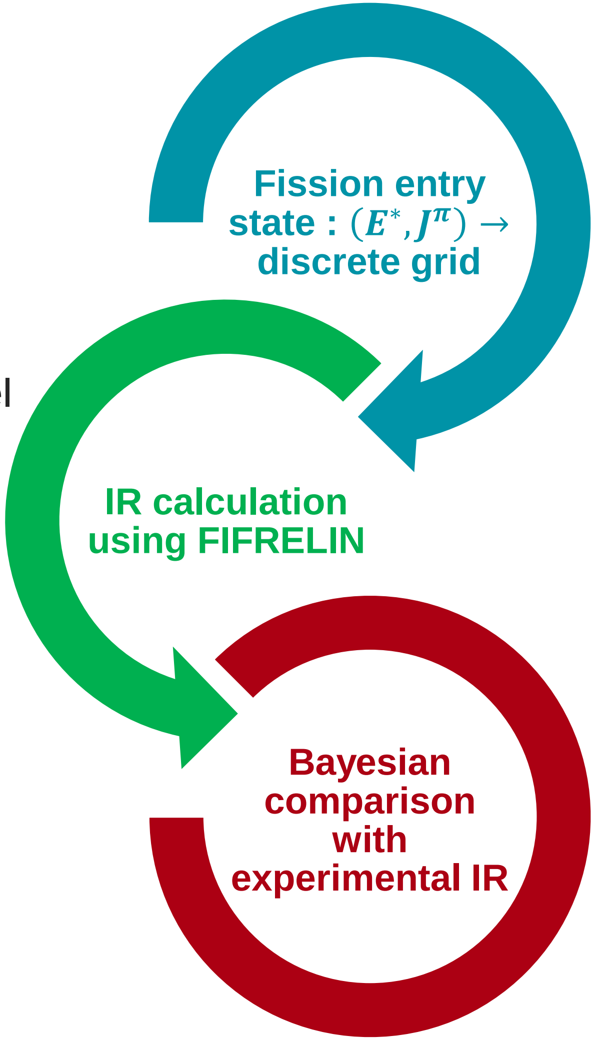
In this work, FIFRELIN (developed by CEA Cadarache) is used **only as a nuclear de-excitation code (step 2)**

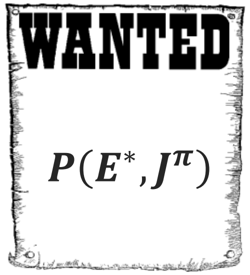
What is required for FIFRELIN :

- experimental level scheme (RIPL-3)
- Model of nuclear density to complete the level scheme (CGCM)
- Model of γ strength function (EGLO)
- Electron conversion coefficients (BrIcc)

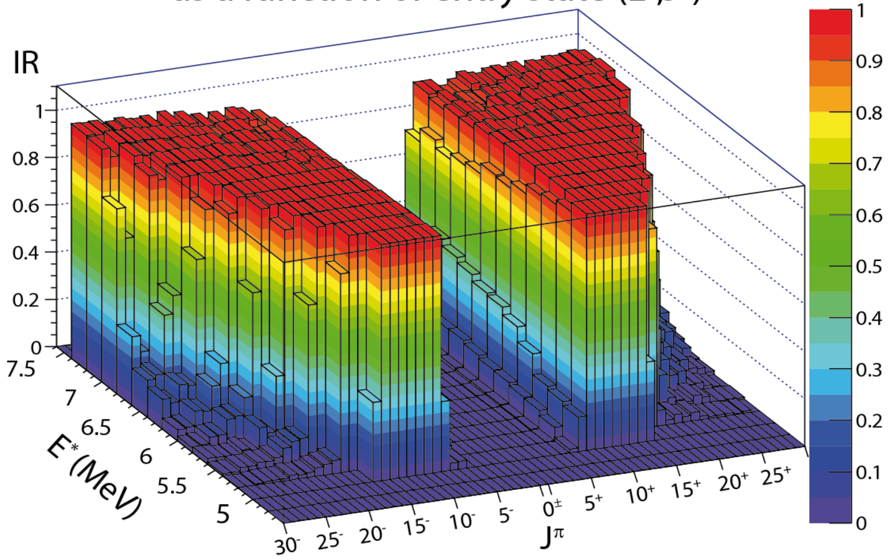
For comparison with experimental results standard spin distribution:

- $IR_{FIF}(E^*, J_{RMS}) = \sum_E \sum_\pi P(\pi) P(J) IR_{FIF}(E^*, J^\pi)$
- $P(J) \propto (2J+1) \exp\left(-\frac{\left(J+\frac{1}{2}\right)^2}{J^2_{cutoff}}\right)$
- $P(\pi) = \frac{1}{2}$

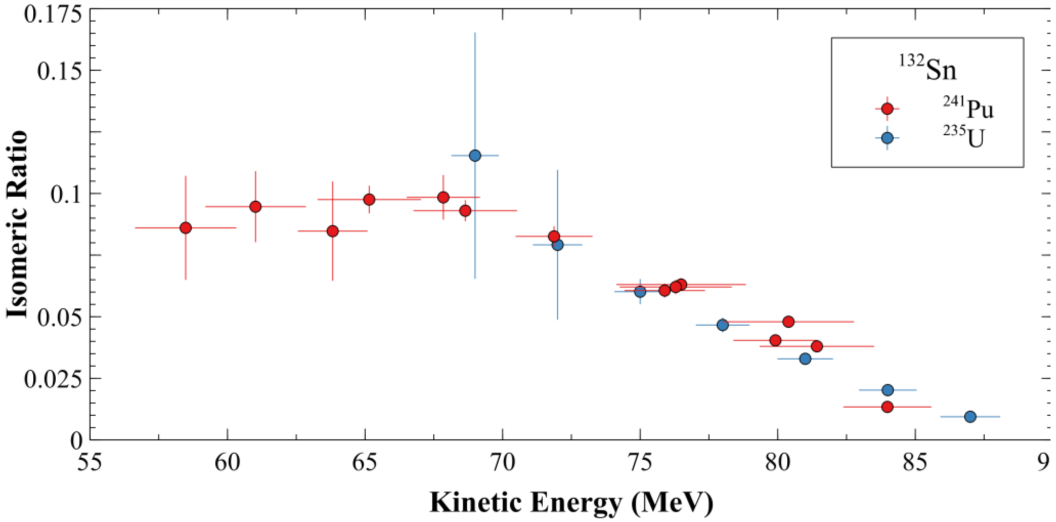


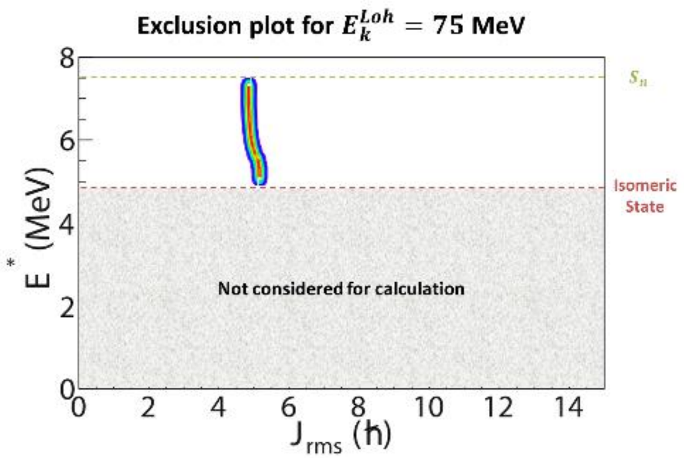


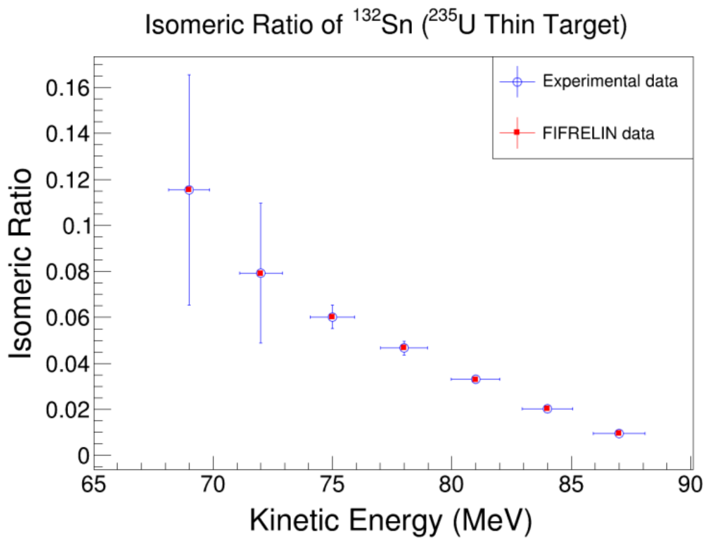
Isomeric Ratio calculated by FIFRELIN as a function of entry state (E^*,J^π)

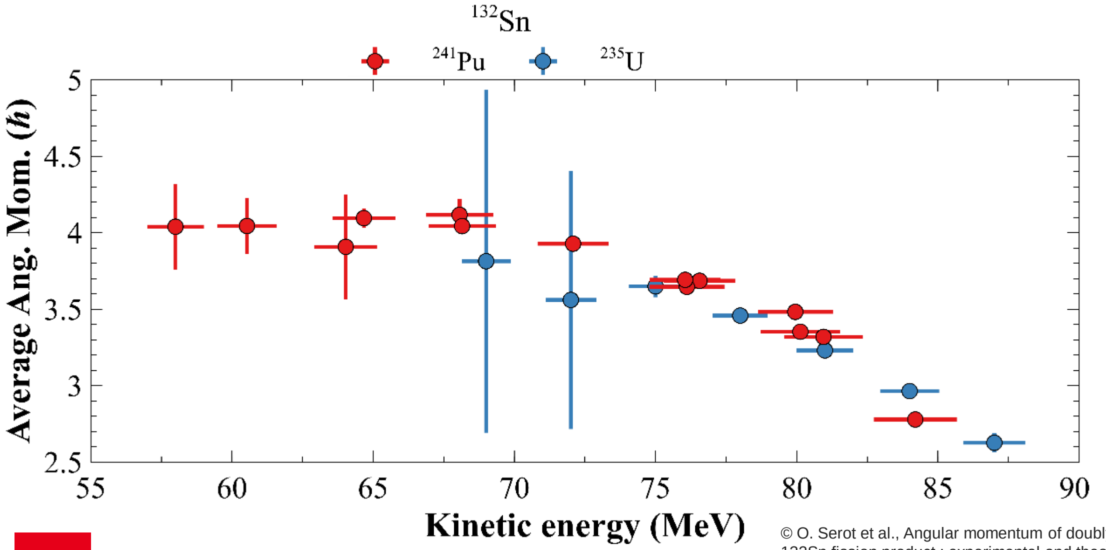


Synthesis on ^{132}Sn work





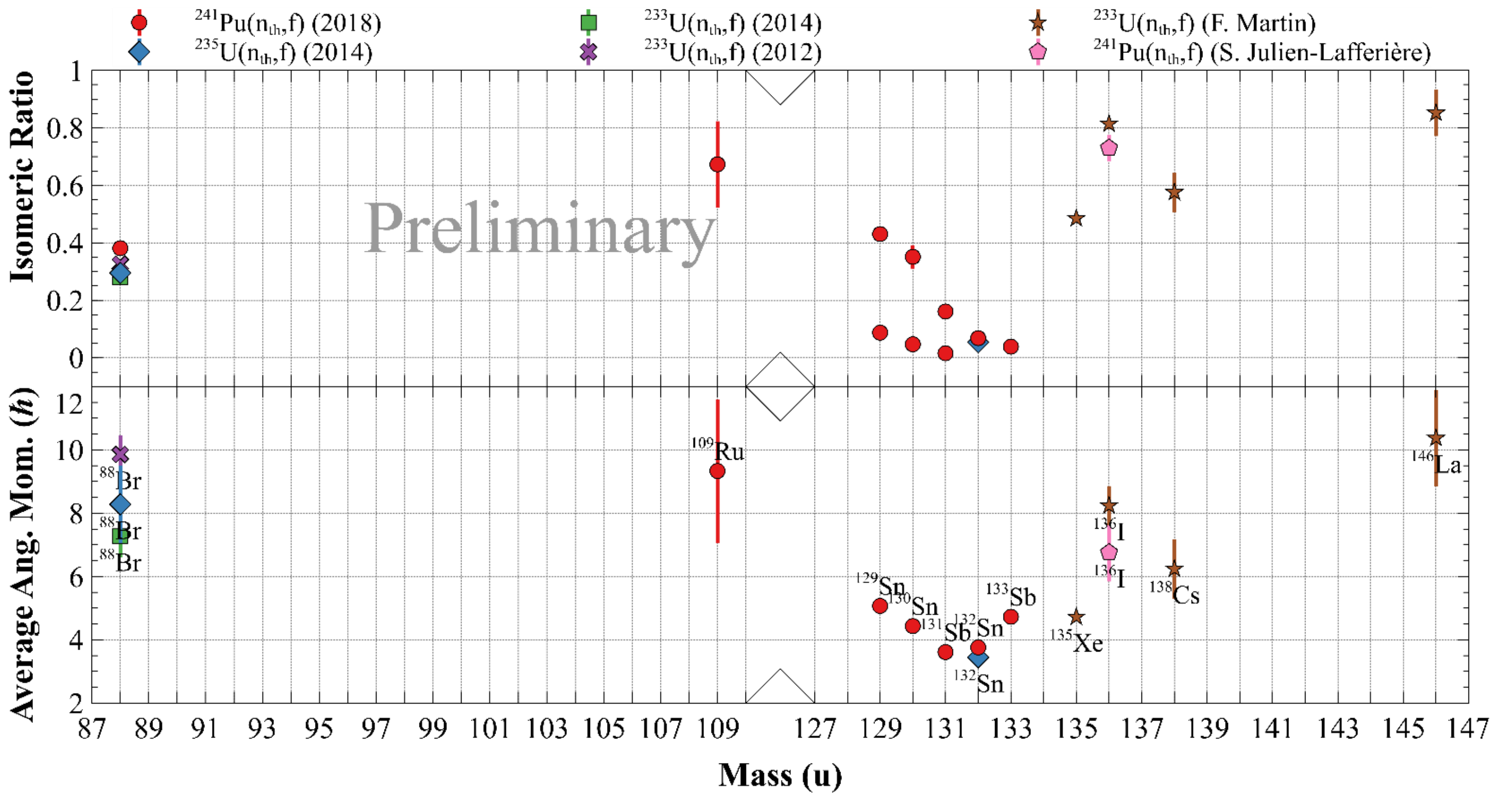


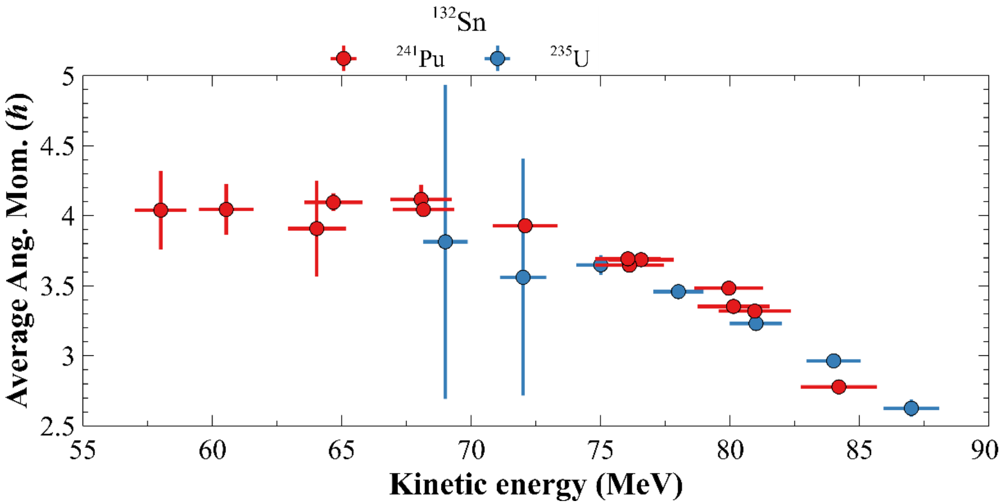


© O. Serot et al., Angular momentum of doubly magic 132Sn fission product : experimental and theoretical aspects, EPJ WoC, 284, 04022 (2023)

- IRs are compared with FIFRELIN calculations starting from arbitrary initial nuclear state
- The derived **average angular momentum** is dependent on the fission fragment **kinetic energy**
- HFB (from P. Marevic et al.) predicts 2.5 $\hbar$ (with ^{239}Pu)
  - Neutron emission ?
  - Thermal excitation ?

Synthesis

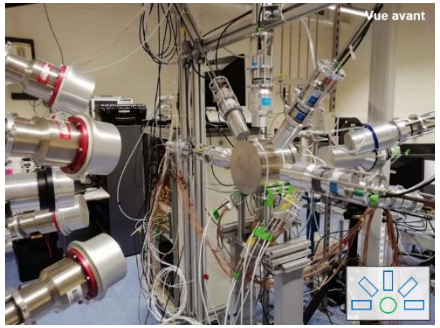




- Isomeric ratios : probe for fission fragment angular momentum
- **Dependency of the derived average angular momentum with the fission fragment kinetic energy**
- Next step : measurement in the light fragment region (part of a thesis 2025-2028)

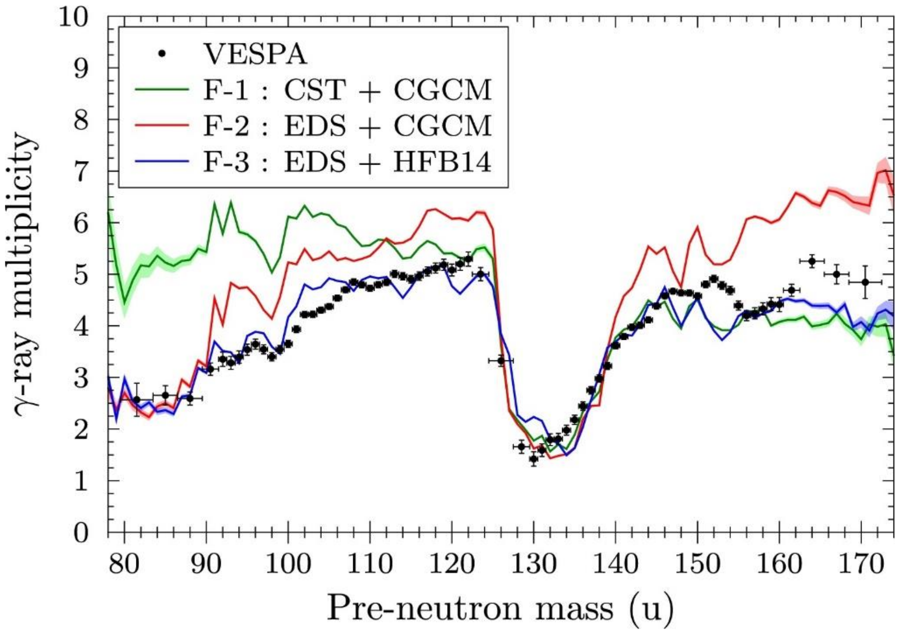
Interpretation using FIFRELIN for prompt γ-rays

Combination	Model of initial angular momentum	Model of level density	[RT_{min}; RT_{min}]	[f_{σ_L}; f_{σ_H}]
F1	Constant	CGCM	[0.45;1.40]	[10.5;8.0]
F2	Energy dependent	CGCM	[0.5;1.40]	[1.7;1.5]
F3	Energy dependent	HFB14	[0.5;1.45]	[1.4;1.3]



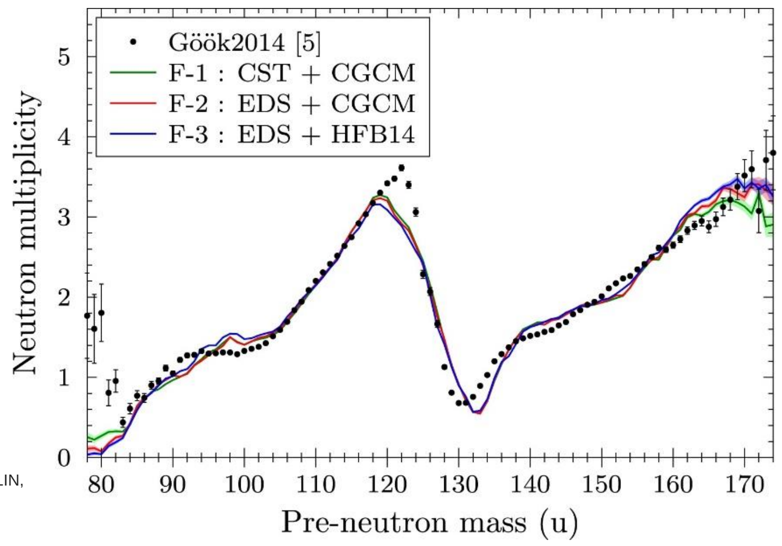
VESPA setup @JRC-Geel

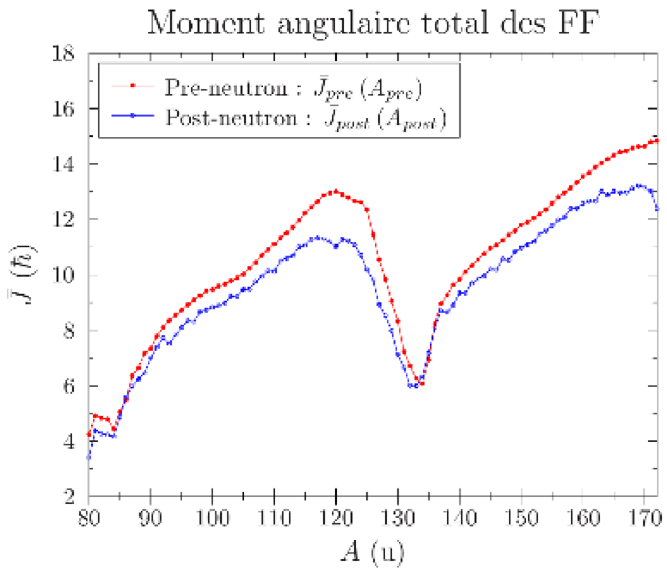
- Twin ionization chamber with Frisch Grid with 252Cf
- 8 LaBr3 for γ
- 7 organic scintillators for neutrons



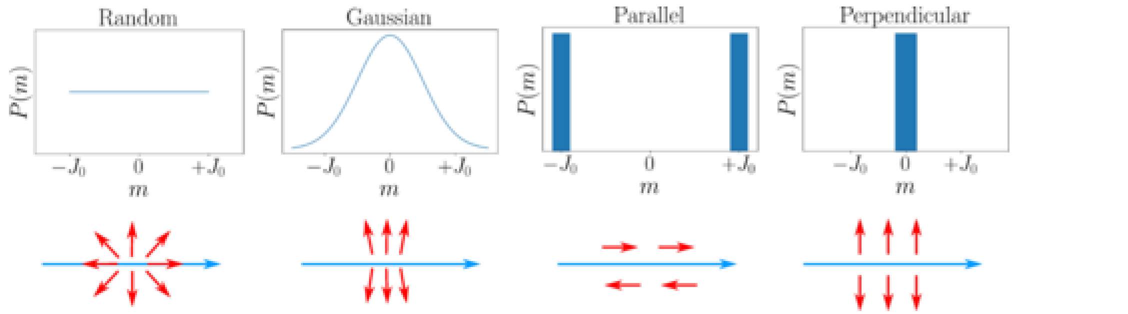
© V. Piau et al., Neutron and gamma multiplicities calculated in the consistent framework of the Hauser-Feshbach Monte Carlo code FIFRELIN, Phys. Lett. B, 837, 137648 (2023)

- F3 is the best combination of models
- Sawtooth behavior seems to raise from energy dependent model
- The scaling is better using HFB14 instead of CGCM level density

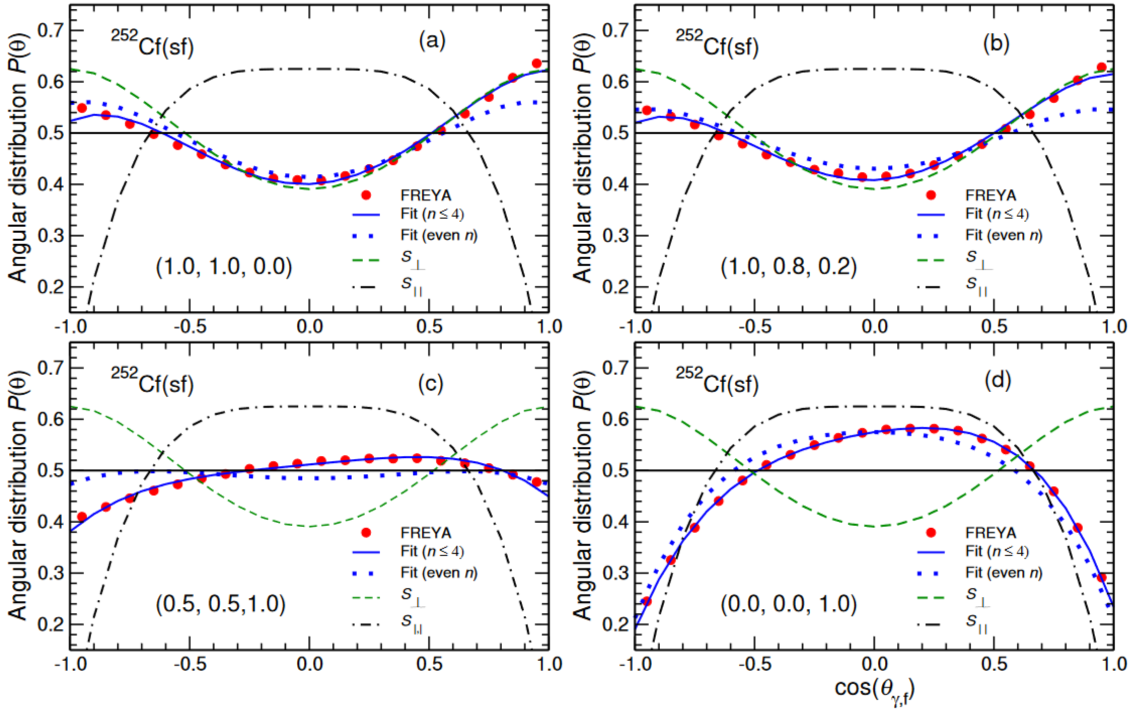


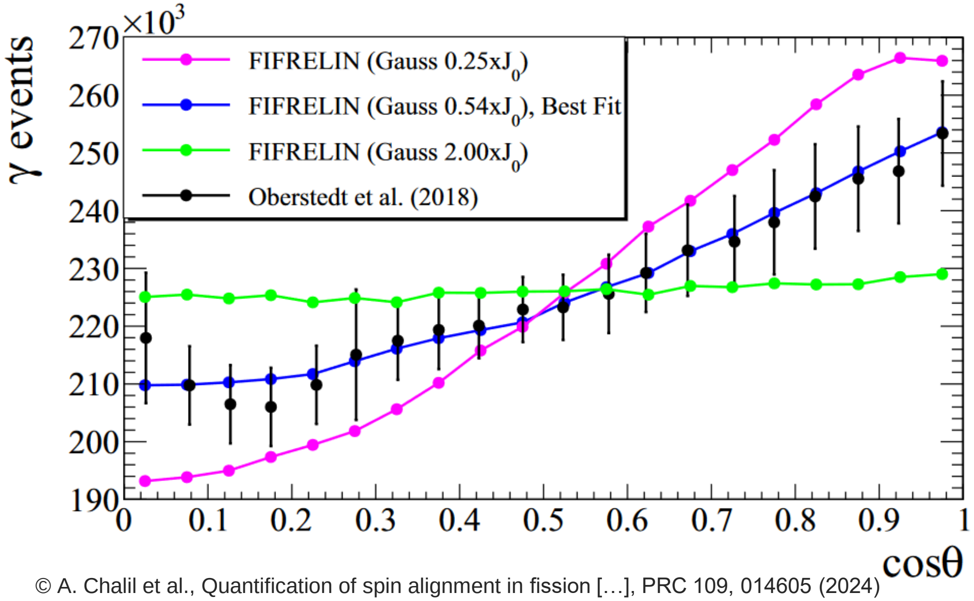


To go further : angular correlation !



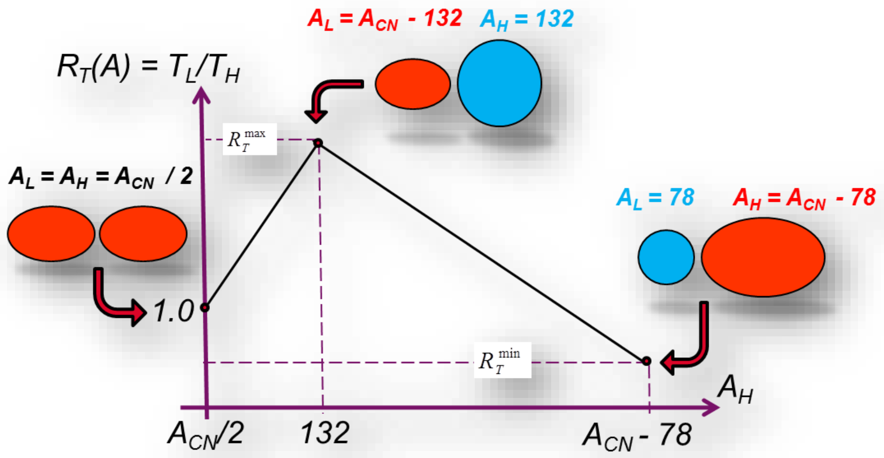
Simulated γ,FF angular correlation from E2 transition and different wriggling/bending/twisting feeding !

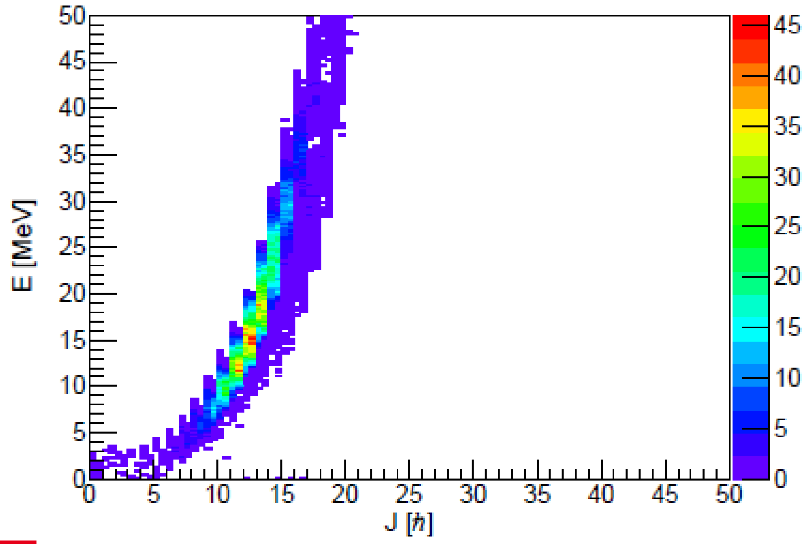


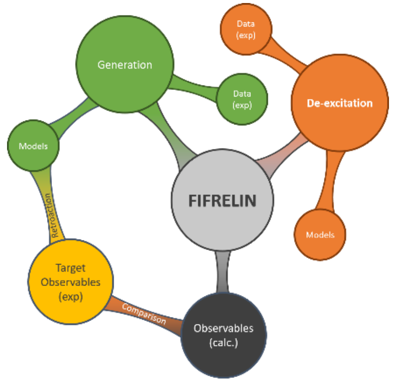


3. On going developments

Machine Learning with FIFRELIN





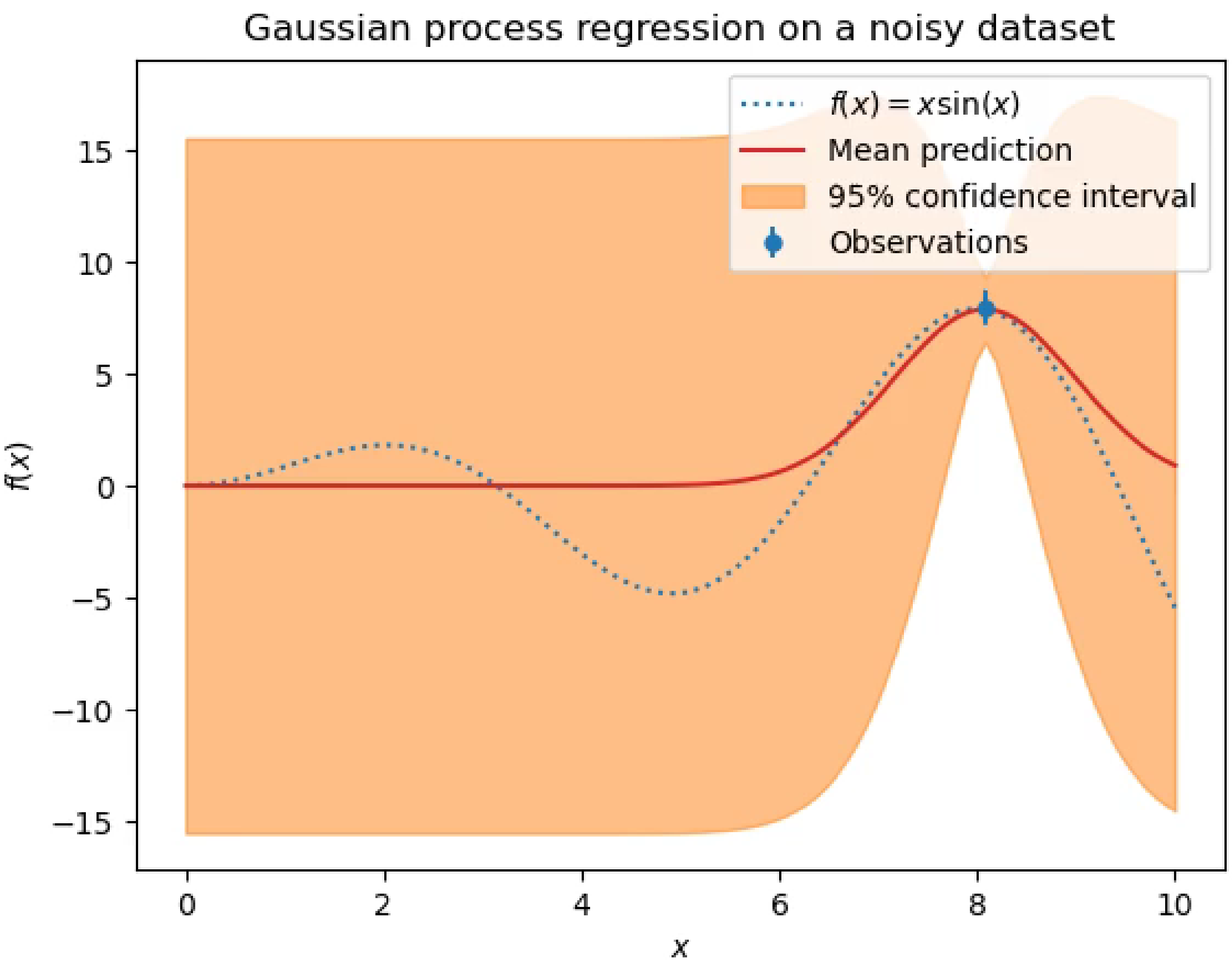


How to determine these 4 parameters ?

- If we consider each of them as independent, and at least 5 points (per dimension) to find their best values, we need $5^4 = 625$ simulations → 4 days
- One way to reduce the number of simulations (time consuming) : Machine Learning
- In this work, we started with Gaussian Process algorithm

GPs

- Can be seen as a more complex way to make interpolation
- Suitable for linear problems!
- Based on prior covariance between data : hyper-parameters are fitted and control the smoothness of the interpolated function
- Not the best option for really high dimensions !



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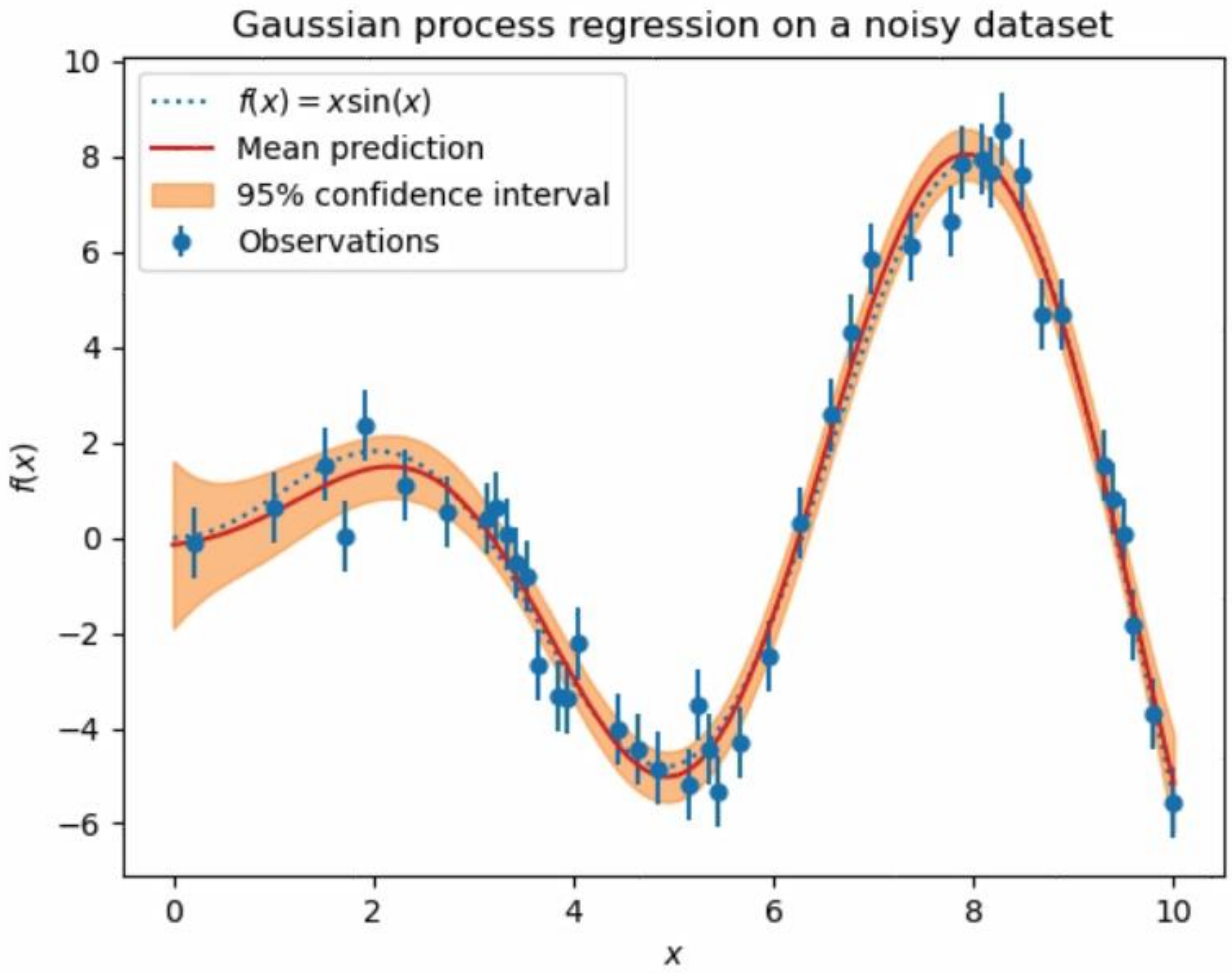
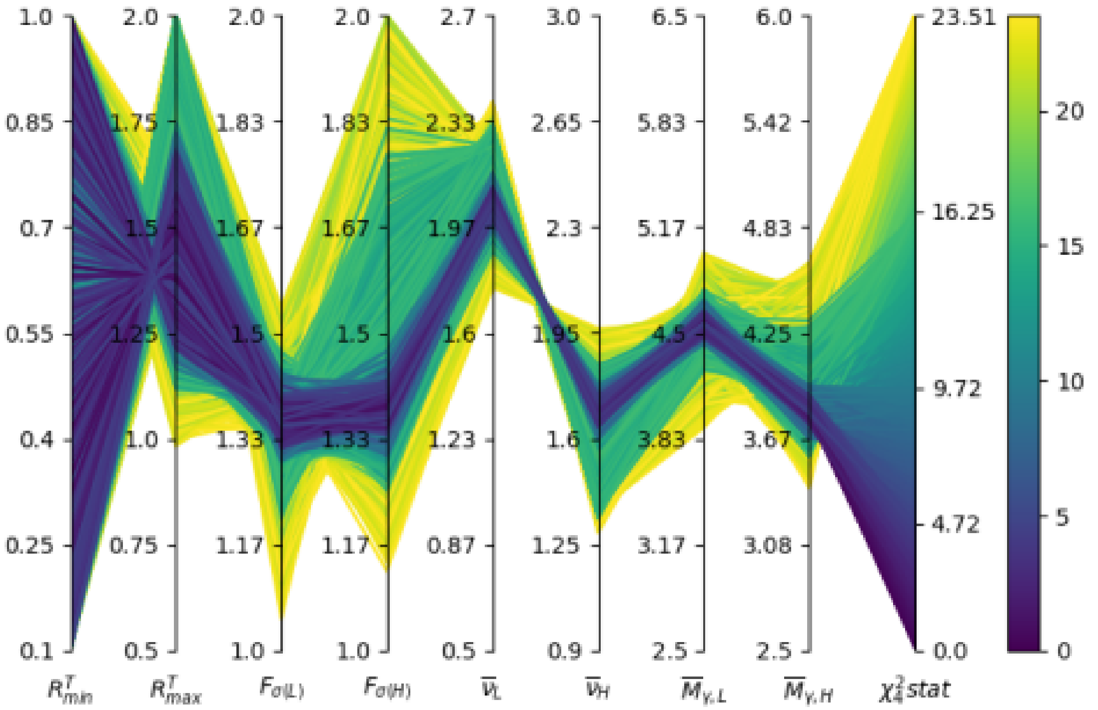
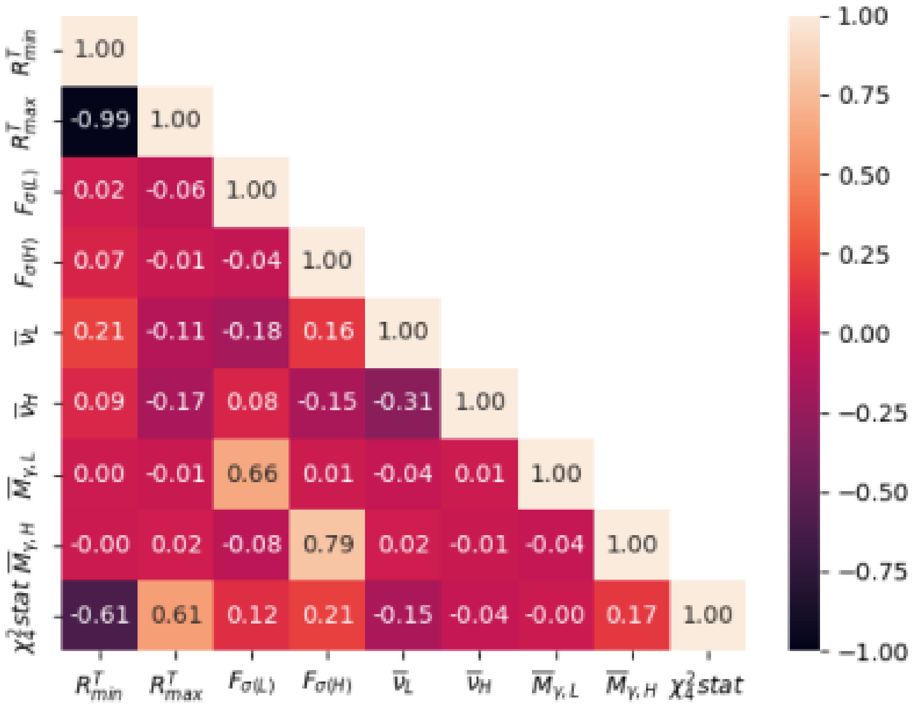


Some results : $^{252}Cf(sf)$



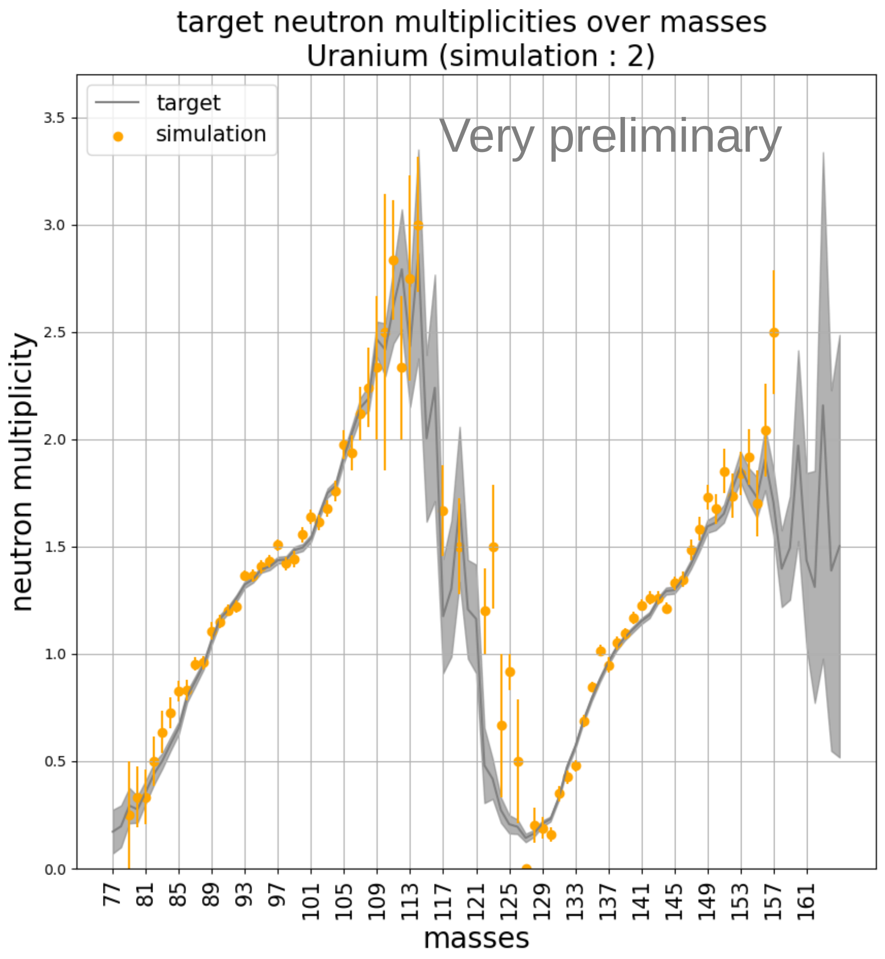


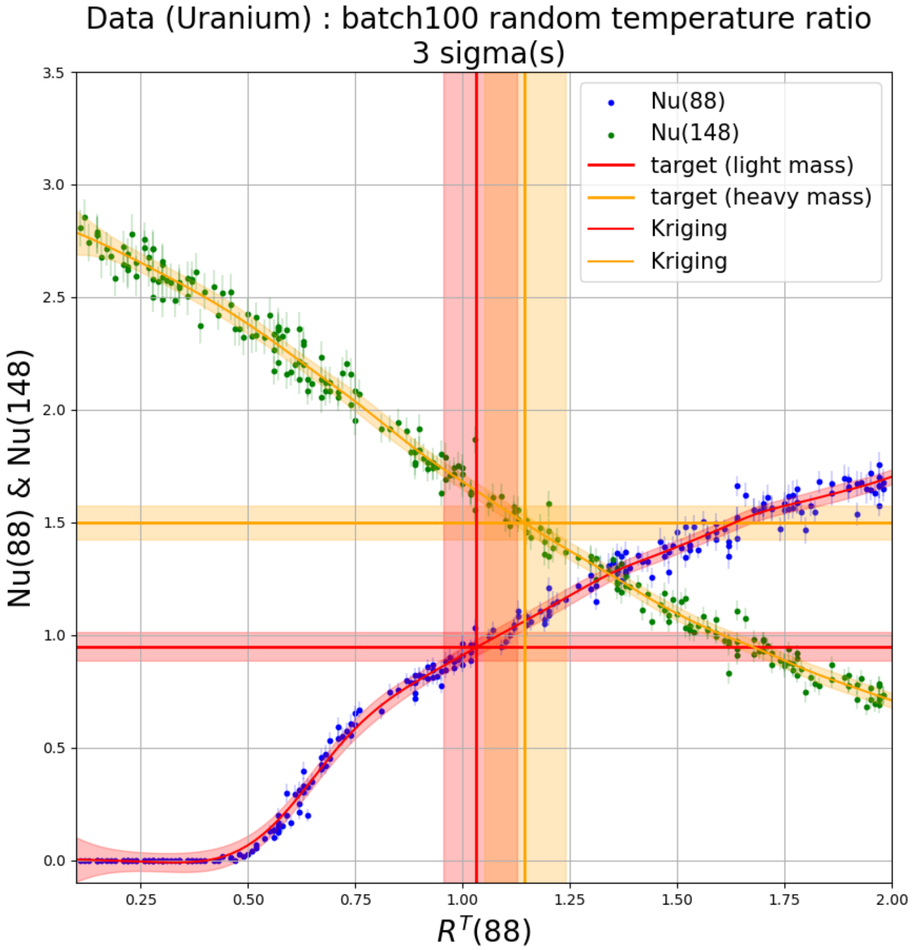
© G. Bazelaire et al., Assimilating fission-code FIFRELIN using machine learning, EPJ Web of Conf. 294,03002 (2024)

- Target : $[\overline{\nu_L}, \overline{\nu_H}, \overline{M_{\gamma_L}}, \overline{M_{\gamma_H}}] = [2.06, 1.70, 4.56, 3.82]$
- In 2h, from scratch, we found an optimum : $[RT_{min}, RT_{max}, f\sigma_L, f\sigma_H]$ = [0.18,1.58,1.38,1.37] thanks to 100 simulations

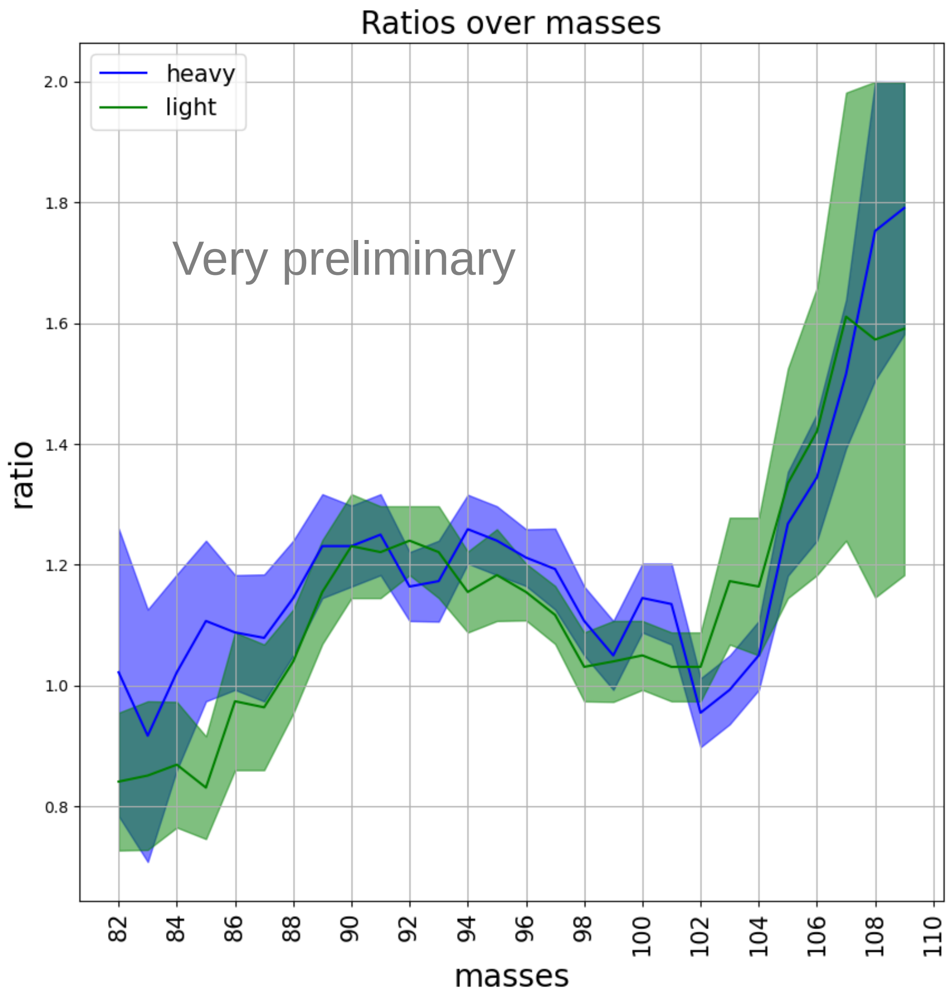
To go further : determination $R_T(A)$ function

- Test on $^{235}U(n_{th},f)$ reaction
- Use $\bar{\nu}(A)$ as target !
- $\bar{\nu}(A)$ and $\bar{\nu}(A_{CN}-A)$ strongly correlated (anti-correlated) to $R_T(A)$





To go further : determination $R_T(A)$ function

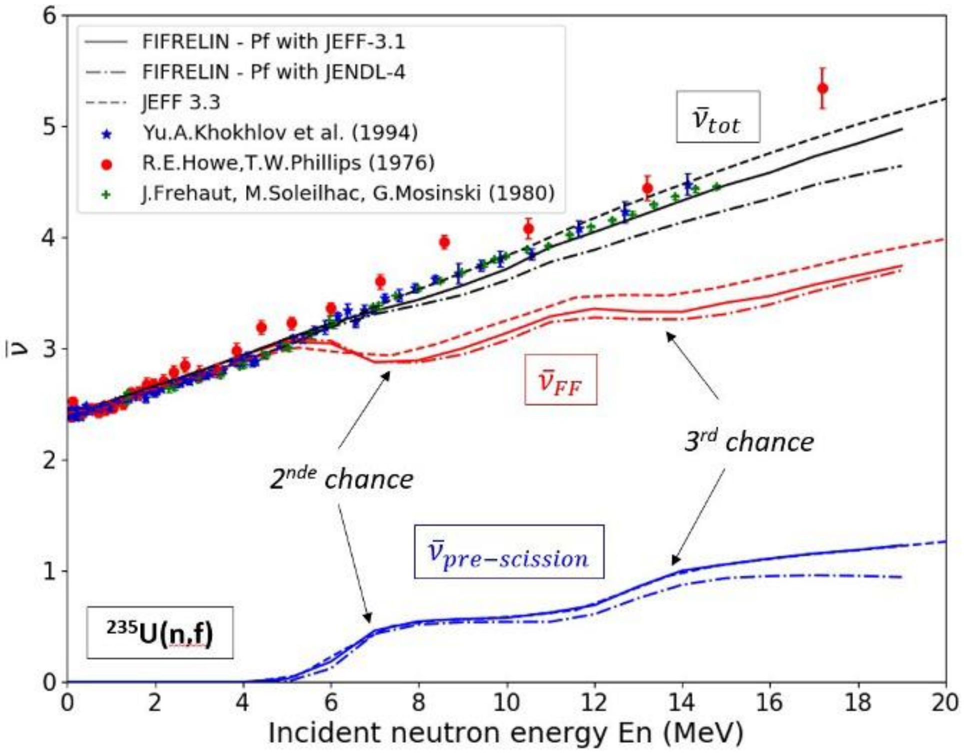


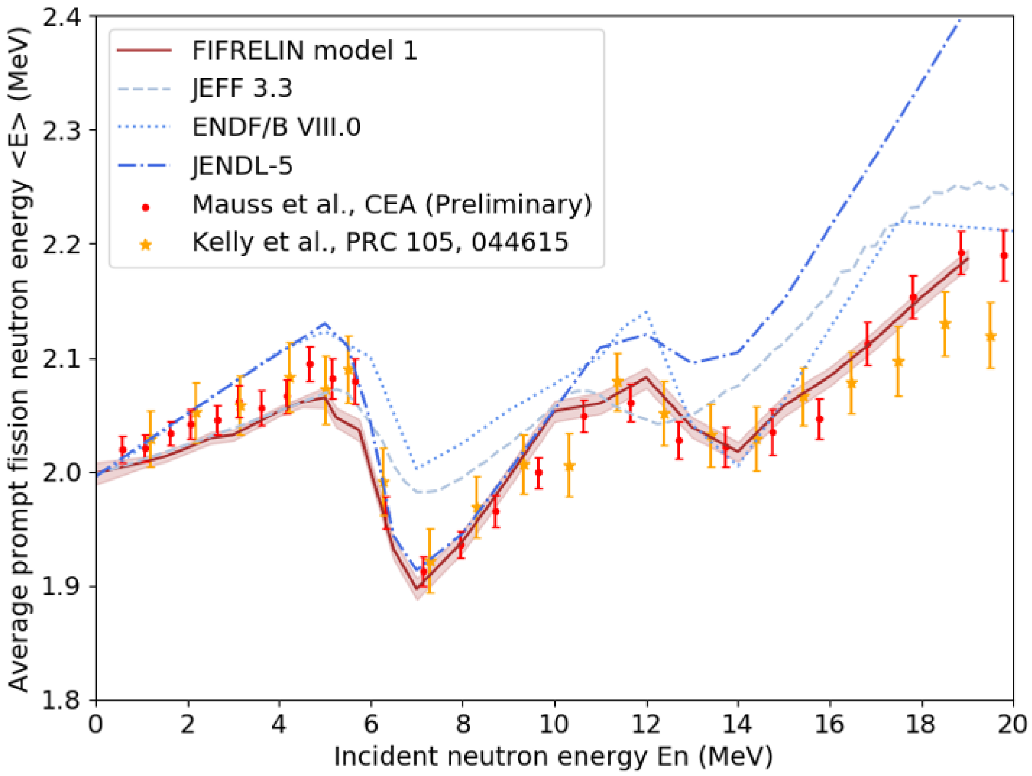
- To reproduce the sawtooth, we need such $R_T(A)$ function
- Can theoretical calculation produce such quantity ?
- Good illustration of the role played by FIFRELIN to “transform” experimental quantity (neutron multiplicity) to physical observable (excitation energy at/nearby scission)

Multi-chance fission

Need a lot of pre-neutron data → GEF is used to provide them + interpolation
Free parameters are also tuned against ν + interpolation
Two models implemented :

- Non analog : based on evaluated partial fission cross section (see results below)
- Analog : calculation of fission width based on Hill-Wheeler formula + competition with other channels (neutron/γ)

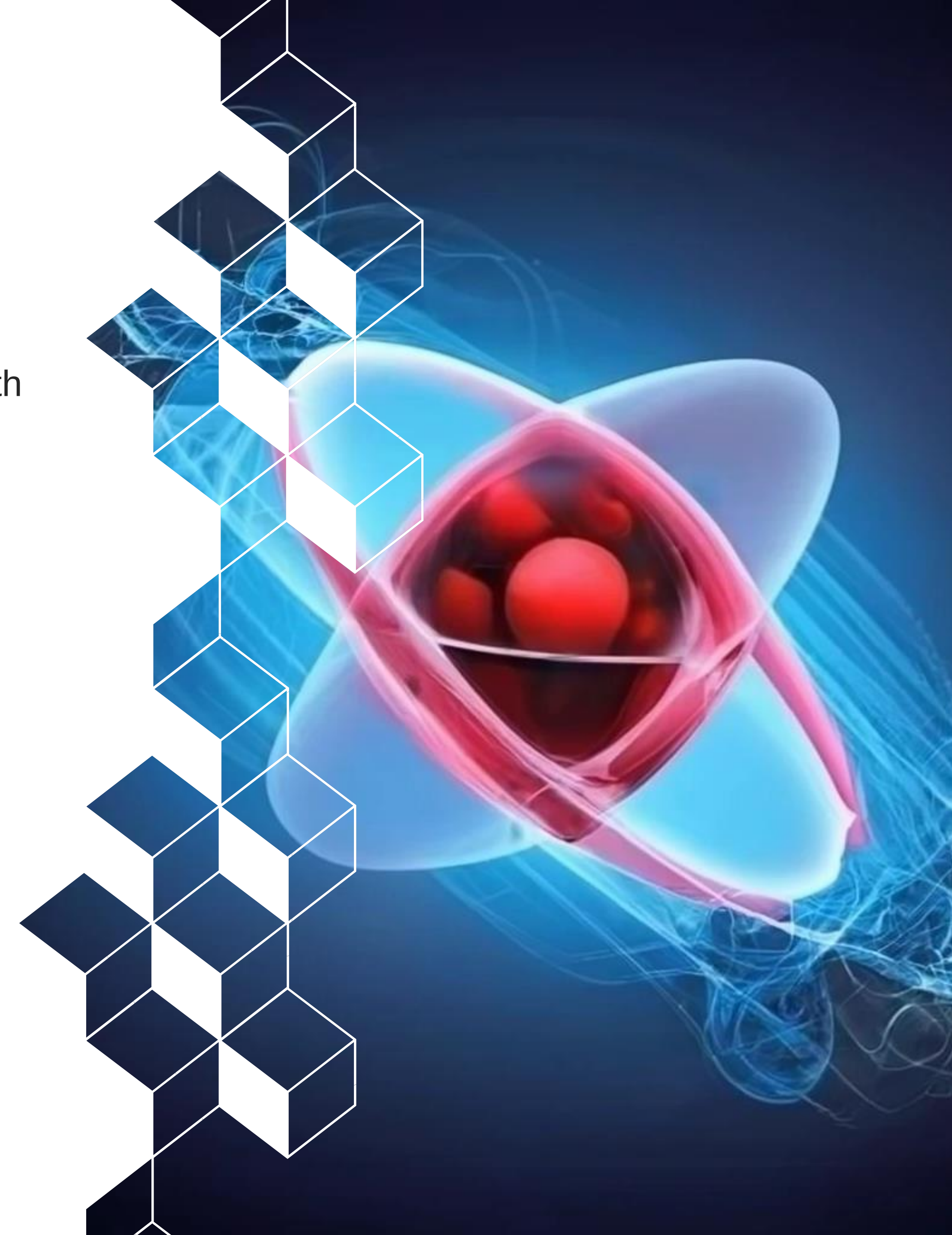




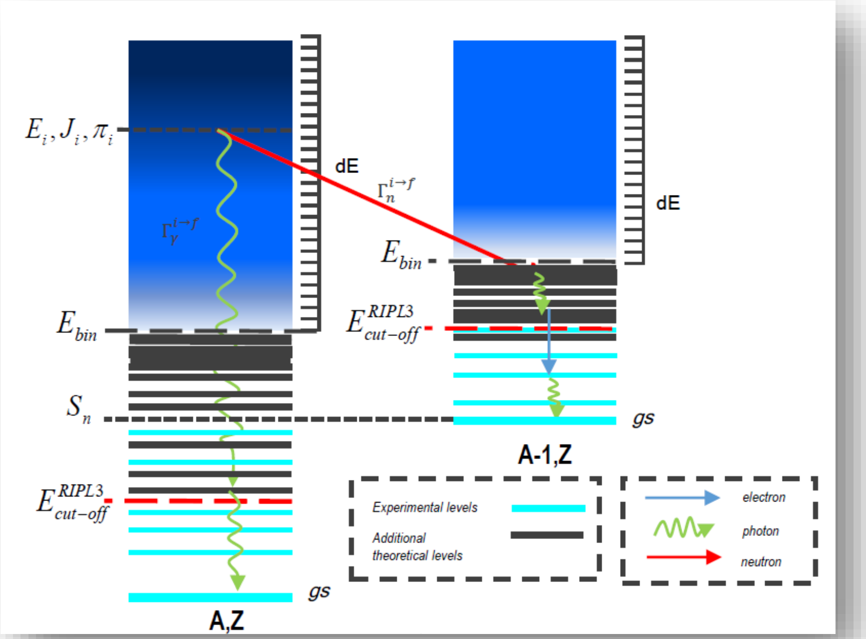
Conclusions

FIFRELIN is a two step Monte Carlo Code with 4 free parameters

- Recent works have generalized electron emission calculation
- Energy dependent angular momentum is crucial for comparison with experimental data
- HFB level densities suits well with experimental data
- Use of machine learning to expand the range of applications of FIFRELIN + more complex initial modelling
- Multi-chance fission implemented in the code
- FIFRELIN is now available at NEA!



Thank you for your attention



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