FIFRELIN: a keystone to Study Nuclear Fission

FIESTA 2024, 11/18-22/2024, Los Alamos

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IRESNE | Positioning in the CEA's Energy Division

Low Carbon Energy Production

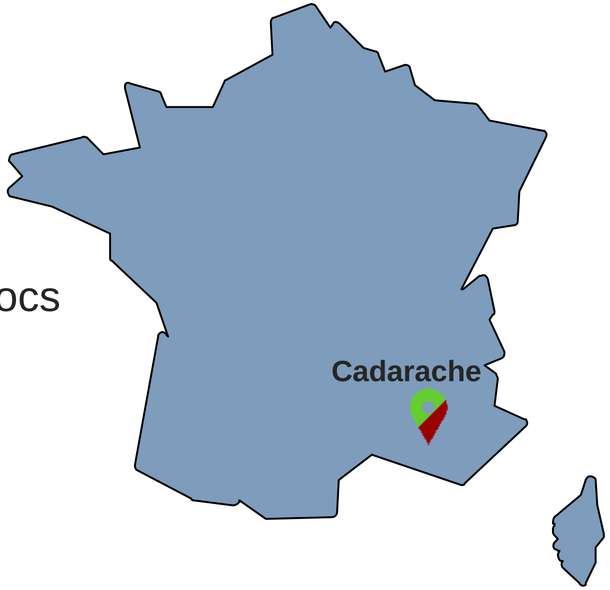
- **Expertise** and **design of solutions** for present and future **nuclear systems** :
  - Technologies
  - Instrumentation and control
  - Nuclear Fuels
  - Reactors
- Low-carbon energy production **applications** involving **nuclear, renewable energy** and **storage**..

900 employees

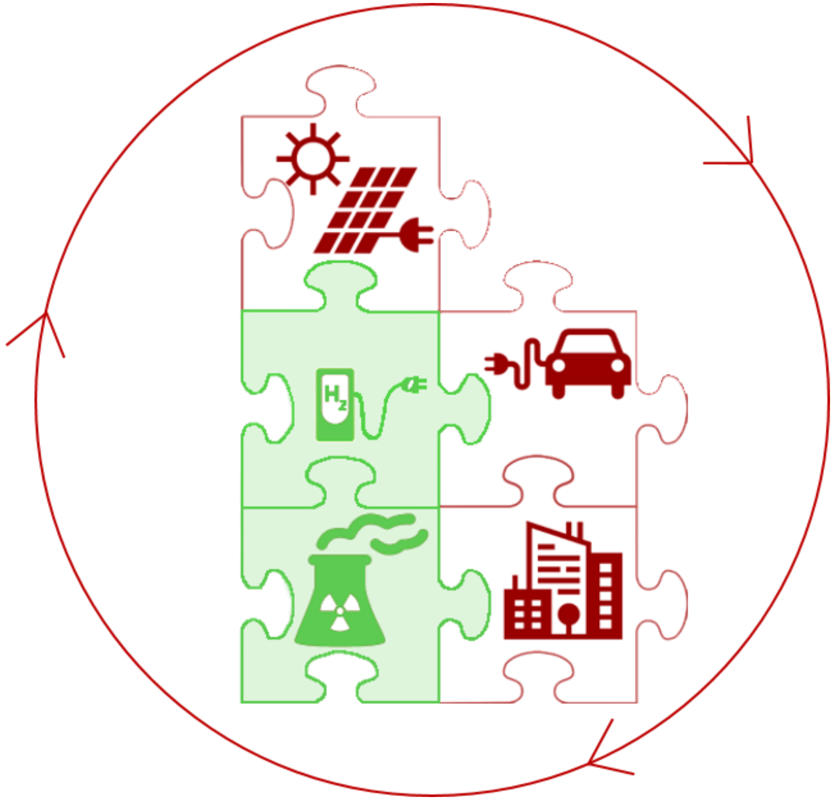
300 experts

150 PhD students and post-docs

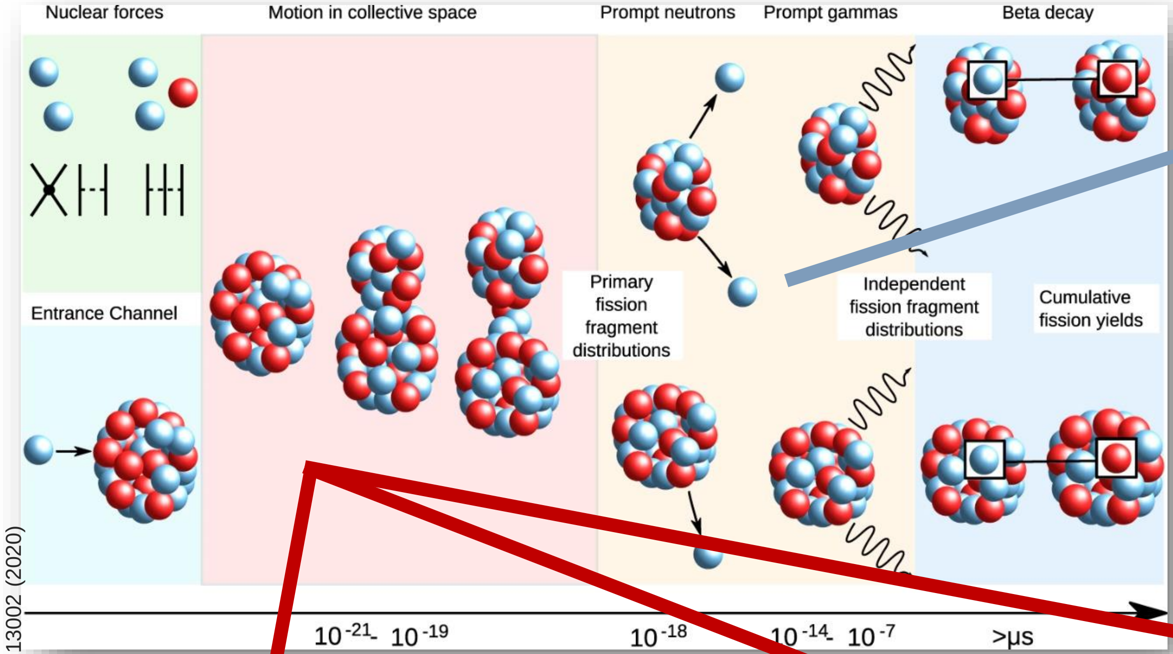
> **50** cooperation agreements



Integrated Energy System



The nuclear fission process



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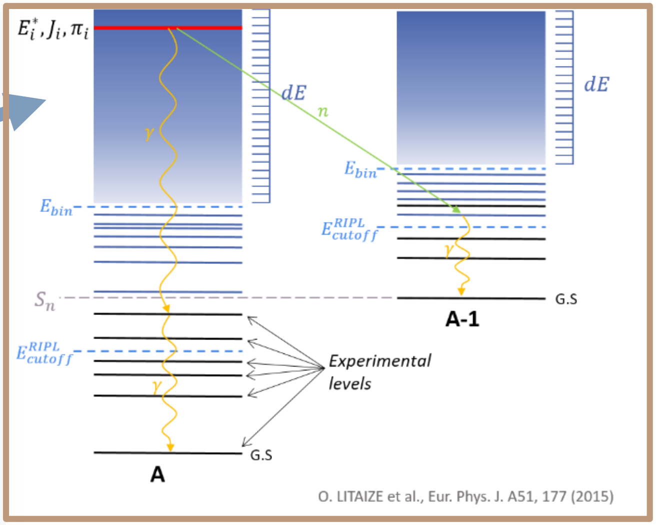
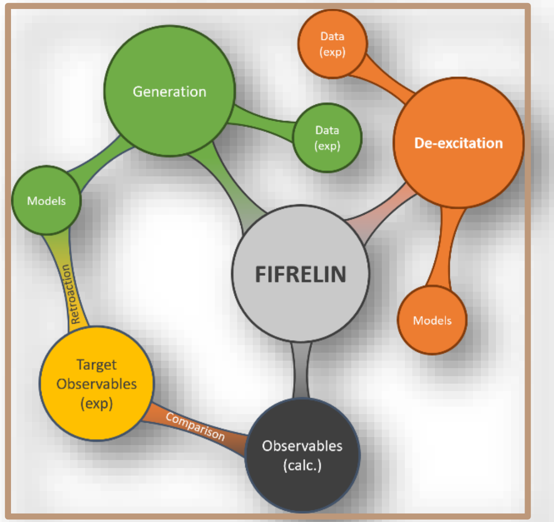
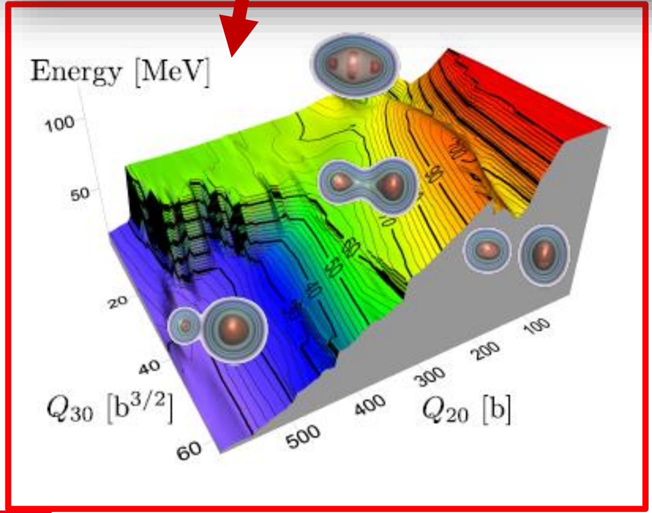




FIFRELIN : generation and de-excitation of fission fragment. Developed by DES/IRESNE



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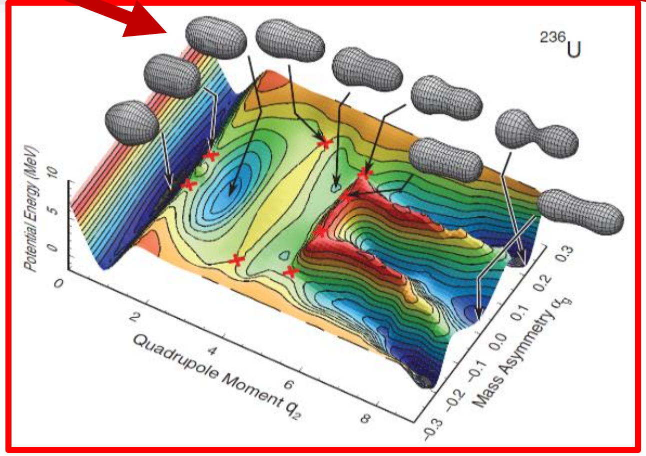
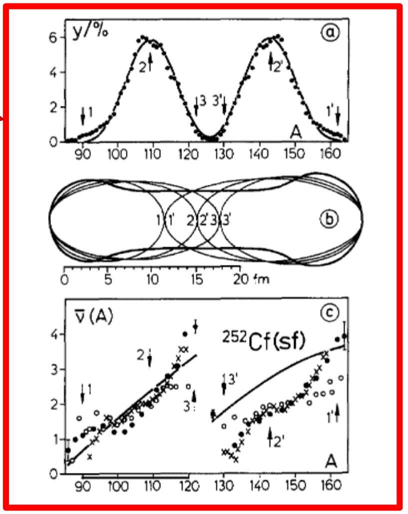


© Ichikawa *et al.*, *Contrasting fission potential energy structure of actinides and mercury isotopes,* Phys. Rev. C 40, 770 (1989)



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

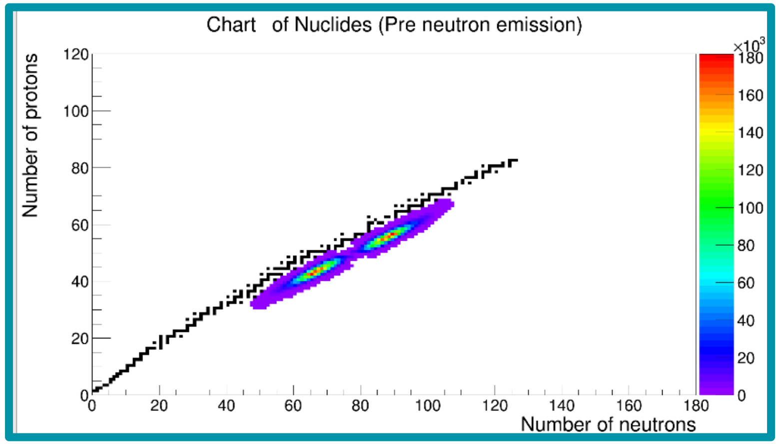
1. Description of FIFRELIN

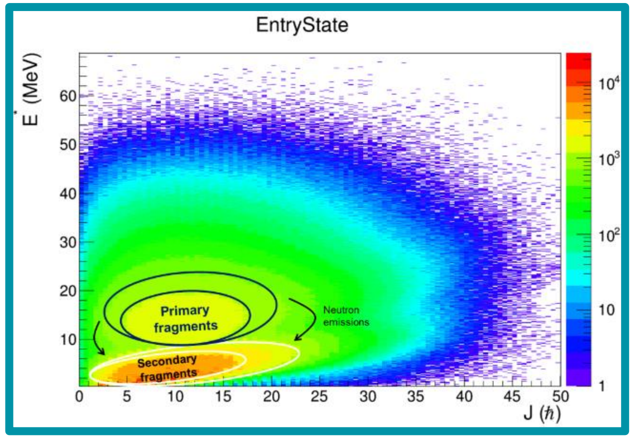
FIFRELIN : a bridge between experimental and theoretical worlds

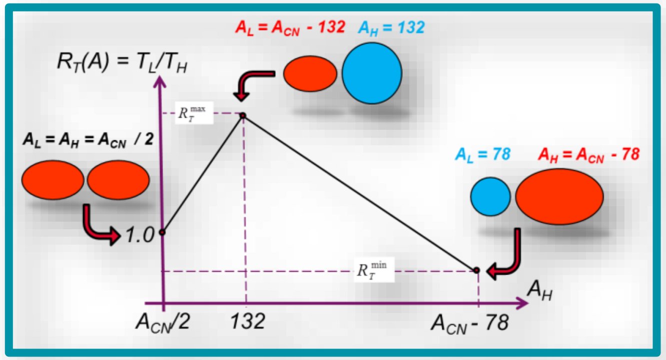
FIFRELIN (FIssion Fragments Evaporation modeLINg)

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

Fission Fragments Generation

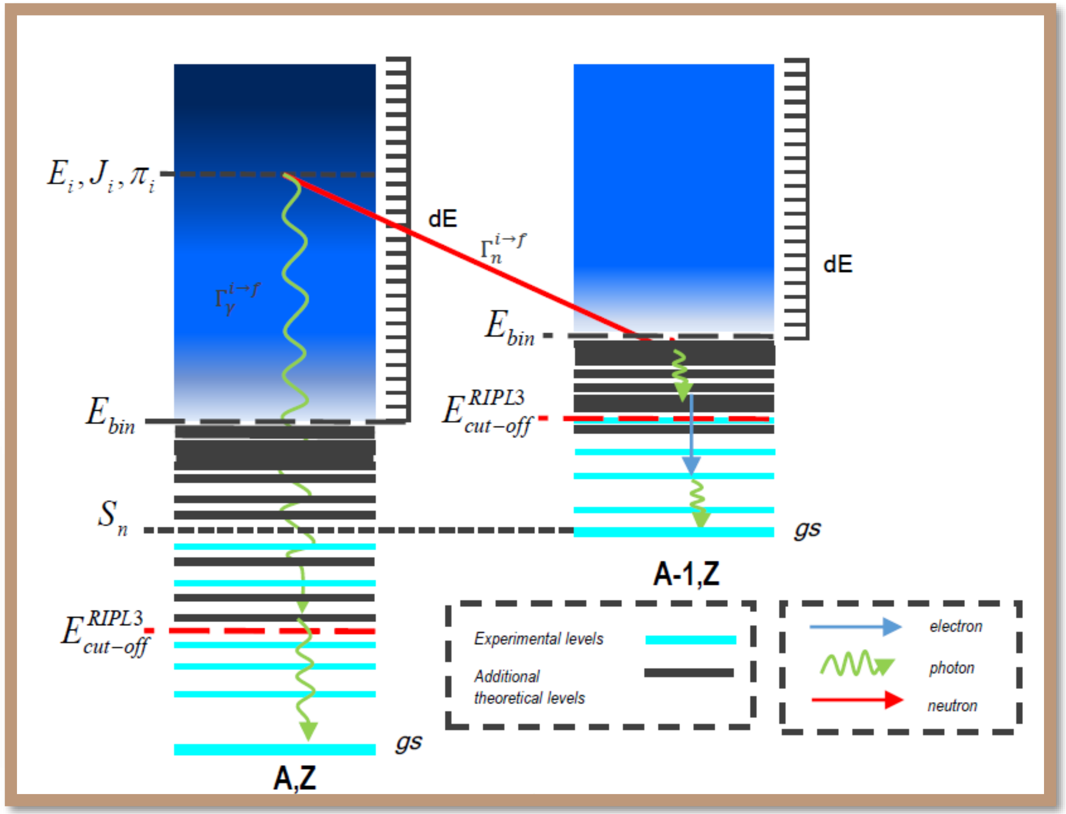






2 steps code

Creation of nuclear levels for given fission fragments and daughters



Fission fragment generation

Ingredient (input files/models) :

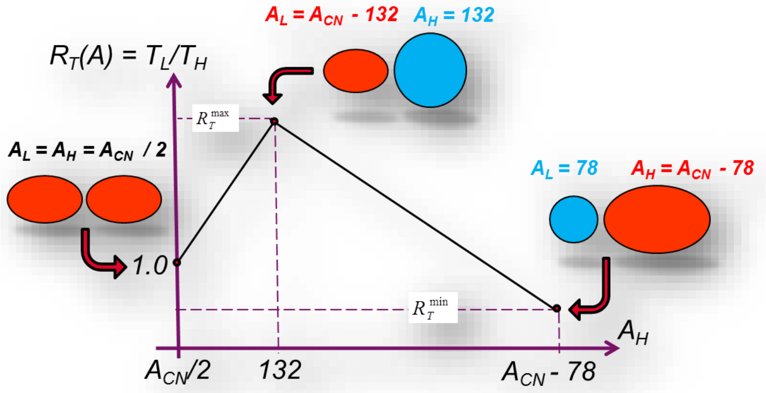
- Pre-neutron mass yields: A (usually obtained from experimental data)
- Nuclear charge calculation: Z (Wahl)
- Pre-neutron emission kinetic energy distributions : KE (usually obtained from experimental data)
- Excitation energy sharing E^* : Temperature Ratio function (2 free parameters)
- Fission fragment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

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

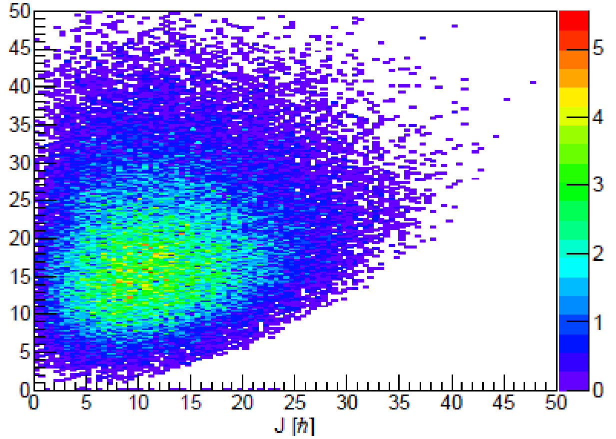
Constant model :

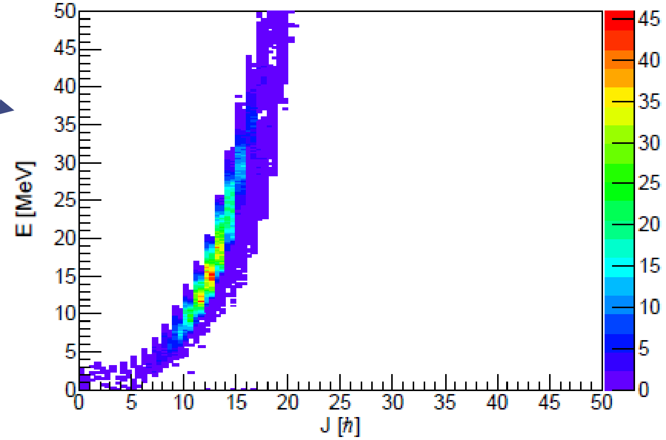
$\sigma_{L,H} = f_{\sigma\, L,H}$ not energy dependant !

Energy dependant model :

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

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





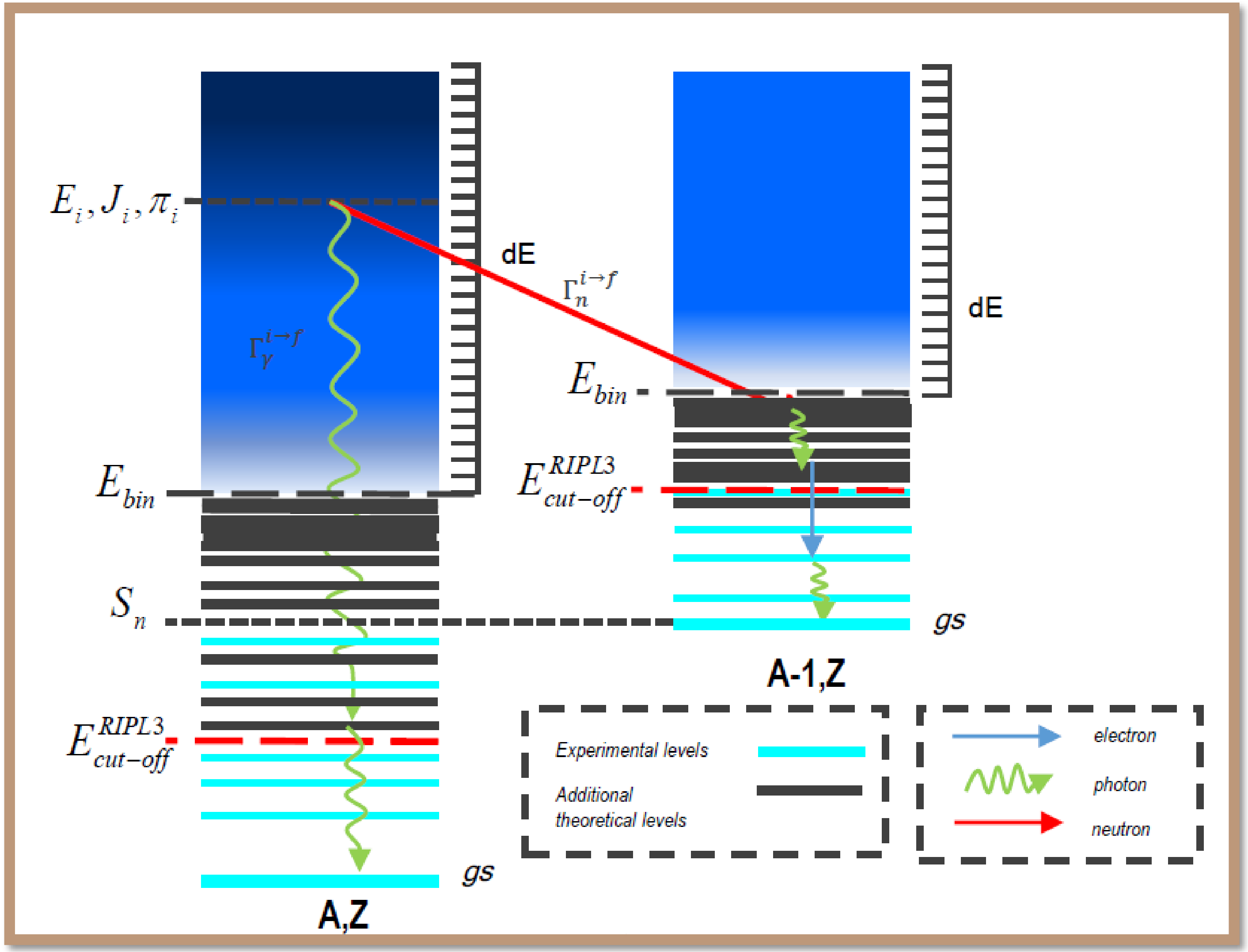
Emission of prompt particles

Ingredient (input files/models) :

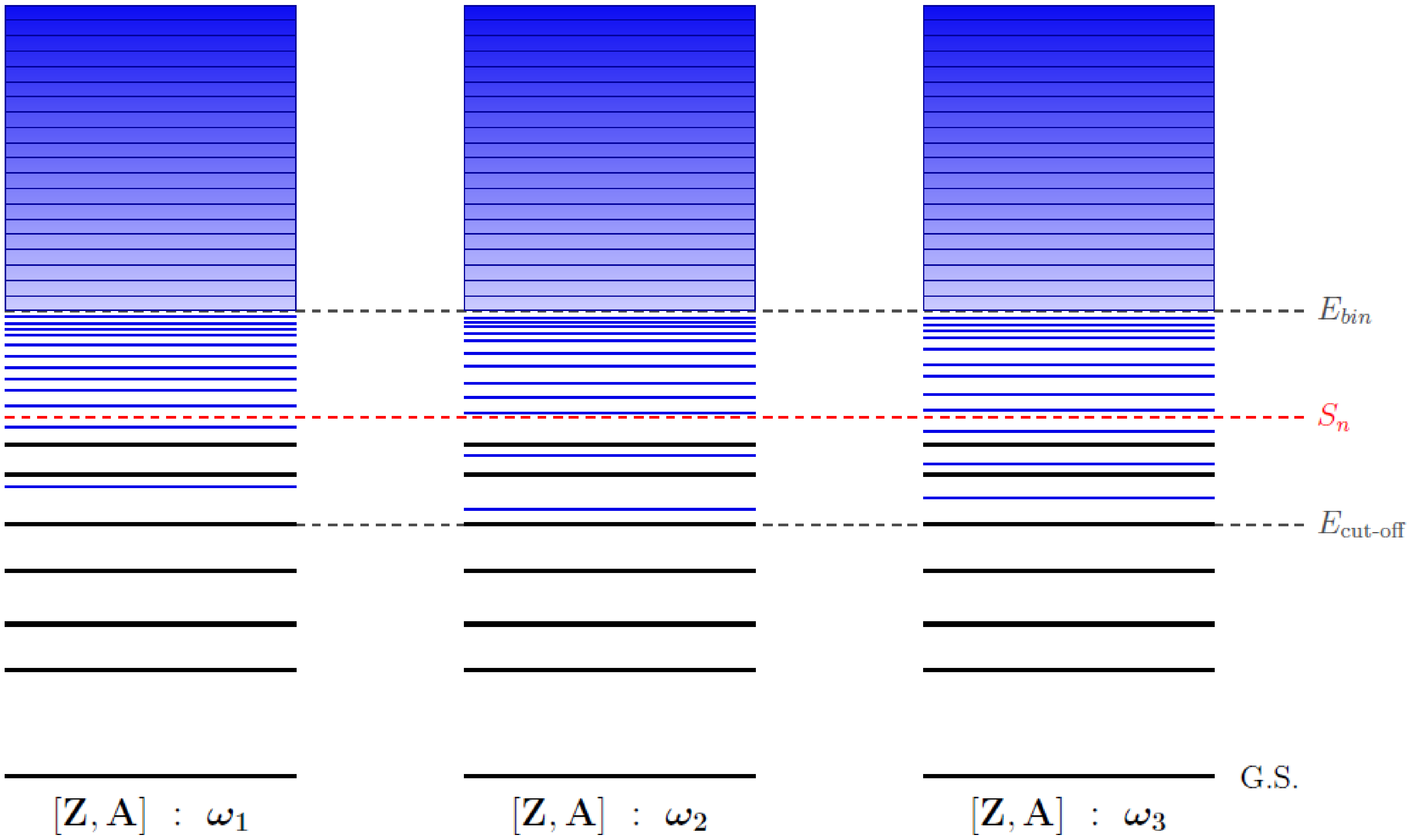
- Experimental nuclear level scheme (RIPL)
- Models of nuclear level density (CGCM, …)
- Models of γ strength function (EGLO, …)
- Neutron transmission coefficients (Koning-Delaroche, …)
- Internal conversion coefficients (BrIcc)

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

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



Multiple level scheme



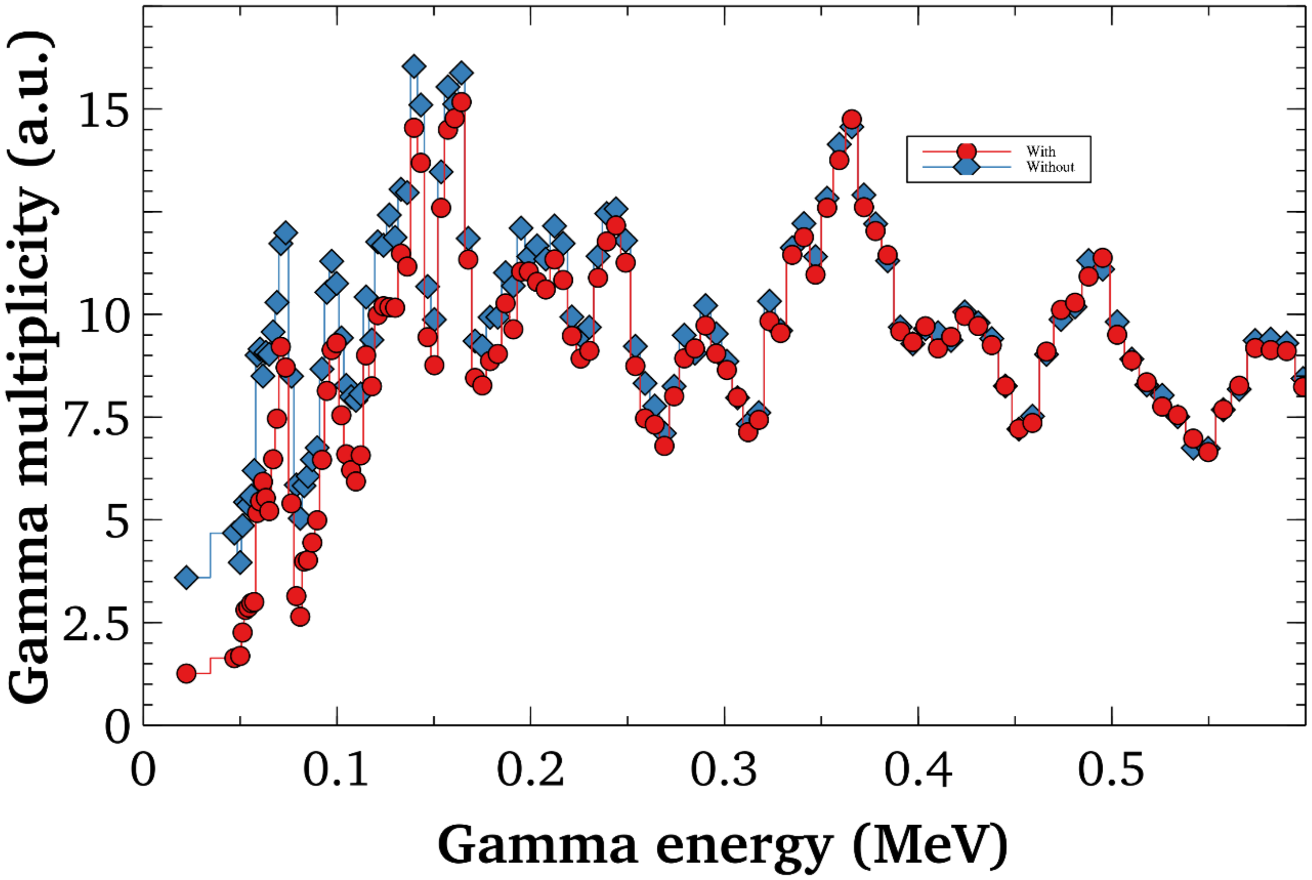
Generalization of electron emission

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

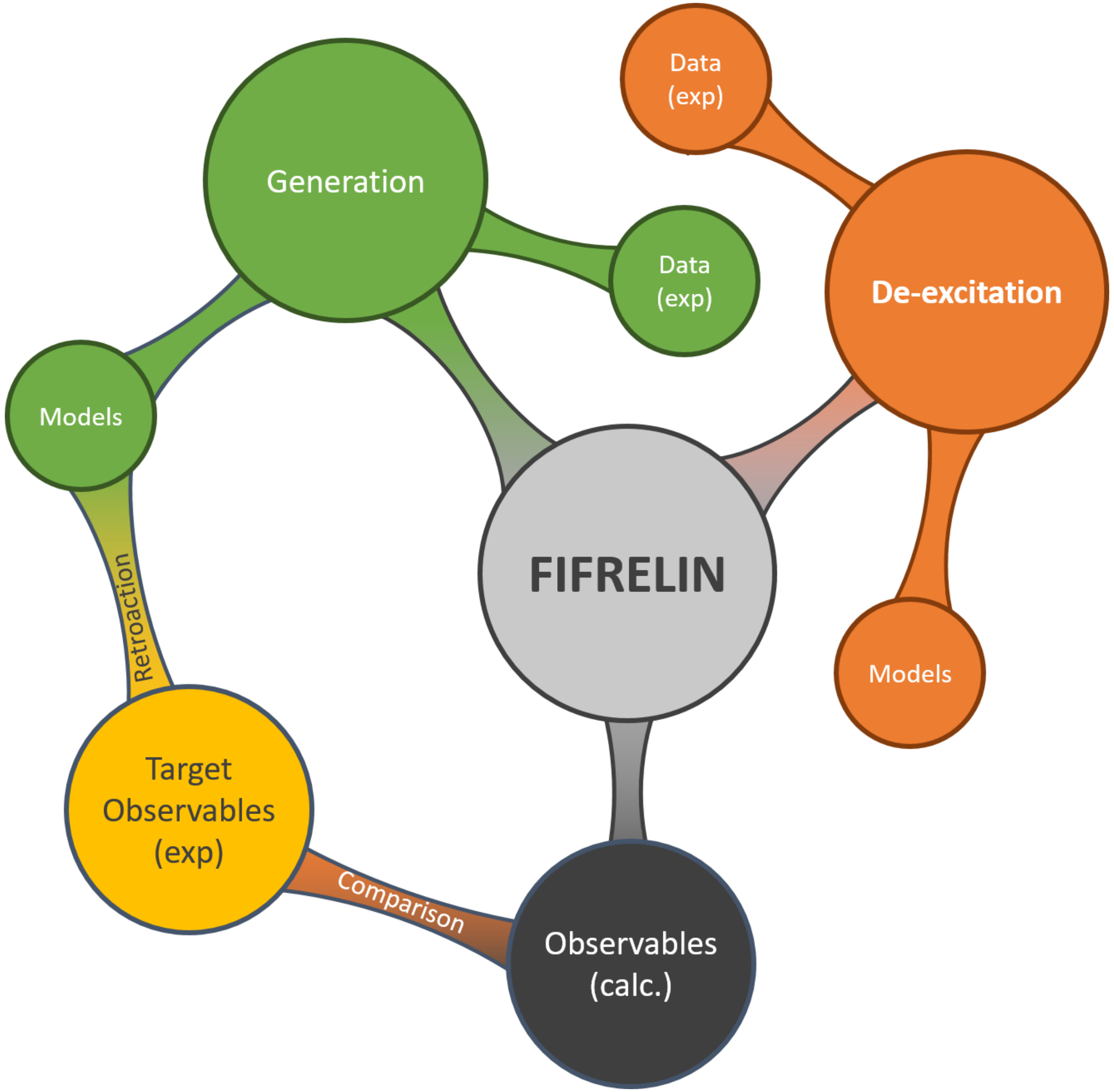
- Now, we have tabulated Internal Conversion Coefficient with BrIcc for
  - $Z = 5 - 110$
  - $E_\gamma = \epsilon_i + 1 - 6000\ keV$ (ϵ_i binding energy of electron on shell i (K,L,M …))
  - $E1 - E6$ and $M1 - M6$
  - Positrons can be emitted !

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

^{252}Cf



How FIFRELIN is working?

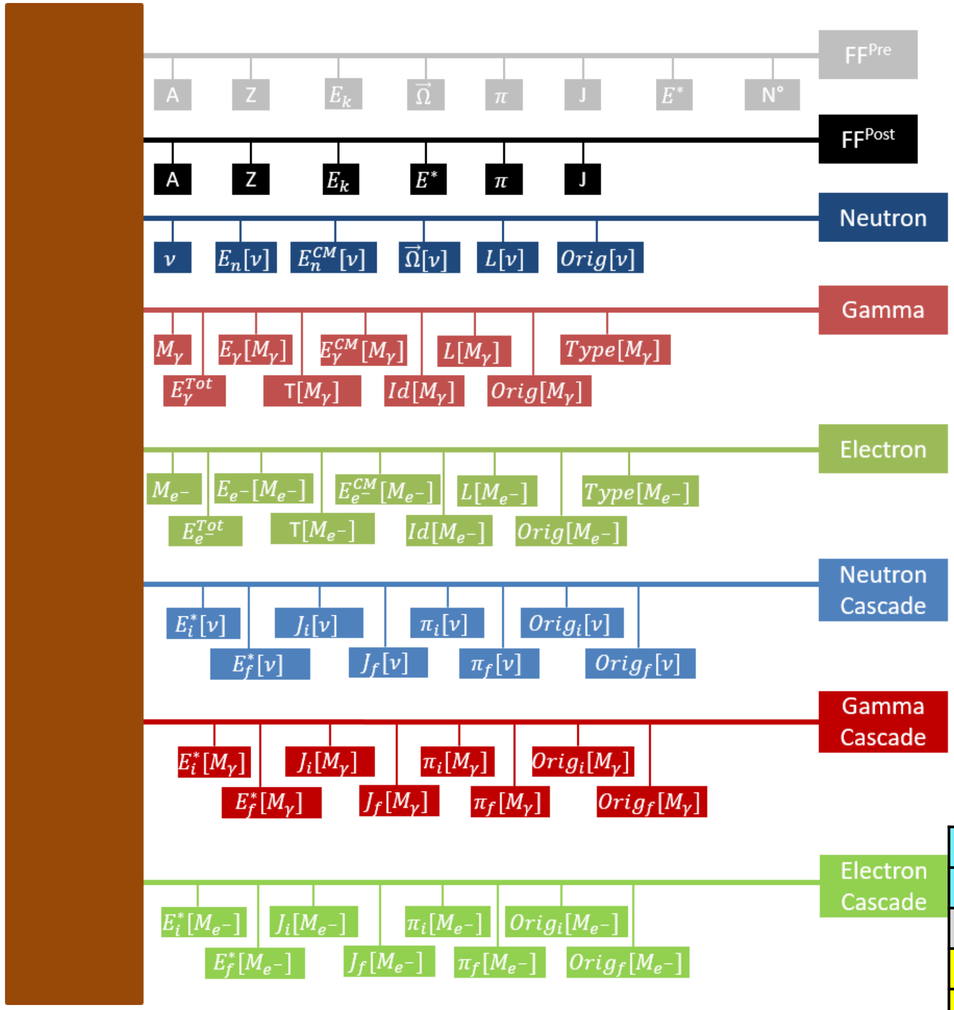


- 4 free parameters to determine excitation energy and angular momentum for each fragment
- Fixed against “target observables” : average neutron multiplicity (light/heavy if existing)

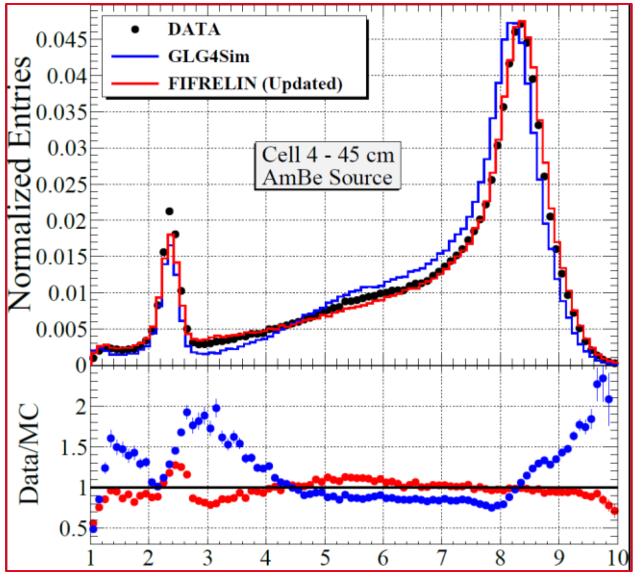
- Limitation : 4D space

Some practical information

- Developed in C++ since 2009
- Highly parallel (OpenMP+MPI)
  - Next step: GPU
- Executable available through NEA (very soon !!)
- 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)

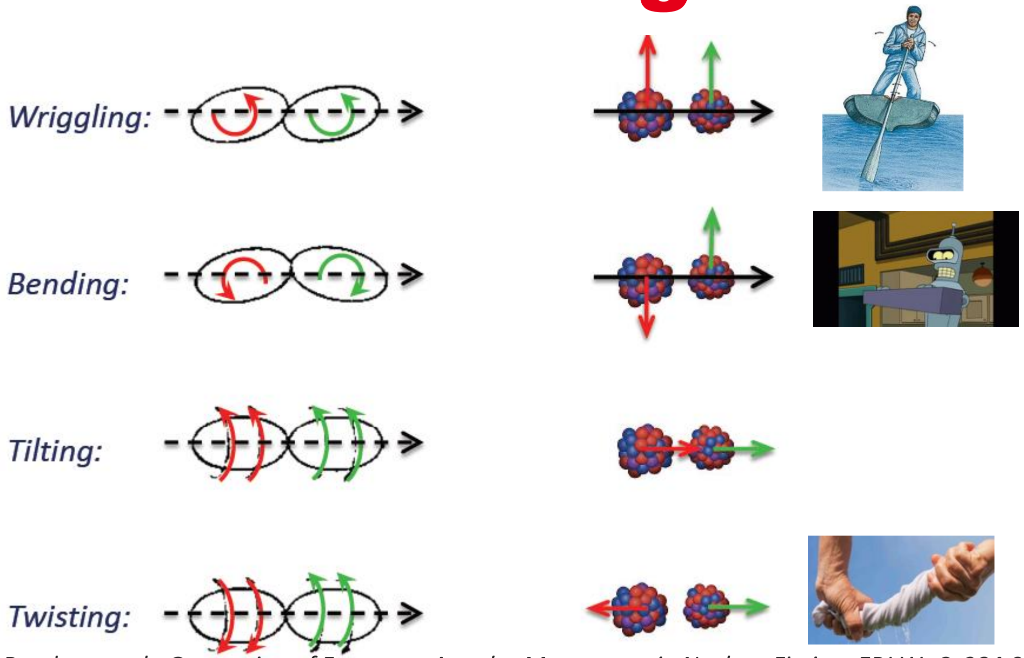


Gd156	(1- , 2-)
Gd158	(1- , 2-)
Al28	(2+, 3+)
Si29	1/2+
Si30	1- (direct)
Si31	1/2+
Na24	(1+, 2+)

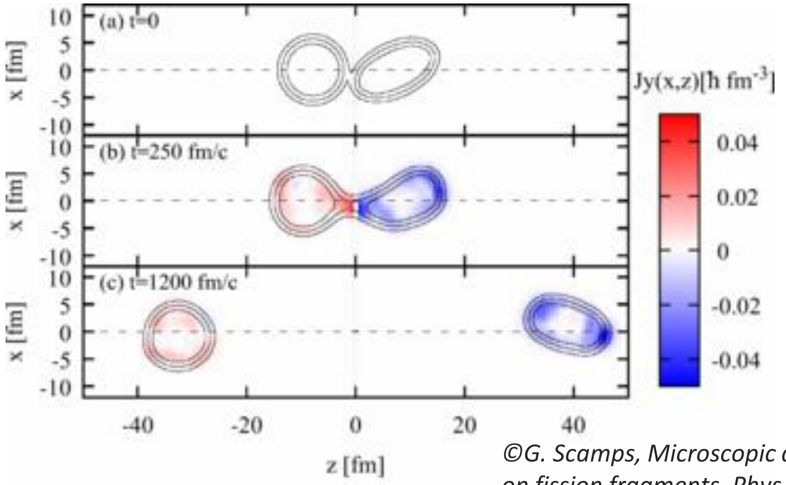
Ge71	1/2+
Ge73	1/2+
Ge74	(4+ , 5+)
Ge75	1/2+
Ge77	1/2+
W183	1/2+
W184	(0- , 1-)
W185	1/2+
W187	1/2+

2. Extraction of angular momentum with FIFRELIN

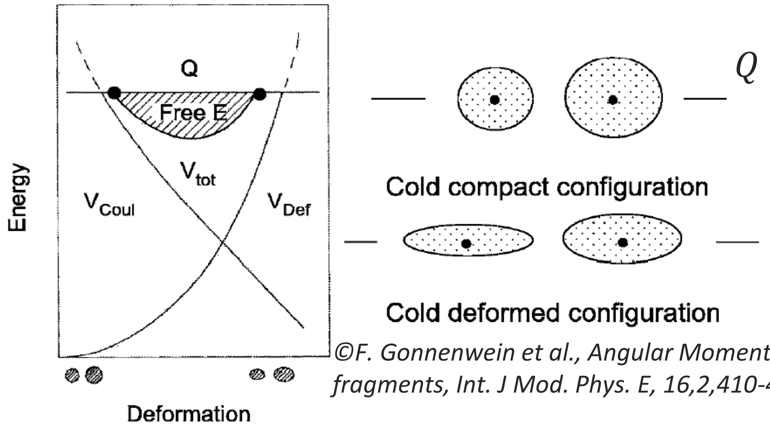
Focus on angular momentum generation



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

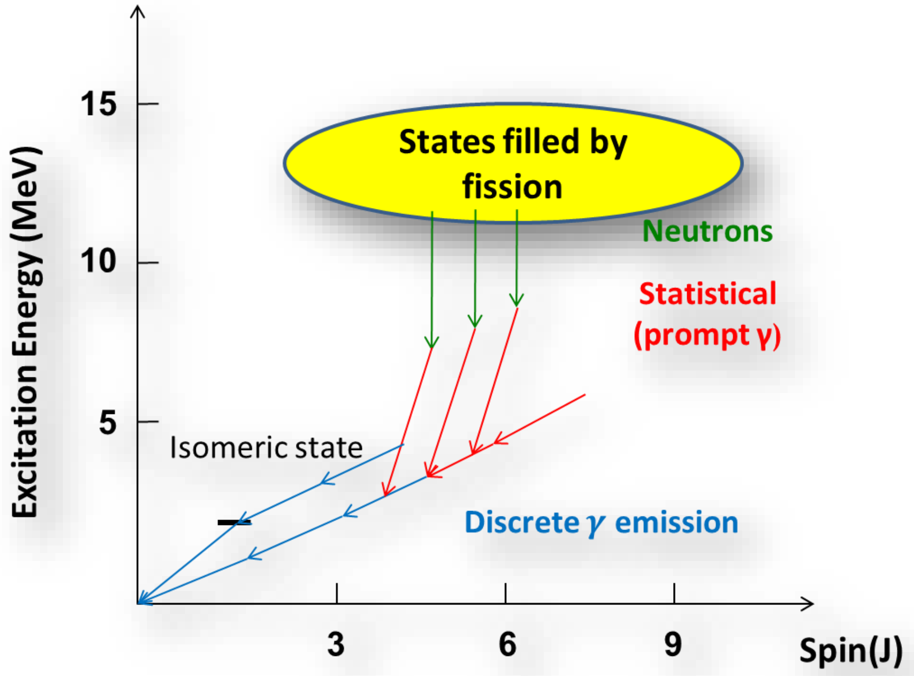


©G. Scamps, Microscopic description of the torque acting on fission fragments, Phys. Rev. C 106, 054614 (2022)

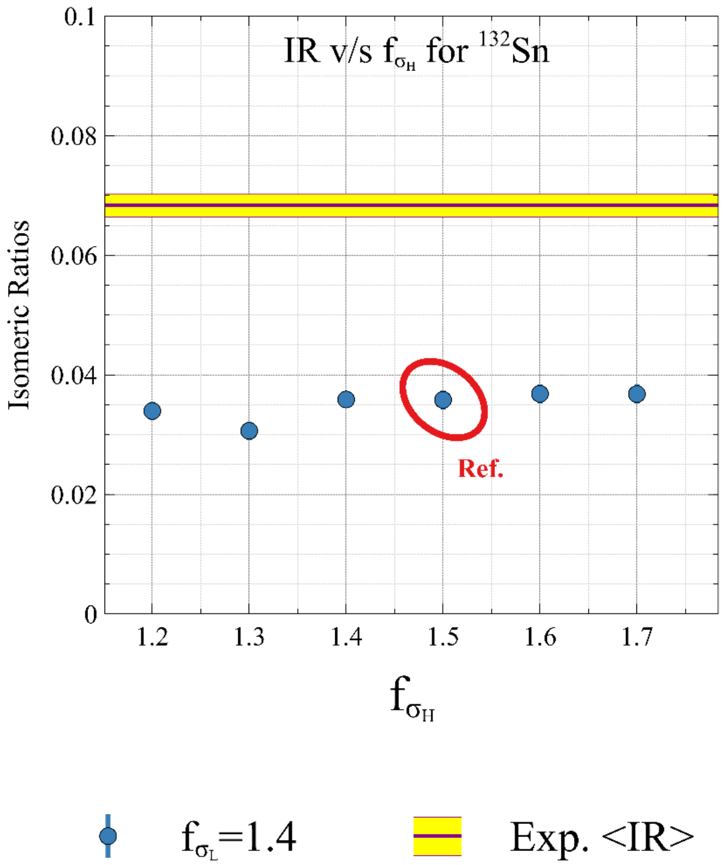


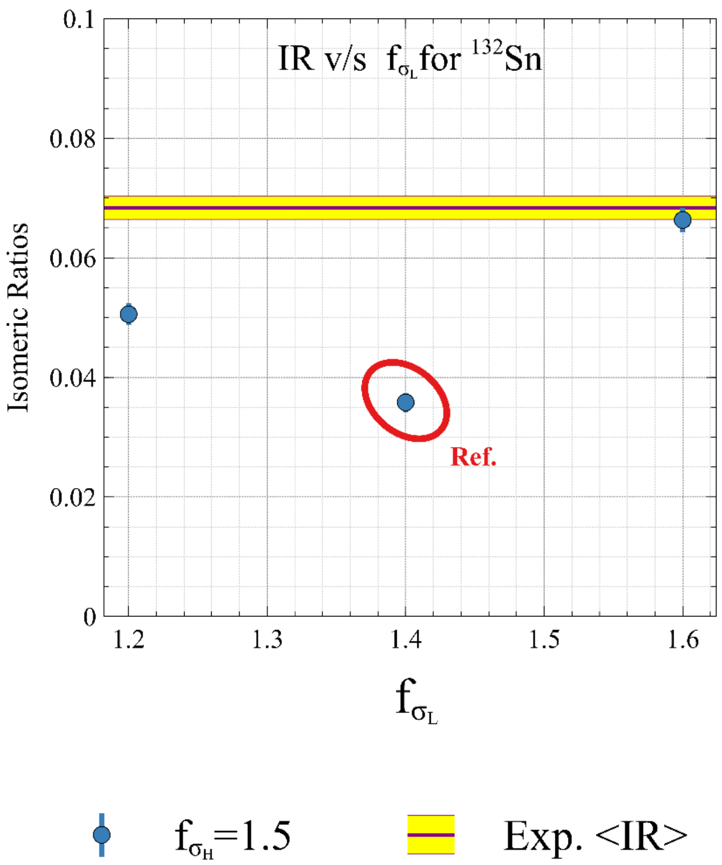
$$Q = E_{int} + V_{Coul} + V_{Def}$$

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



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}
- Can be explained by nucleons exchange at scission (TDHFB) → role of deformation energy?
- Thermal excitation ?
- Role of the rotational energy in the total energy excitation sharing ?
- Correlation between both fragments arise naturally !

Direct determination of angular momentum with FIFRELIN decay

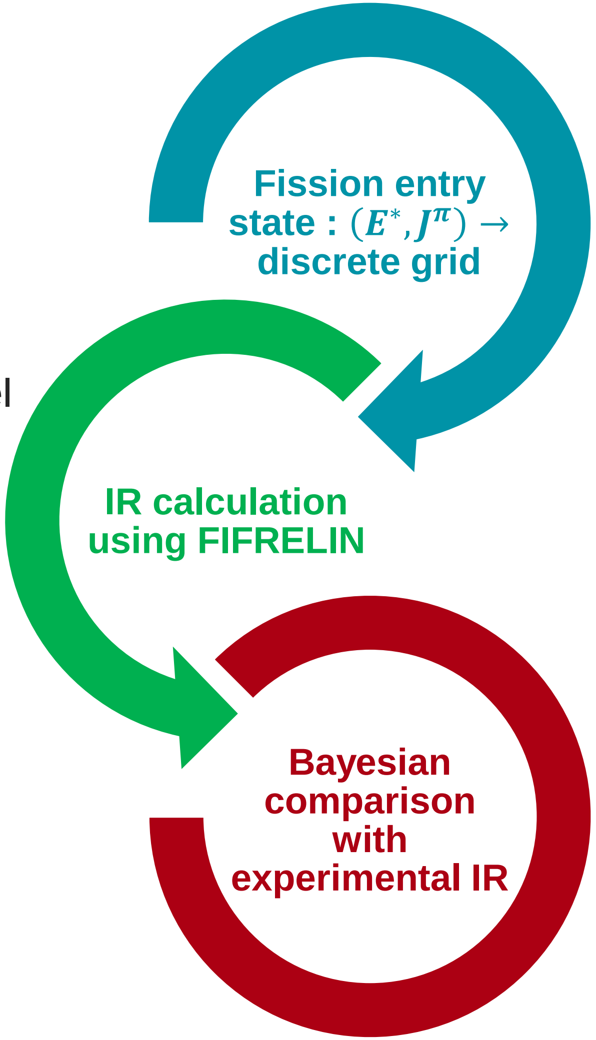
In this work, FIFRELIN (developed by CEA Cadarache) is used **only as a nuclear de-excitation code (step 2)**

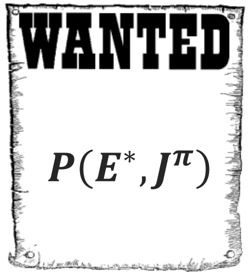
What is required for FIFRELIN :

- 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)

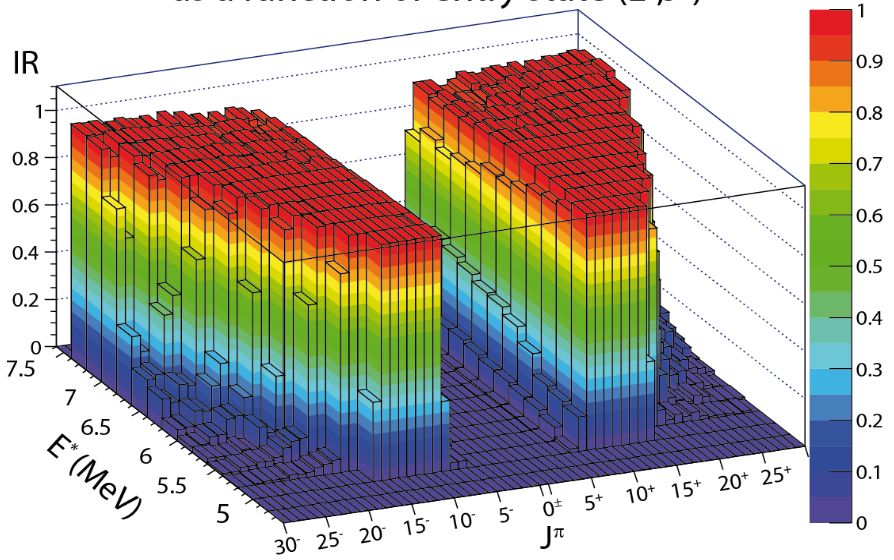
For comparison with experimental results standard spin distribution:

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

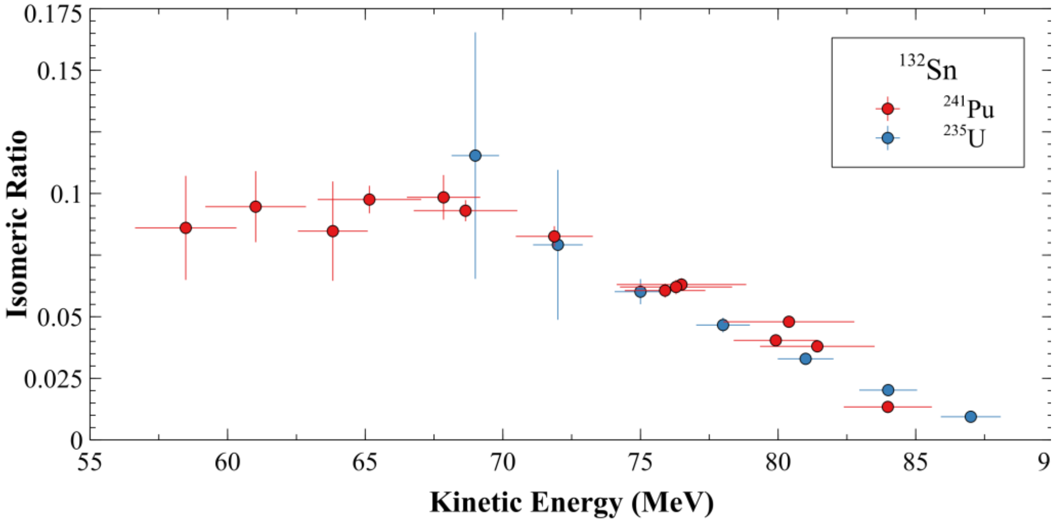


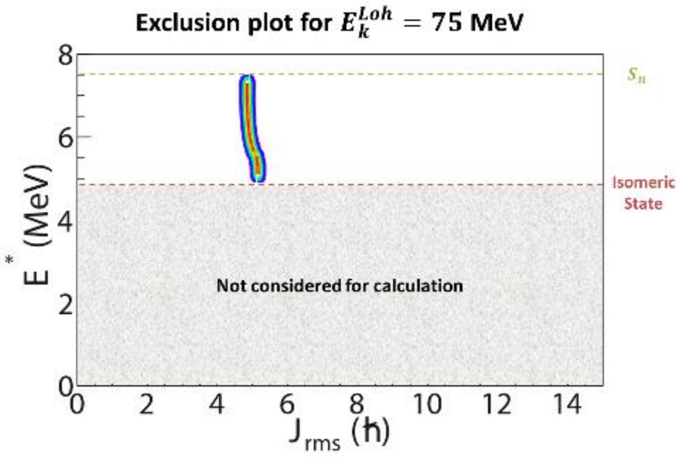


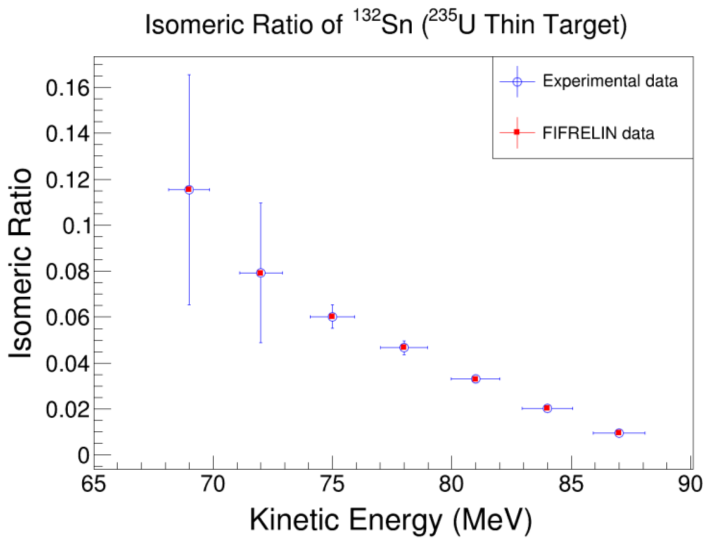
Isomeric Ratio calculated by FIFRELIN as a function of entry state (E^*, J^π)

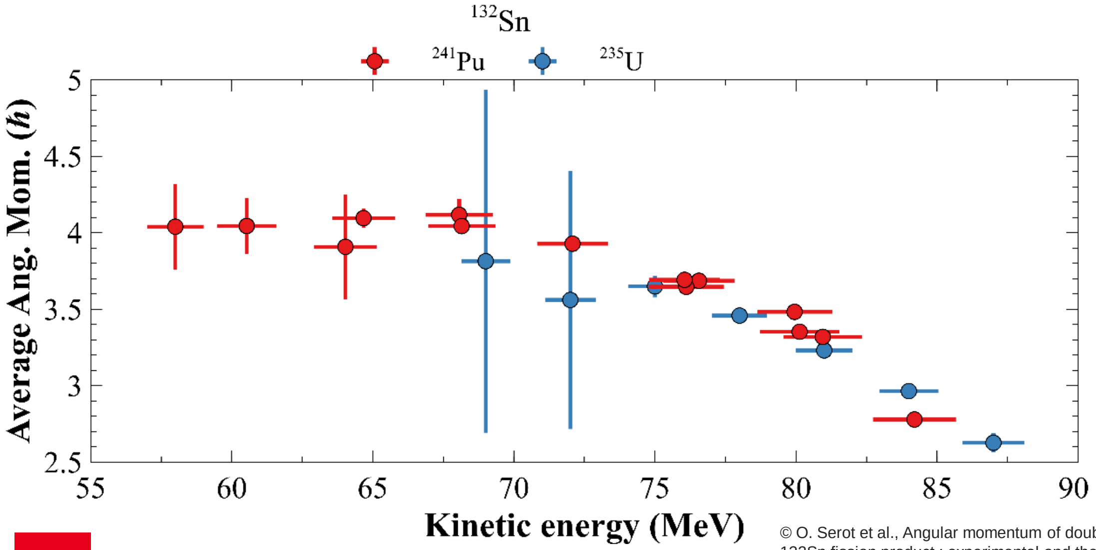


Synthesis on ^{132}Sn work







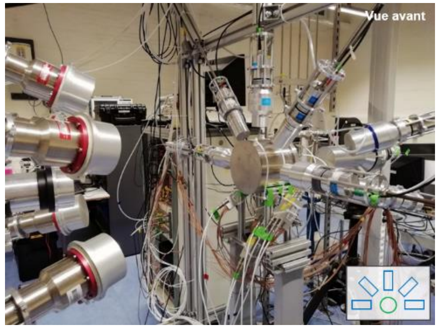


© O. Serot et al., Angular momentum of doubly magic 132Sn fission product : experimental and theoretical aspects, EPJ WoC, 284, 04022 (2023)

- 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 ?

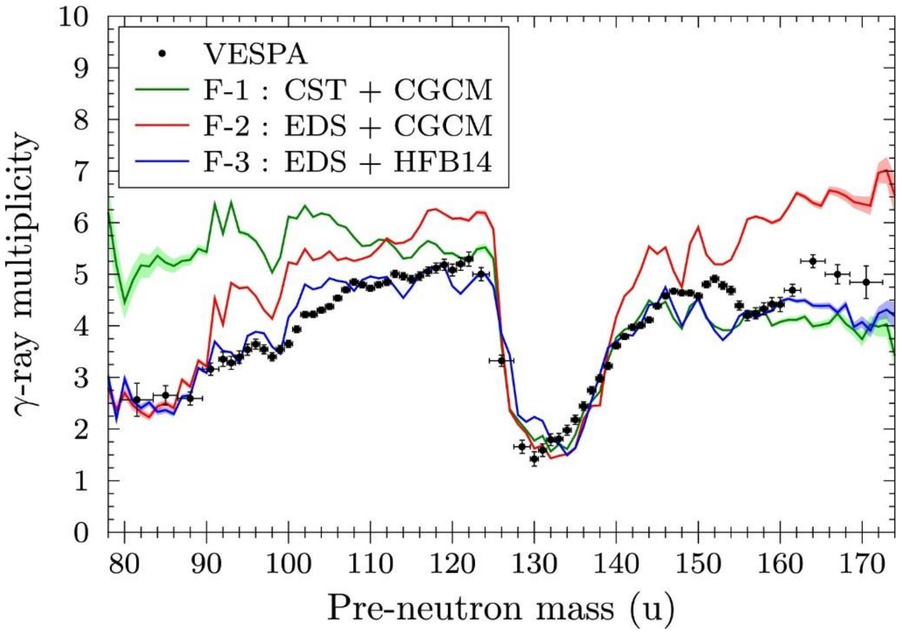
Interpretation using FIFRELIN for prompt γ-rays

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]

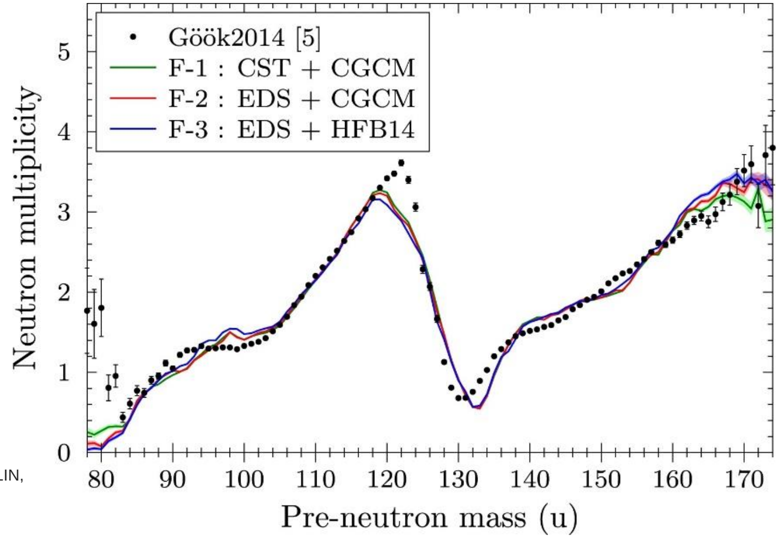


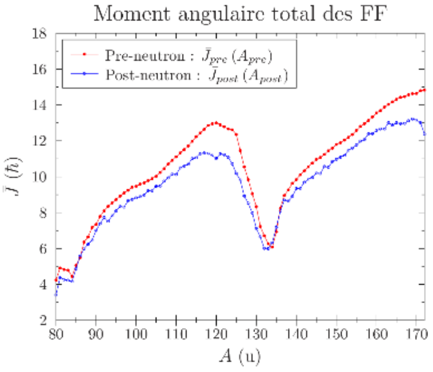
VESPA setup @JRC-Geel

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



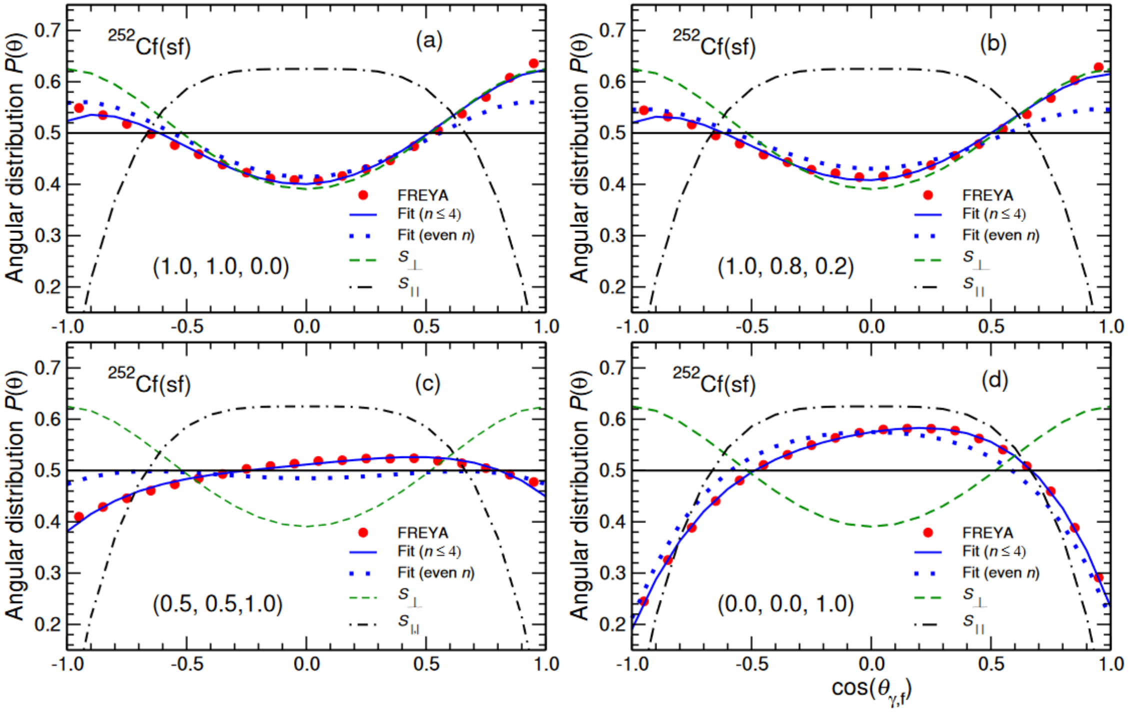
- F3 is the best combination of models
- Sawtooth behavior seems to raise from energy dependent model
- The scaling is better using HFB14 instead of CGCM level density





To go further : angular correlation !

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



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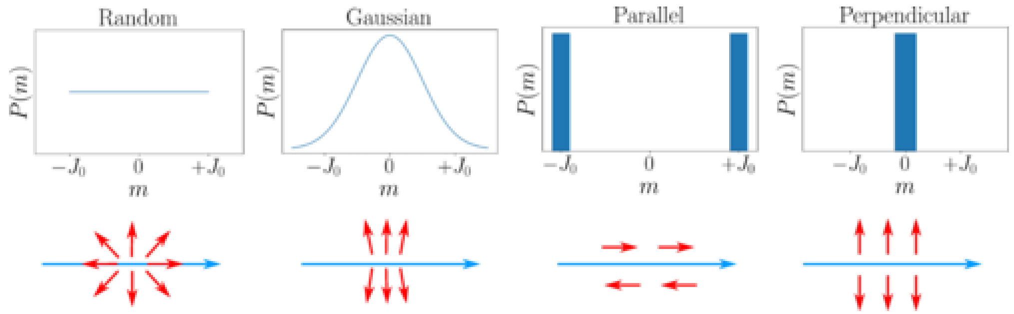
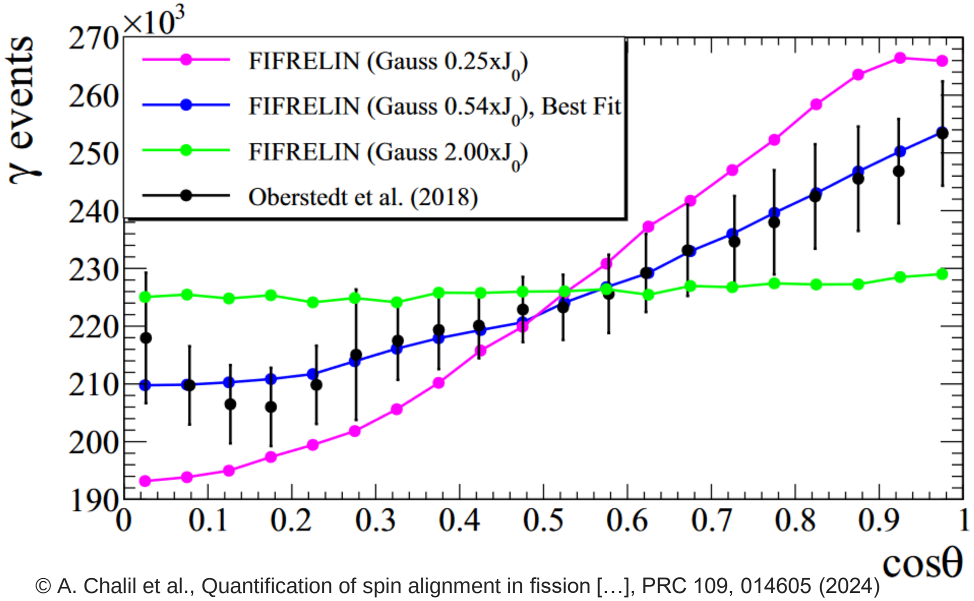


Mix + motion + neutron emission

Twisting/Tilting

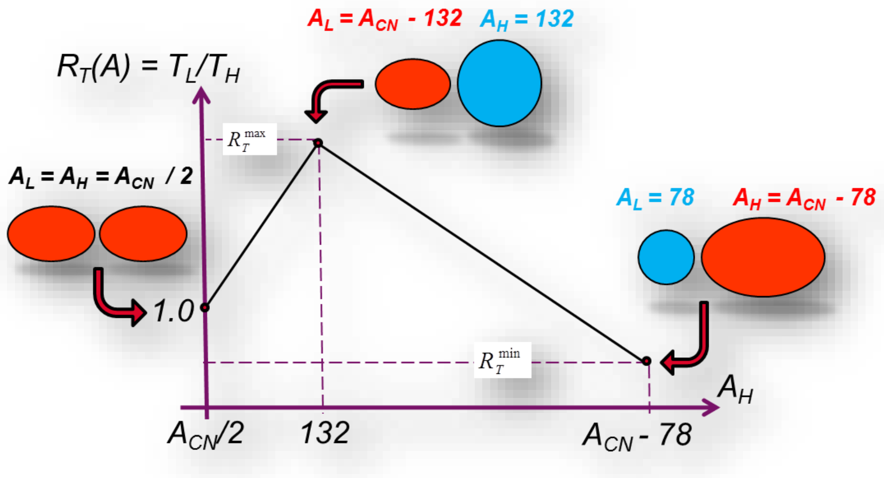
Wriggling/bending

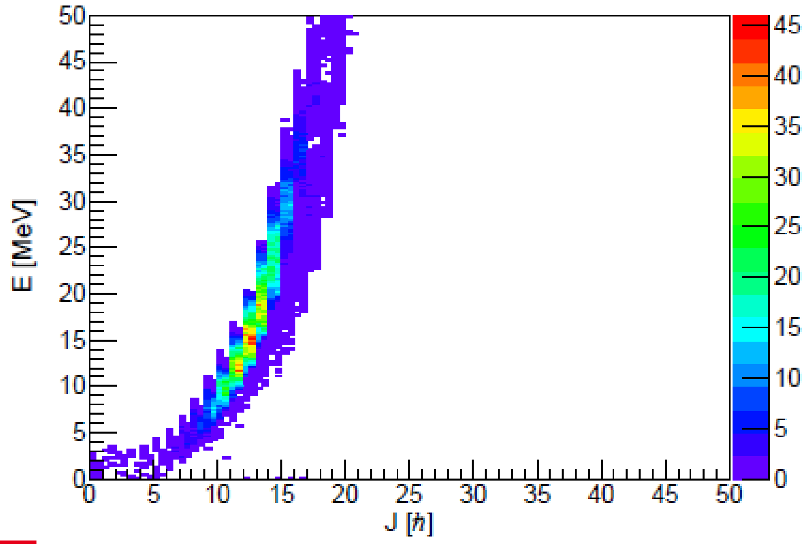


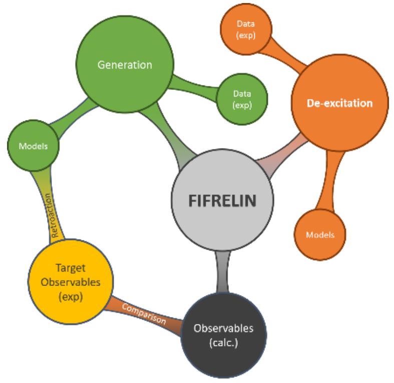
© A. Chalil et al., Quantification of spin alignment in fission […], PRC 109, 014605 (2024)

3. On going developments

Machine Learning with FIFRELIN





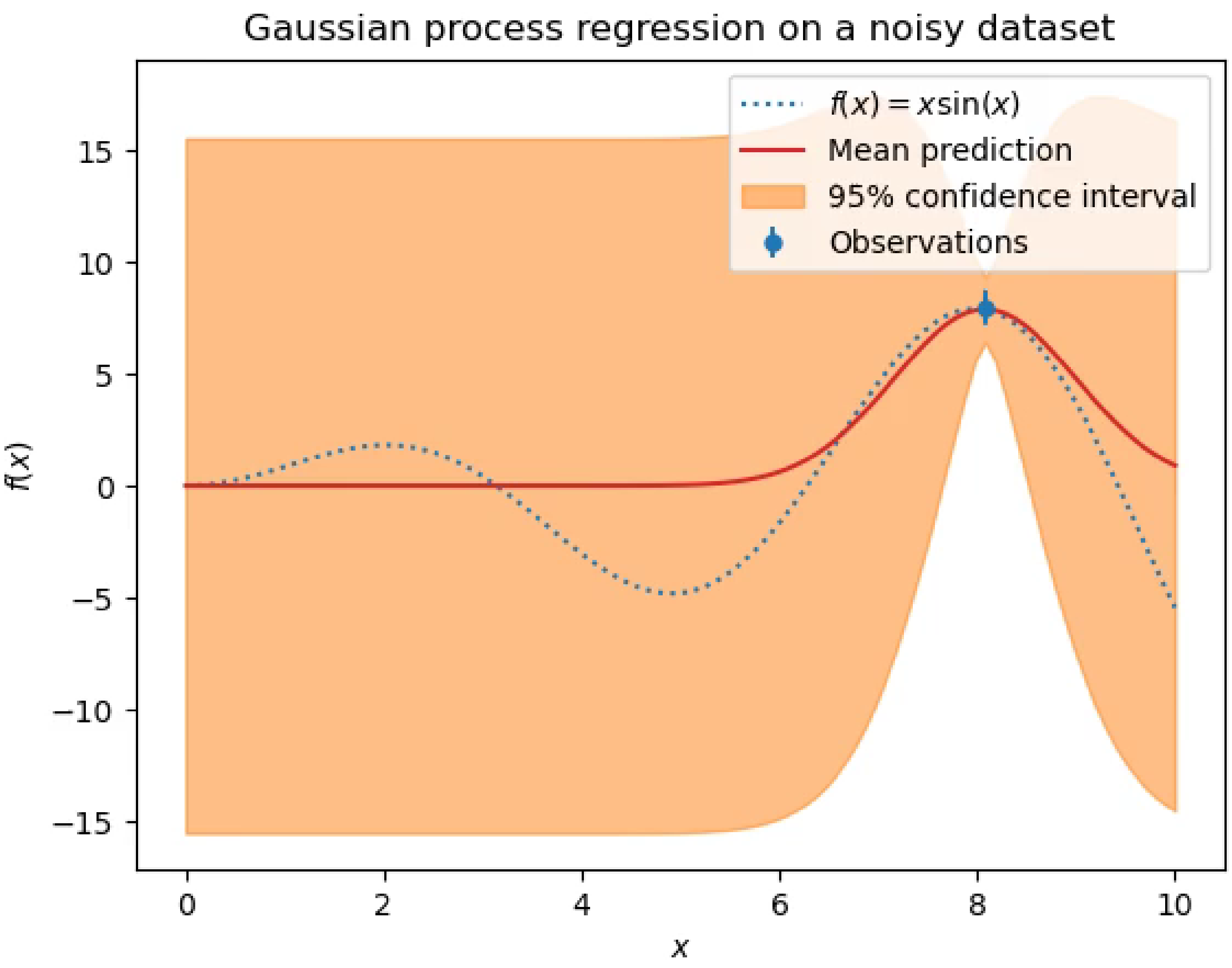


How to determine these 4 parameters ?

- 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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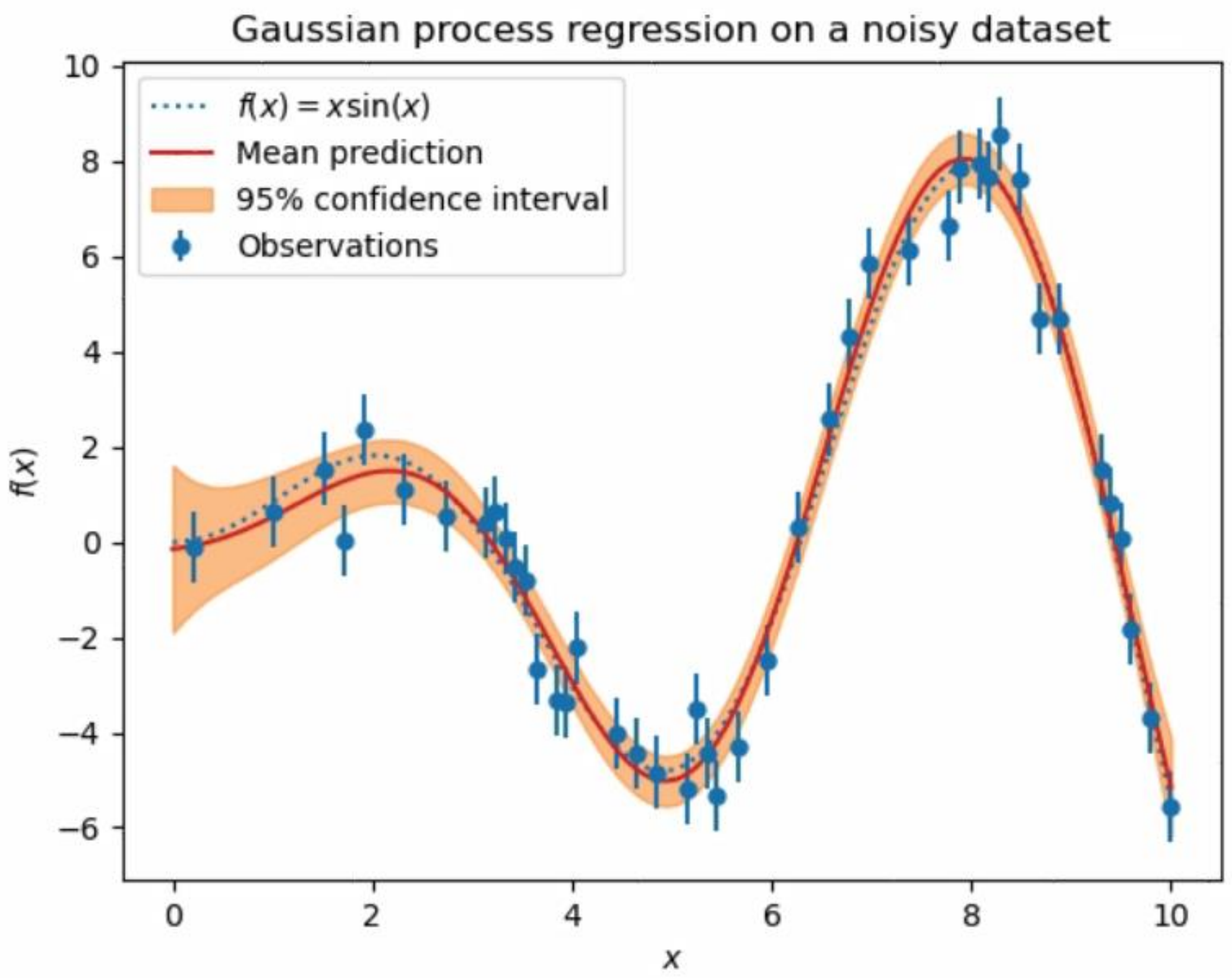
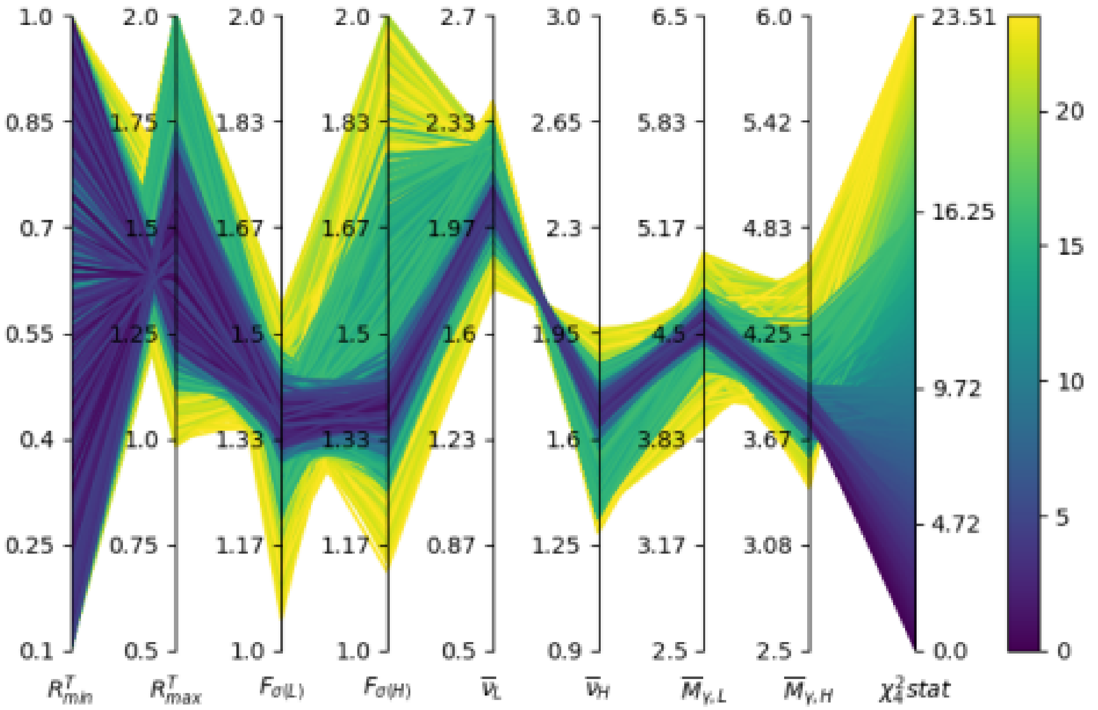
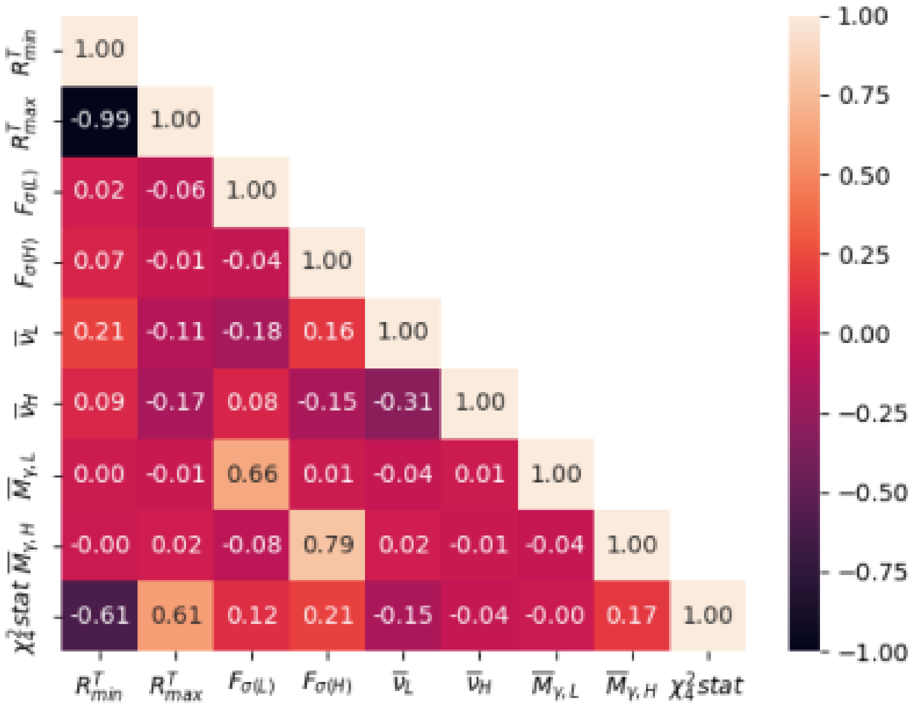


Some results





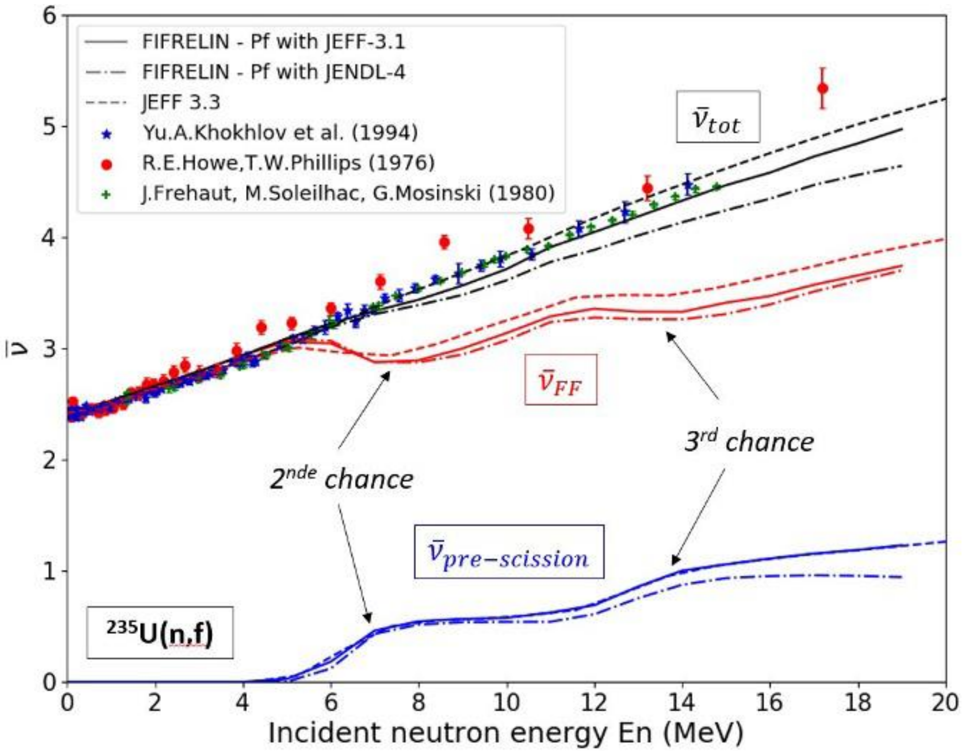
© G. Bazelaire et al., Assimilating fission-code FIFRELIN using machine learning, EPJ Web of Conf. 294,03002 (2024)

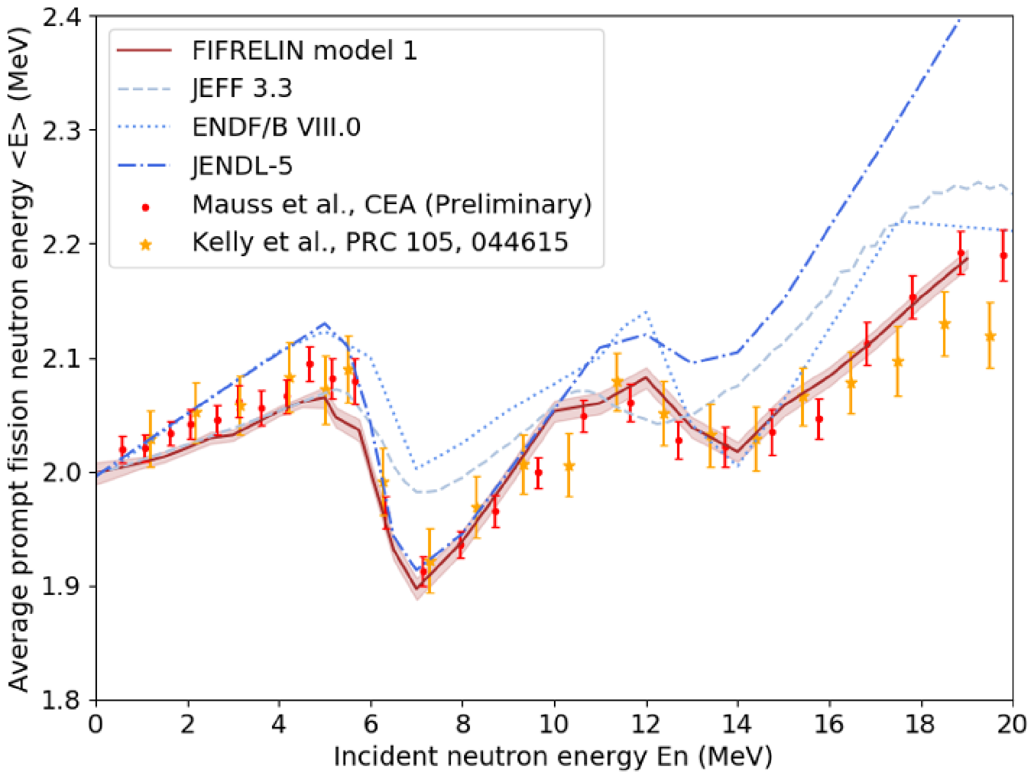
- Target : $[\overline{\nu_L}, \overline{\nu_H}, \overline{M_{\gamma_L}}, \overline{M_{\gamma_H}}] = [2.06, 1.70, 4.56, 3.82]$
- In 2h, from scratch, we found an optimum : $[RT_{min}, RT_{max}, f\sigma_L, f\sigma_H]$ = [0.18,1.58,1.38,1.37] thanks to 100 simulations

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 bellow)
- Analog : calculation of fission width based on Hill-Wheeler formula + competition with other channels (neutron/γ)



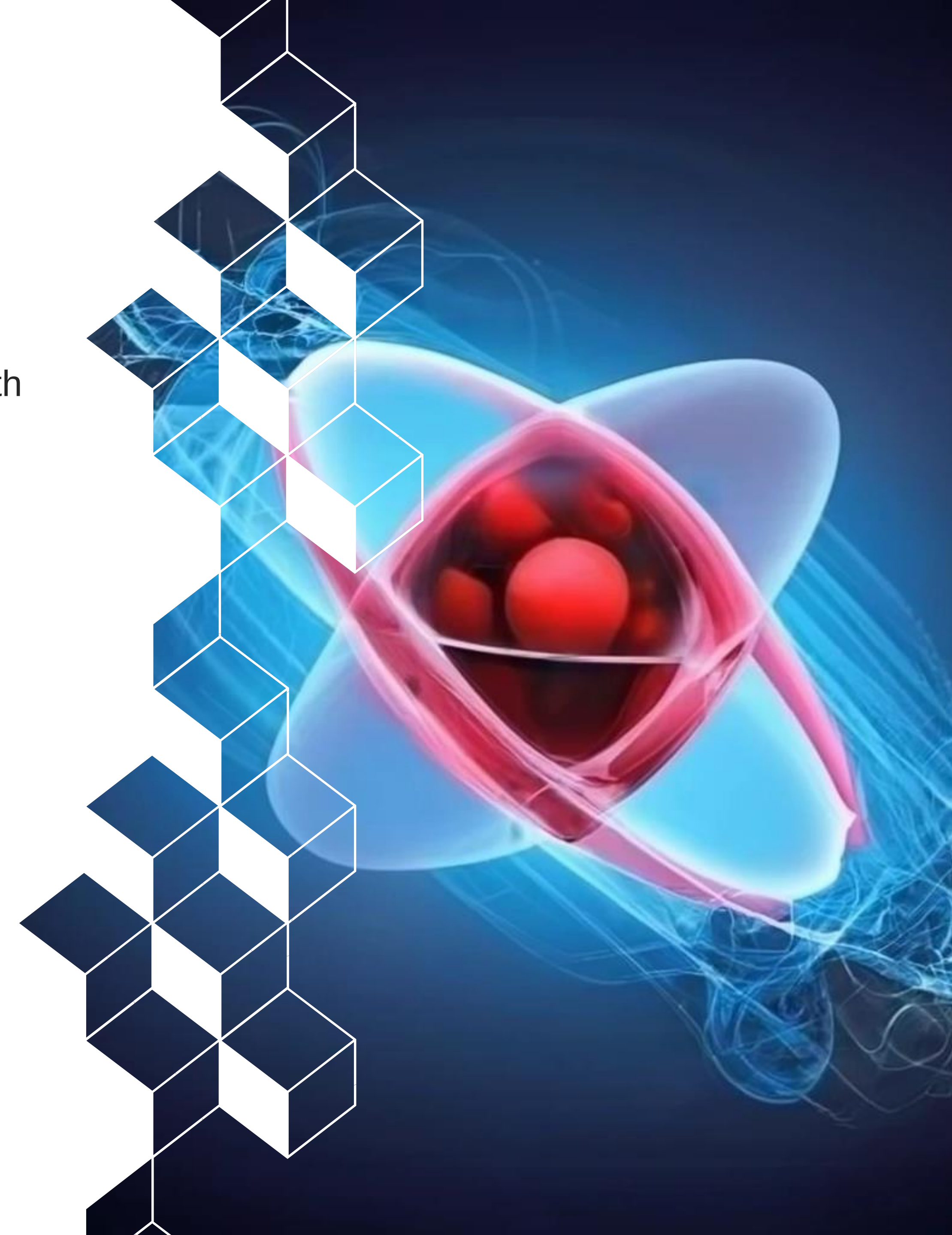


© M. Sabathé et al., Implementation of a multi-chance fission model in FIFRELIN for 235U(n,f) reaction, EPJ Web of Conf. 294,03001 (2024)

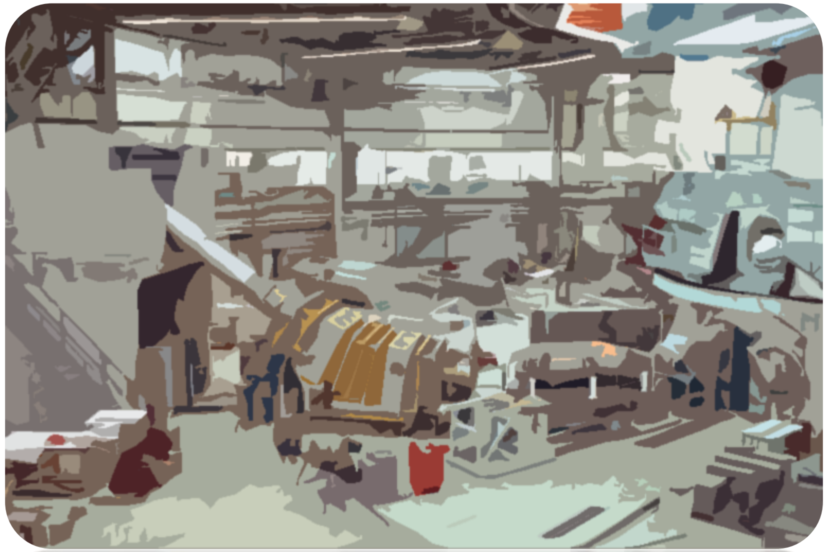
Conclusions

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 go expand the range of applications of FIFRELIN + more complex initial modelling
- Multi-chance fission implemented in the code
- FIFRELIN will be soon available, stay tuned !



Thank you for your attention



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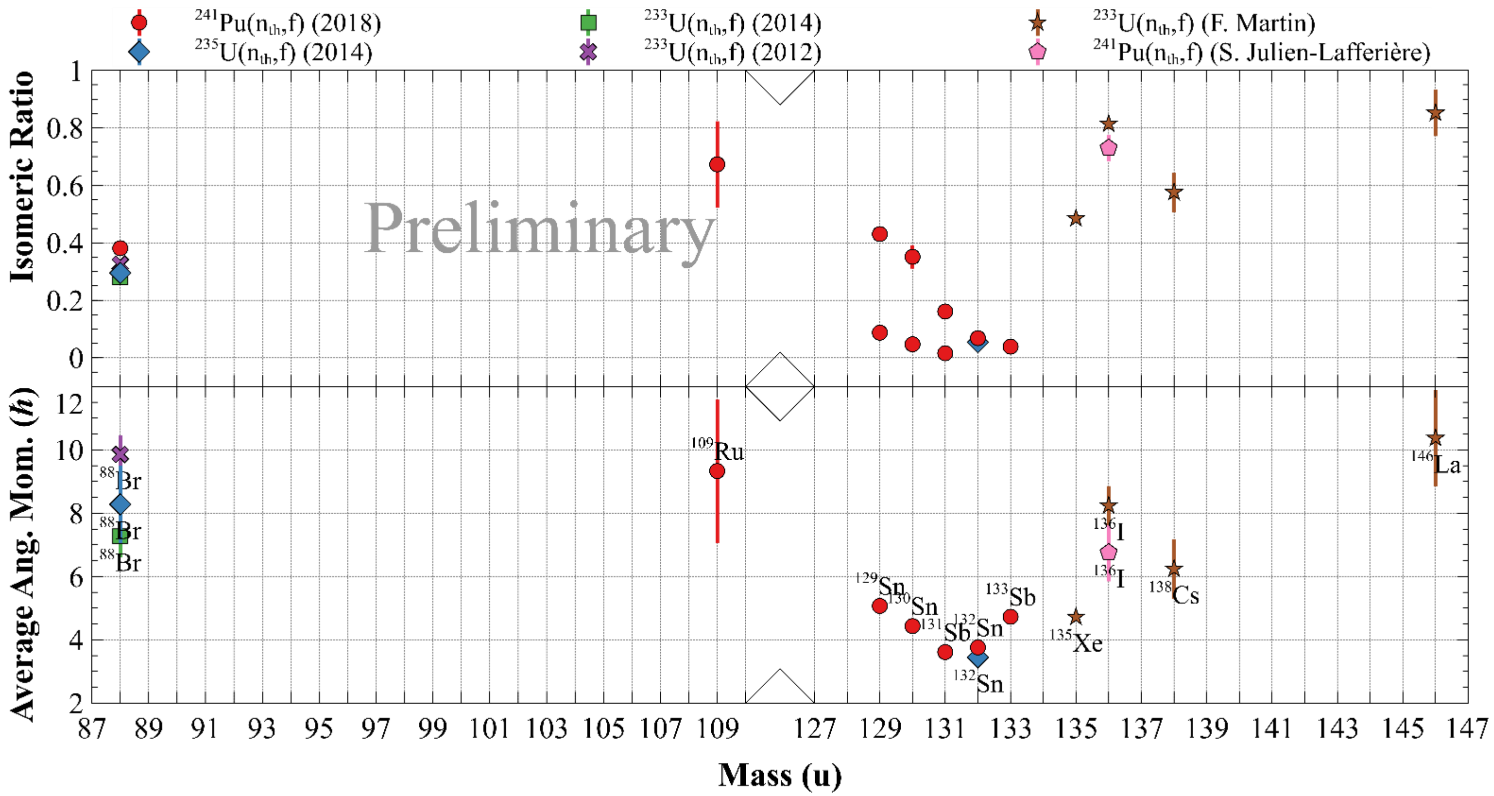
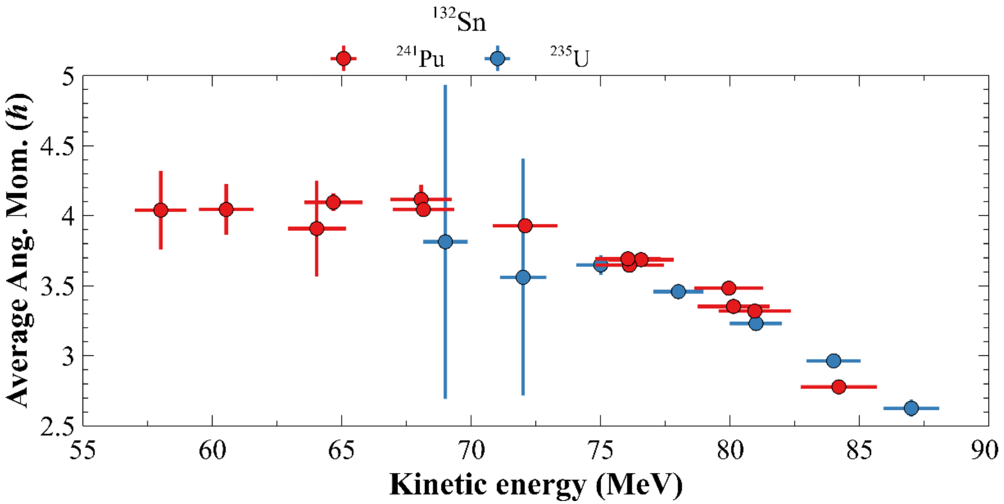
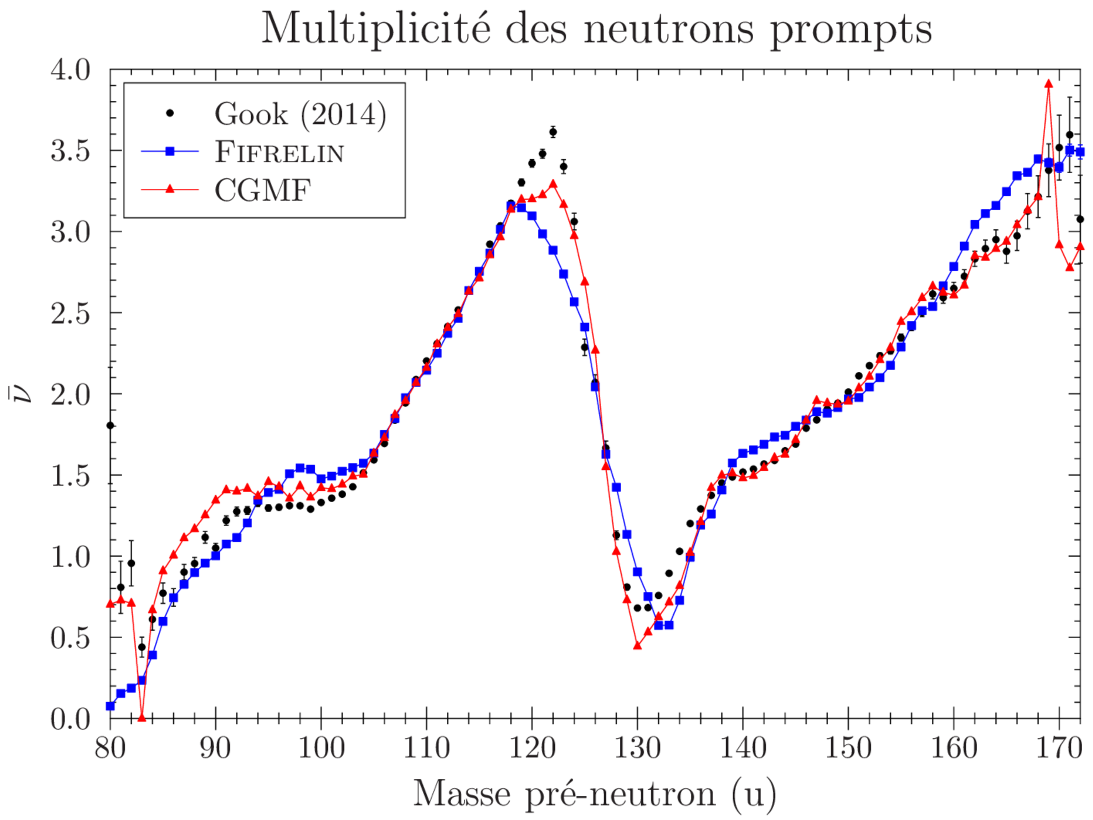
Synthesis

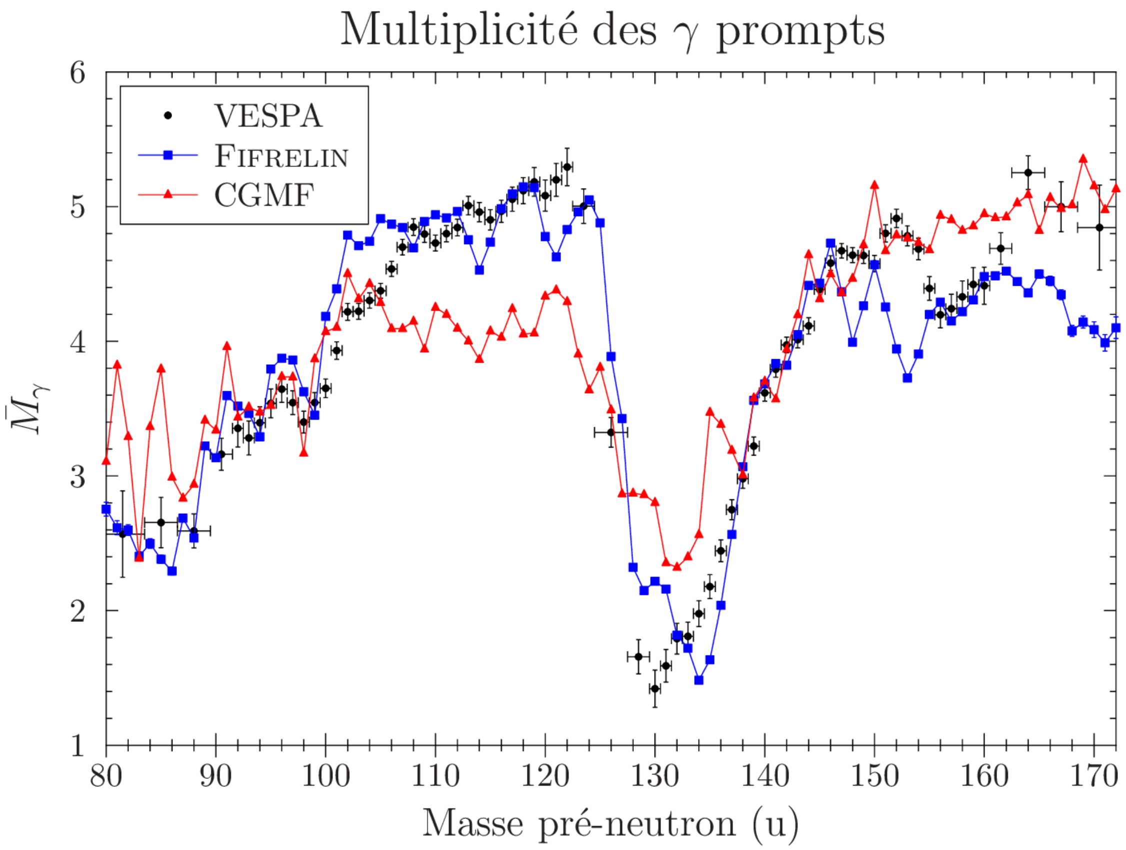




- Isomeric ratios : probe for fission fragment angular momentum
- **Dependency of the derived average angular momentum with the fission fragment kinetic energy**
- Next step : measurement in the light fragment region (part of a thesis 2025-2028)

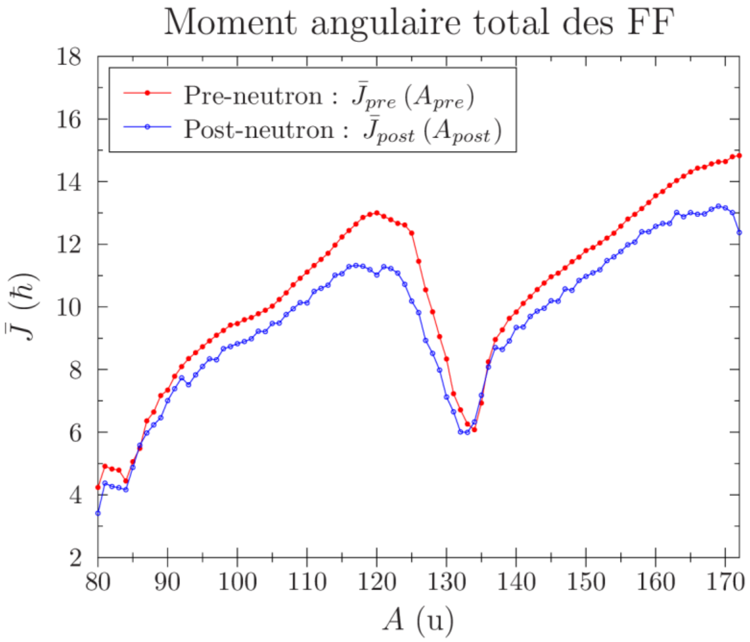
Comparison with CGMF

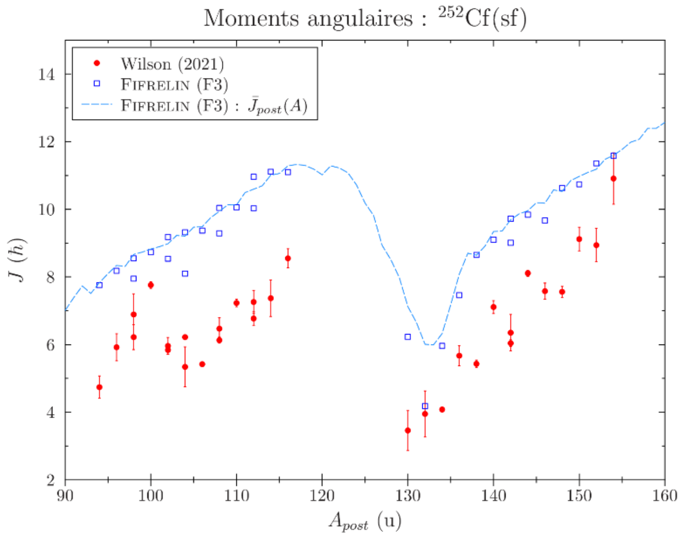


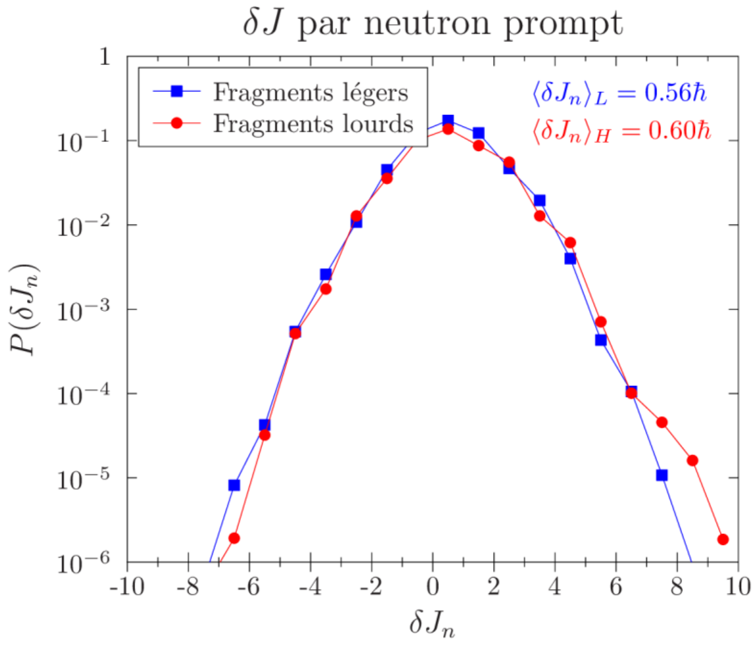


Others

	Light Fragment	Heavy Fragment
Pre-neutron	$\langle J \rangle_L = 10.79\ \hbar$	$\langle J \rangle_H = 10.57\ \hbar$
Post-neutron	$\langle J \rangle_L = 9.61\ \hbar$	$\langle J \rangle_H = 9.39\ \hbar$







Excitation Energy, Multiplicity, Temperature