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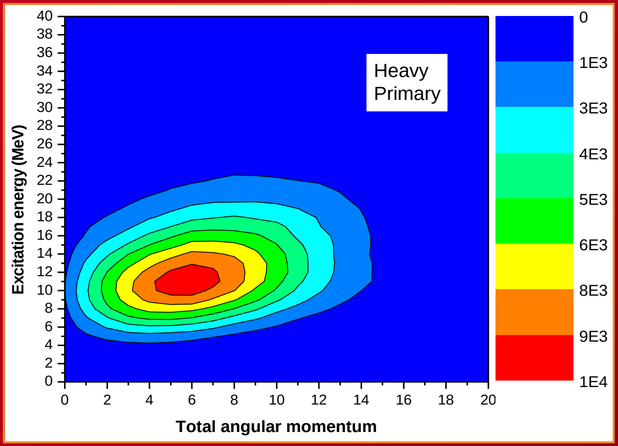

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Modeling fission in FIFRELIN

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P(ND)²-2 Perspectives on Nuclear Data for the Next Decade,
14-17 october, 2014, BIII, France

- **Context**
- Models in FIFRELIN
- Fission observables: comparison with experiments
- Beyond common observables
- Perspectives

Codes for simulating fission fragment de-excitation

- **Madland-Nix** model @ LANL, USA (*neutrons / PFNS + Nubar)* 1982
- **Point-by-Point** model @ Bucharest Univ., Romania (extended MN+) ~2000
- **GEF** code @ CENBG, France (*from CN to Fiss. Obs.*) ~2010
- **CGMF** code @ LANL, USA (Fiss. Obs. / -W or -*HF* model) ~2005
- **FREYA** code @ LLNL, USA (Fiss. Obs. / -*W* model) ~2010
- **FIFRELIN** code @ CEA, France (Fiss. Obs. / -*W* or -*HF* model) ~2010

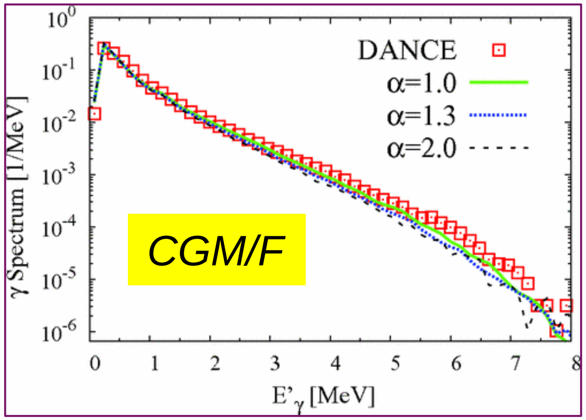
Deterministic + Monte Carlo (GEF, CGMF)

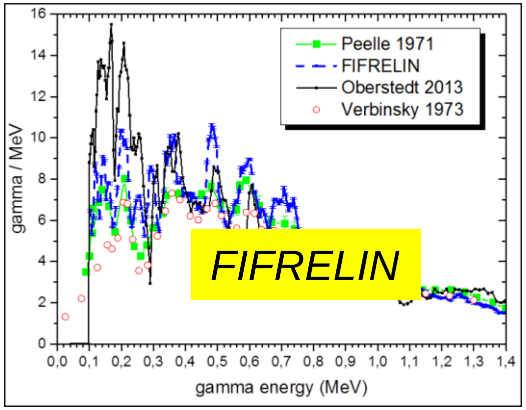
Monte Carlo (FREYA, FIFRELIN)

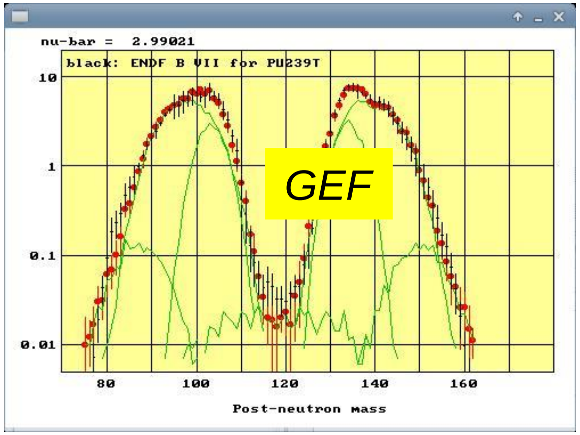
- ✓ Monte Carlo method was used at the end of the 1950's to simulate the de-excitation of hot nuclei (high energy, high spin) : *Dostrovsky et al., Phys. Rev.* ***111****, 1659 (1958), Phys. Rev.* ***116****, 683 (1959), Phys. Rev.* ***118****, 781 (1960), Phys. Rev.* ***119****, 2098 (1960)*.
- ✓ Application to fission in the 1960's 1970's: *Gordon et al. Phys. & Chem. of Fission, vol. II, 73 (1965)*, *Gavron, Nucl. Instr. Meth.* ***115****, 93 (1974), 99 (1974)*.

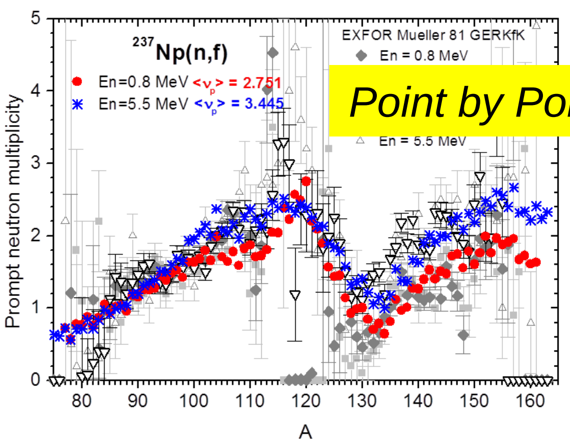
Main contributions of Monte Carlo codes

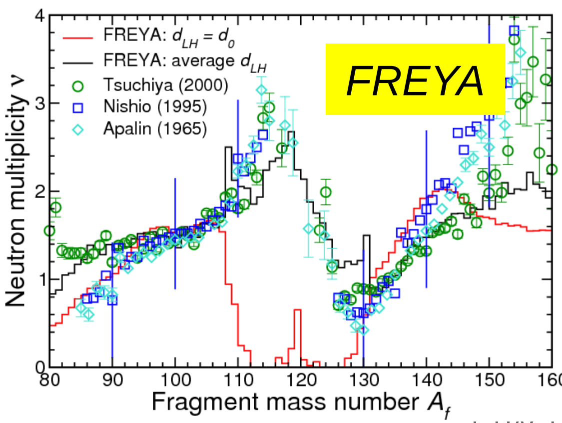
- Distributions, correlations between fission observables,
- Complete and consistent set of calculated fission observables: neutron spectra and multiplicities as well as gamma spectra and multiplicities in addition of prompt energy release, post neutron yields, …











- Context
- **Models in FIFRELIN**
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Definitions

- Prompt emission : before β^- decay
- Prediction : By establishing the '*as better as possible*' calculation scheme (models, model parameters, hypothesis…) we can reproduce some given 'target observables' (global quantities, e.g. $\overline{\nu_L}$, $\overline{\nu_H}$) and then look at other ones (predicting them):

  $P(\nu)$, $P(M_\gamma)$, $\overline{\nu}(TKE)$, …

Hypothesis

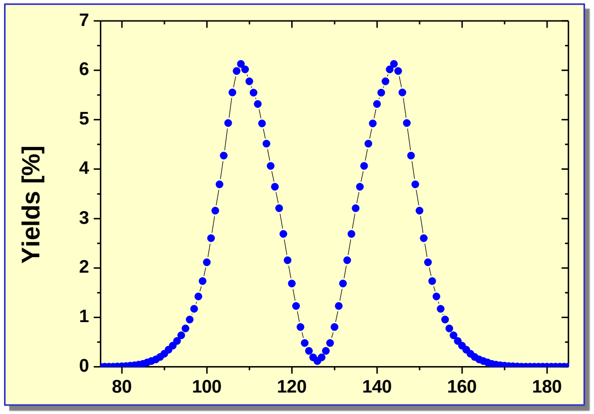
- Binary Fission
- n/γ/e$^-$ emission after FF full acceleration (fragments have recovered their gs deformation)
- NEDA (*A. Matsumoto et al., J. of Nucl. Sc. and Tech. 49, 782 (2012)*) *not accounted for.*
- SN (*N. Carjan et al., Phys. Rev. C 85, 044601 (2012)*) *not accounted for.*

Fission Fragment characteristics sampling

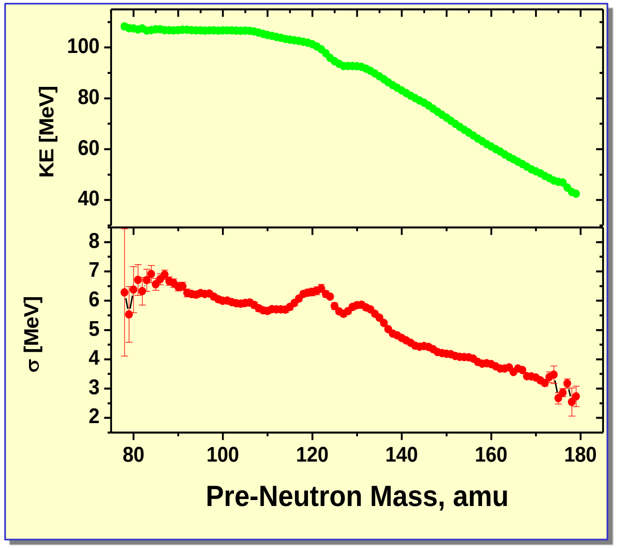
1. Mass (*A*)
2. Kinetic Energy (*KE*)
3. Nuclear Charge (*Z*)
4. Spin, Parity (J^{π})
5. Excitation Energy (*E**)

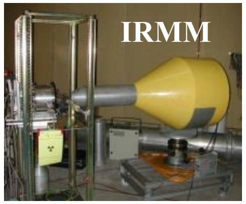
can be reconstructed from a set of fission mode parameters (MM-RNR)

1 Pre-neutron mass yields from experiment or fission modes

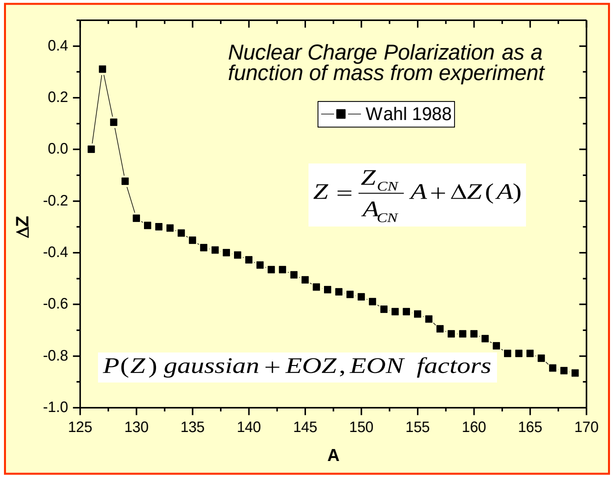


2 Pre-neutron kinetic energy distributions as function of mass from experiment or fission modes

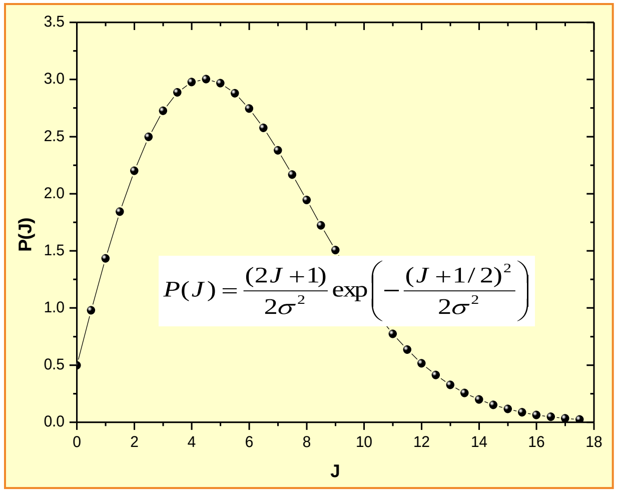




3 Nuclear Charge as a function of mass (Wahl model)



4 Spin distribution from models



5 Excitation energy sharing between fragments

At scission:

intrinsic excitation energy
+ deformation energy + collective excitation

$$TXE = a_{sc}T_{sc}^2 + E_{def} + E_{coll}$$

After full acceleration:

the rotational energy is not included
in the intrinsic excitation energy

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

A part of excitation energy at scission is converted in ***rotational energy (collective excitation)***

Rotating deformed Liquid Drop model

$$E_{rot} = \frac{\hbar^2 J(J+1)}{2\mathfrak{I}}$$

only the intrinsic excitation energy corresponding to

$$TXE - (E_{rot}^L + E_{rot}^H)$$

is partitioned through

$$E_{L,H}^* = a_{L,H}T_{L,H}^2$$

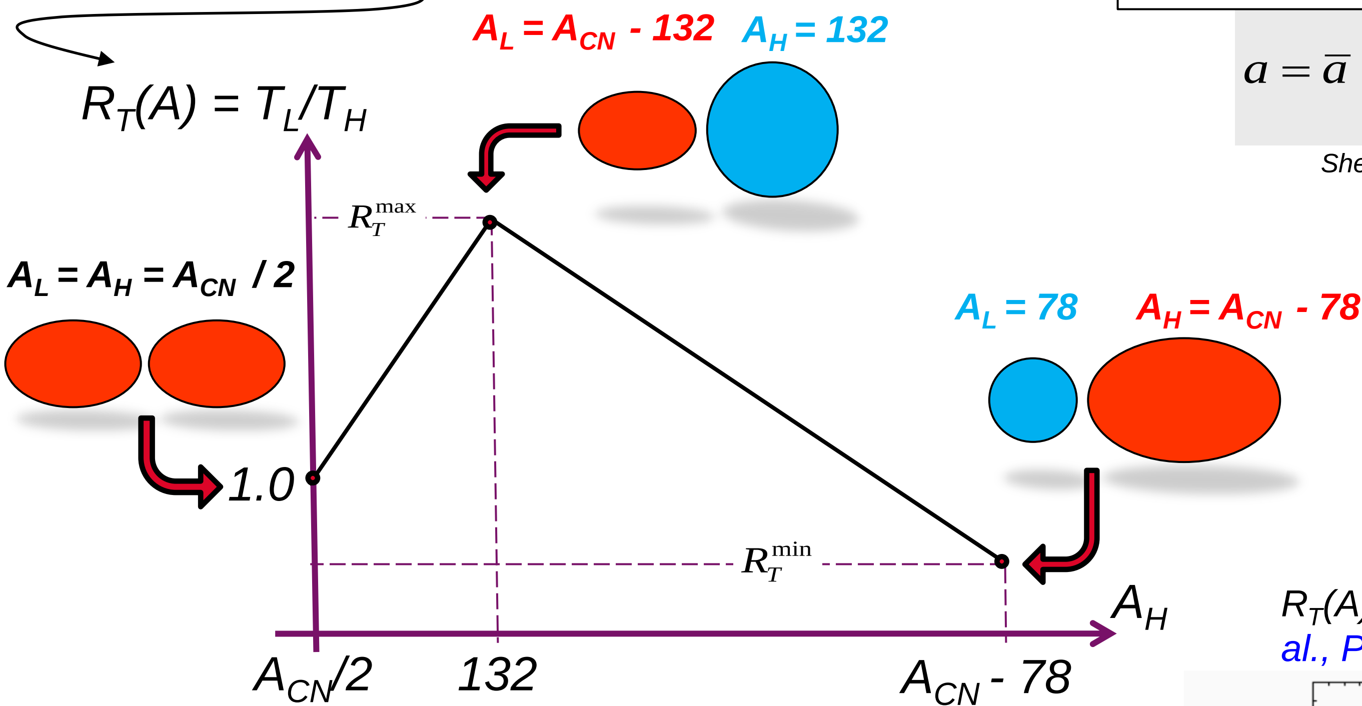
$$\forall L, H \quad E^* = a\, T^2$$

Ignatyuk prescription

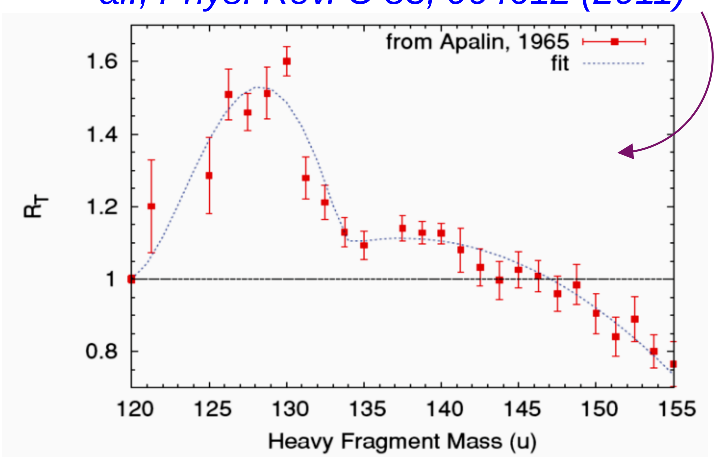
$$a = \bar{a}\left(1 + \delta W \frac{\left(1 - e^{-\gamma U^*}\right)}{U^*}\right)$$

Shell corrections, pairing, …

$R_T(A) = T_L/T_H$



$R_T(A)$ succesfully tested by Talou et al., Phys. Rev. C 83, 064612 (2011)



- ❑ **Max $R_T(A_H{=}130)$?**
- ❑ **$R_T(Z)$?**
- ❑ **R_T^m**

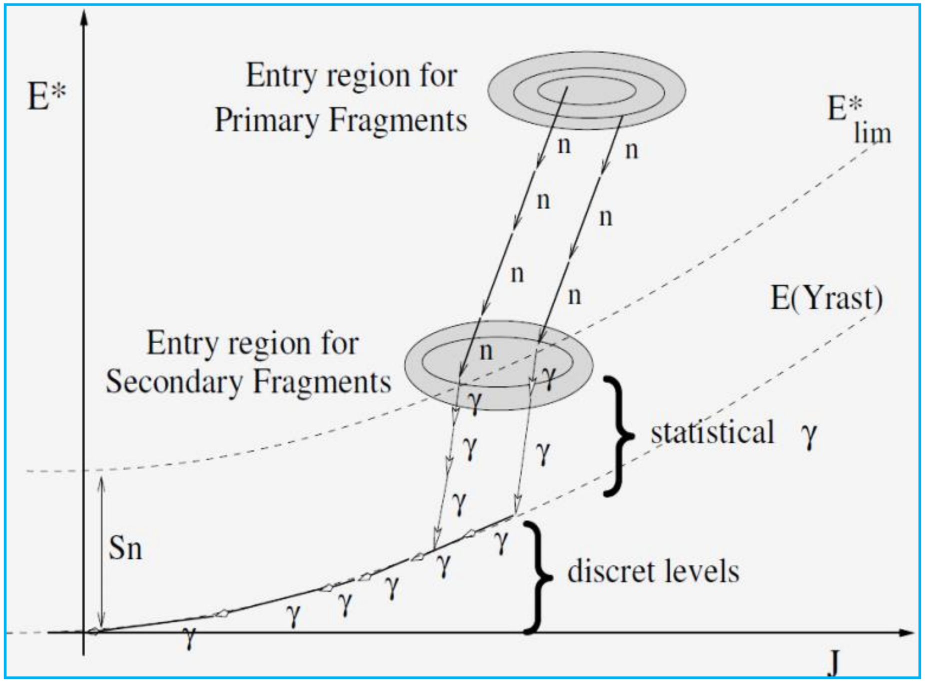
Fission Fragment deexcitation (Weisskopf or Hauser-Feshbach models)

Weisskopf evaporation theory for neutron emission
+ DICEBOX like MC scheme for gamma emission ('Nuclear Realization')

- Residual nuclear temperature *T(A-1,Z,E*)*
- *Step by step temperature dependent neutron spectrum*
- Neutron emission down to $S_n(J) = S_n + E_{rot}(J)$
- Gamma emission :
  - *Level densities*

    CGCM,CTM,HFB-tabulated
  - *Strength functions*

    SLO,EGLO, QRPA (from HFB or HF+BCS)
  - *Experimental level schemes from RIPL-3*



Fission Fragment deexcitation (Weisskopf or Hauser-Feshbach models)

*D. Regnier et al., Phys. Proc. **47**, 47 (2013)*

'Hauser-Feshbach' statistical theory for n/γ emission

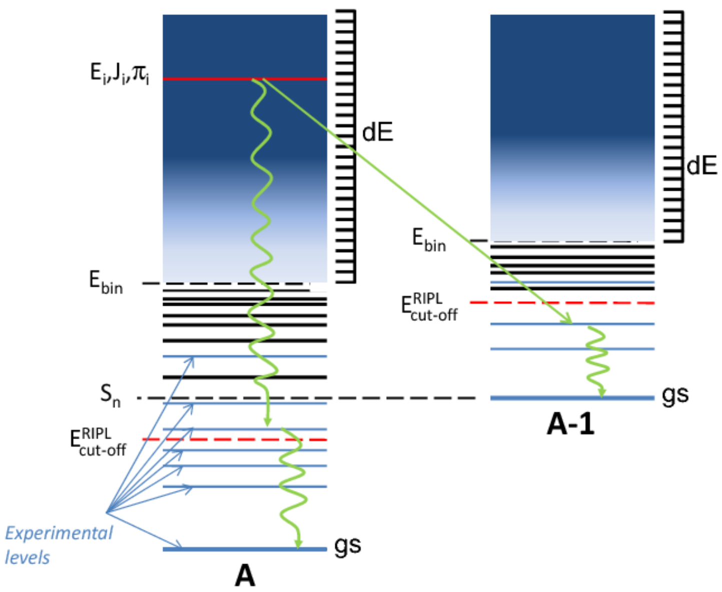
$$P_n = \frac{\Gamma_n}{\Gamma_\gamma + \Gamma_n}$$

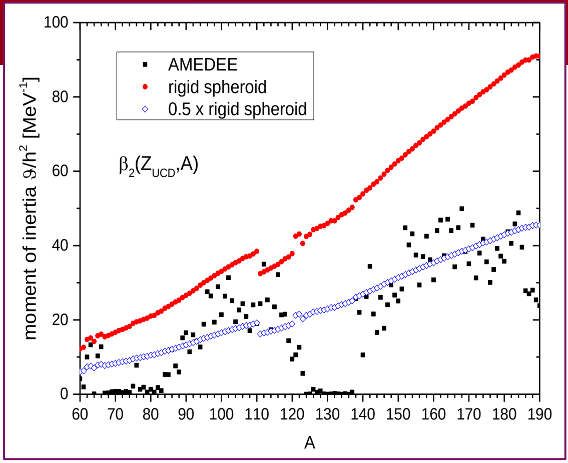
- Neutron transmission coefficients from :
  Talys/Ecis code (Koning-Delaroche, Jeukenne-Lejeune-Mahaux *OMP* from RIPL-3)

$$P_\gamma = \frac{\Gamma_\gamma}{\Gamma_\gamma + \Gamma_n}$$

- Gamma transmission coefficients (as previously described)
  - *Level densities*
    CGCM,CTM,HFB-tabulated
  - *Strength functions*
    SLO,EGLO, QRPA (from HFB or HF+BCS)
  - *Experimental nuclear level schemes*

NB*: Experimental nuclear level schemes* taken from RIPL-3 are completed with models from $E_{cut\text{-}off}$ up to an energy E_{bin} corresponding to a given level density (default: 5.10^4 MeV^{-1}). E_{bin} is the starting point for bin description.





Free parameters of the simulation (the big 5!)

- ***Fraction (k) of the rigid spheroid moment of inertia*** $\mathcal{I}$

involved in the rotational energy formula $E_{rot} = \hbar^2 J(J+1)/(2\mathcal{I})$

models for $\mathcal{I}$

- Rigid spheroid : $\mathcal{I} = k \times \mathcal{I}_{rig.} = k \times 2/5\, AMR^2(1+0.31\beta_2 + \cdots)$
- Hydrodynamical system : $\mathcal{I} = k \times \mathcal{I}_{fluid} = k \times (9/8\pi)\, AMR^2 \beta_2{}^2$
- From AMEDEE data base : $\mathcal{I} = \mathcal{I}_{AMEDEE}$ [Hilaire et al. Eur. Phys. J. A**33**, 237 (2007)]

- ***Initial fission fragment total angular momenta*** $P(J) = \frac{(J+1/2)}{\sigma^2} \exp\left(-\frac{(J+1/2)^2}{\sigma^2}\right)$

- $\sigma^2 \sim \mathcal{I}\, T/\hbar^2$ *[used in previous studies: Litaize et al., Phys. Proc. 31, 51 (2012)]*
- $<\sigma_L>$, $<\sigma_H>$
- *<J>(A) → σ(A)*
- *<J>(A,E*) → σ(A,E*)*

- ***Extrema values of the temperature ratio*** $R_T(A)$ R_T^{min} , R_T^{max}

(!) Calculated values may change a little from a presentation to another due to releases of the code

- Context
- Models in FIFRELIN
- **Fission observables: comparison with experiments**
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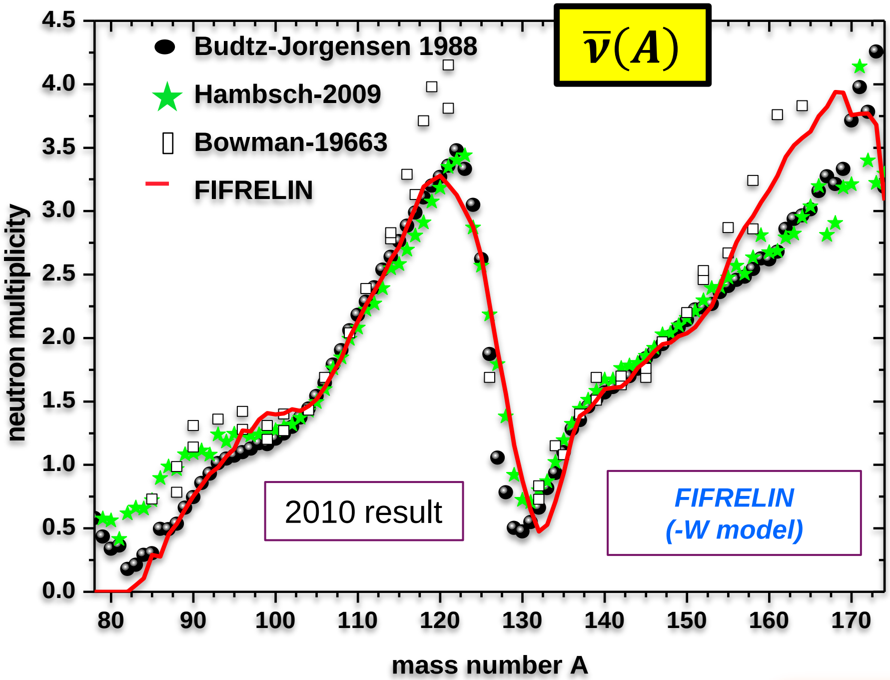
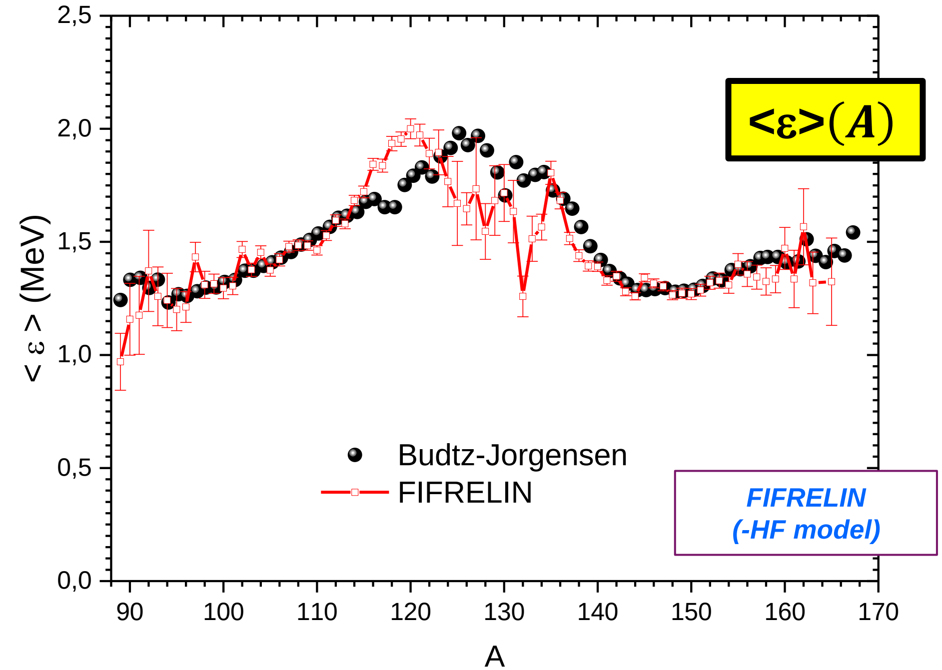
Fission Observables: comparison with experiment

Average prompt neutron multiplicity as a function of pre-neutron mass



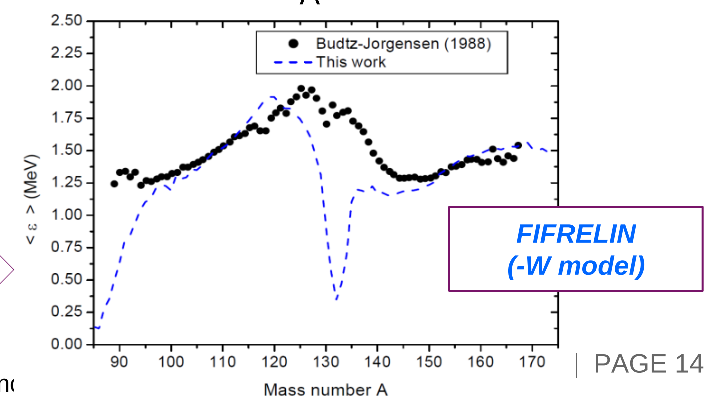
Average prompt neutron energy in CM as a function of pre-neutron mass



	$<\nu_L>$	$<\nu_H>$	$<\nu>$
Vorobyev 2004	2.05	1.70	3.76 ± 0.03
FIFRELIN '2010'	2.06± *0.005*	1.70± *0.005*	3.76± *0.005*

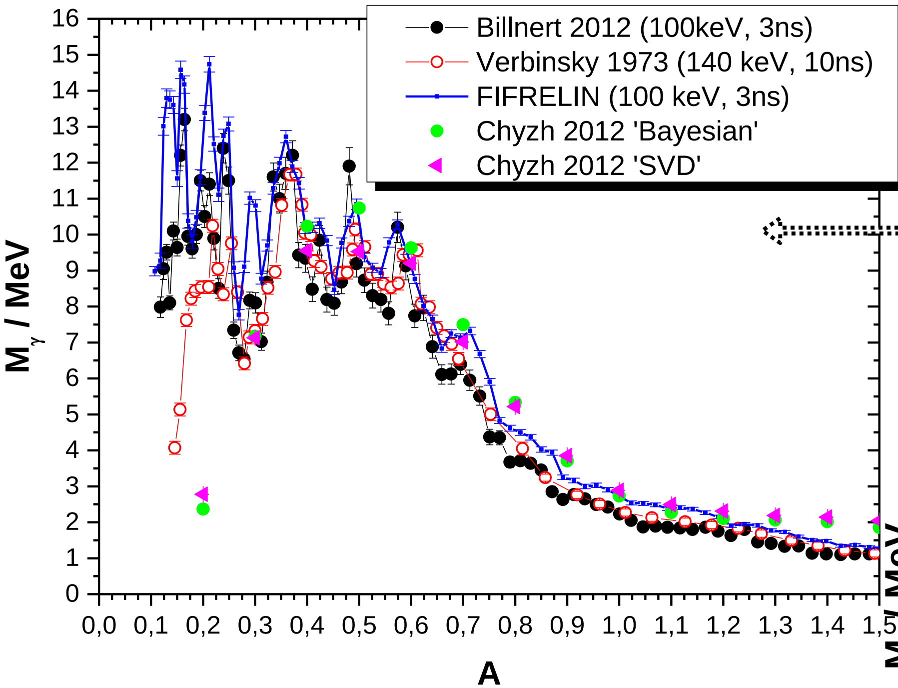
^{252}Cf (sf)

2010 result



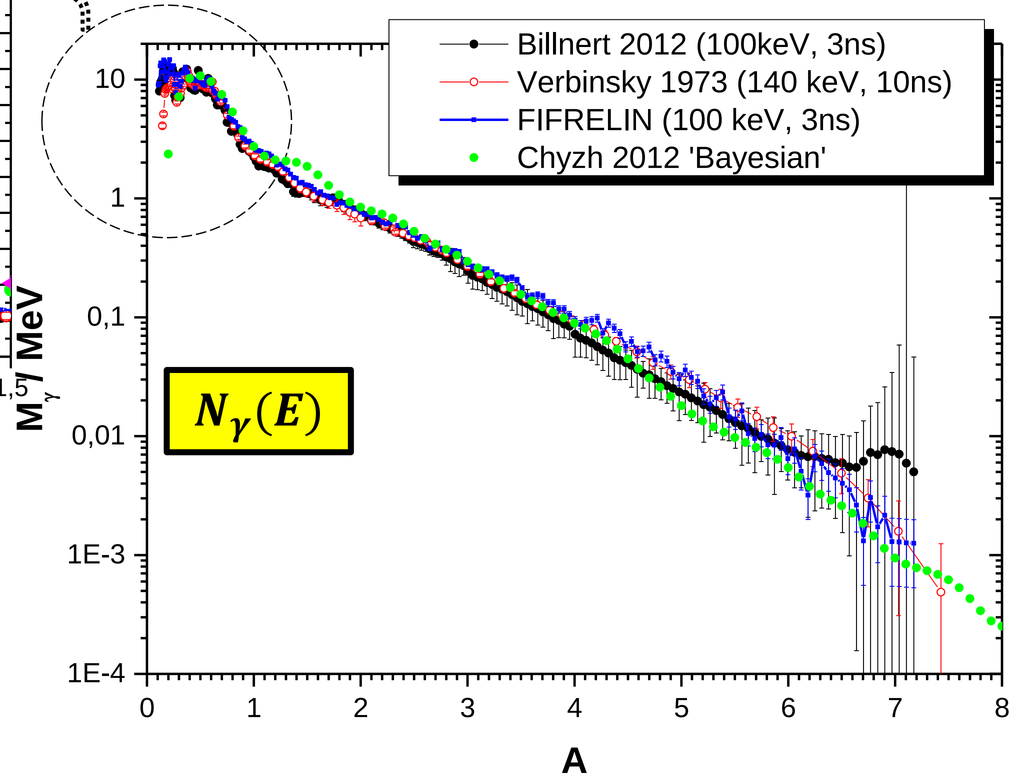
*O. Litaize, O. Serot, Phys. Rev. C **82**, 054616 (2010)*

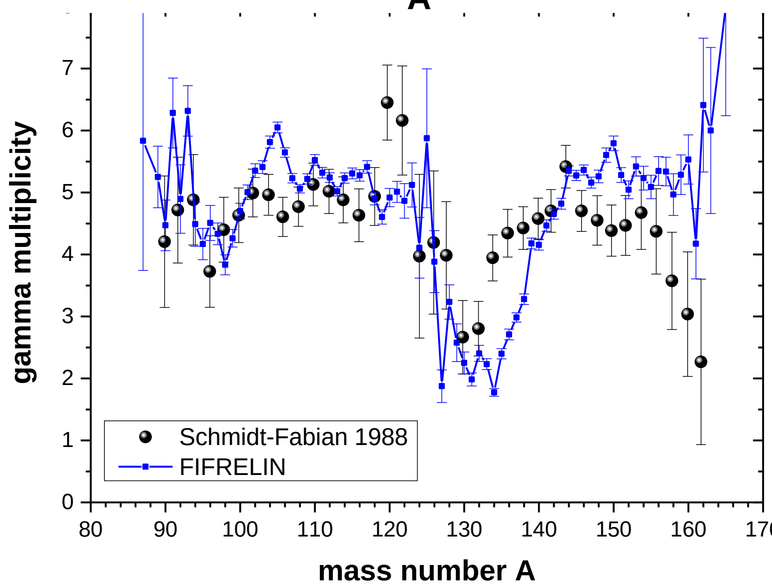
Fission Observables: comparison with experiment



Prompt fission gamma spectrum

^{252}Cf (sf)

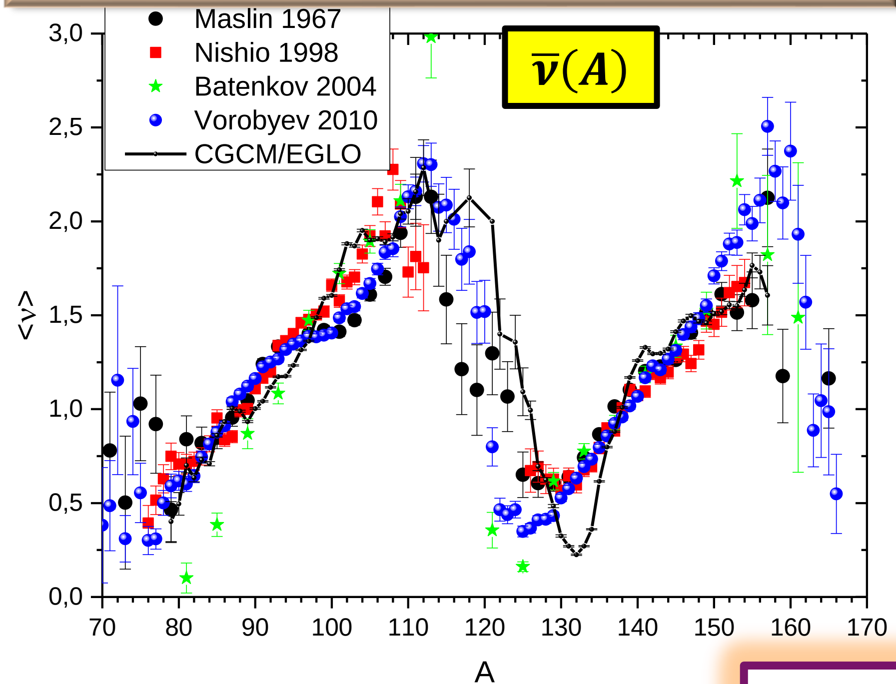




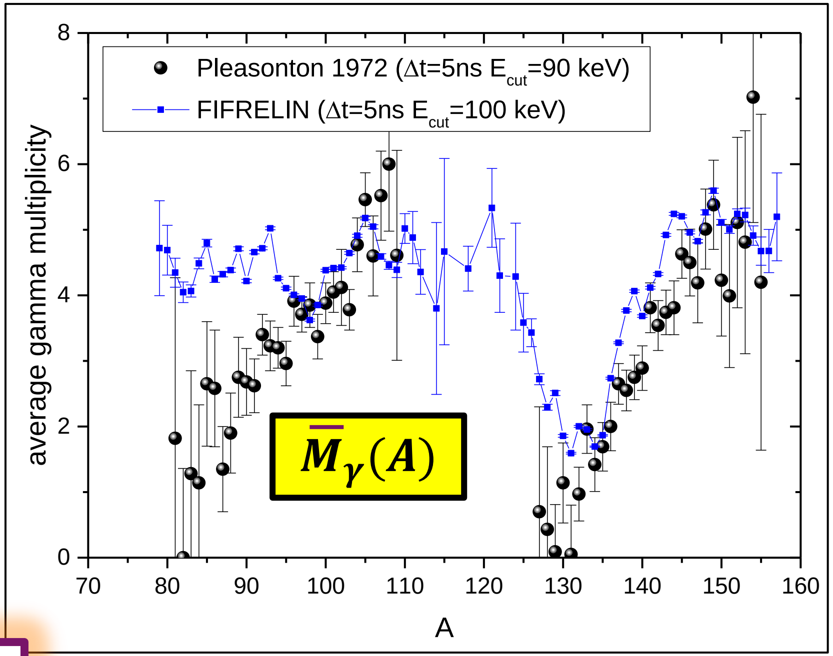
Average prompt gamma multiplicity as a function of pre-neutron mass

Fission Observables: comparison with experiment

Average prompt *neutron* multiplicity as a function of pre-neutron fragment mass



Average prompt *gamma* multiplicity as a function of pre-neutron fragment mass



$^{235}U(n_{th},f)$

Neutron average quantities

	$<\nu_L>$	$<\nu_H>$	$<\nu>$
Nishio 2004	1.42	1.01	2.43 ± 0.03
FIFRELIN	1.41 ± *0.001*	1.02± *0.001*	2.43 ± *0.001*

Gamma average quantities

	Threshold	ΔT	$<M_\gamma>$ (γ/f)	$<E_\gamma^{tot}>$ (MeV)	$<\varepsilon_\gamma>$ (MeV)
Oberstedt 2013	100 keV	5 ns	8.19 ± 0.11	6.92 ± 0.09	0.85 ± 0.02
FIFRELIN	100 keV	5 ns	8.04 ± 0.01	7.02 ± 0.01	0.875 ± 0.001

Fission Observables: comparison with experiment

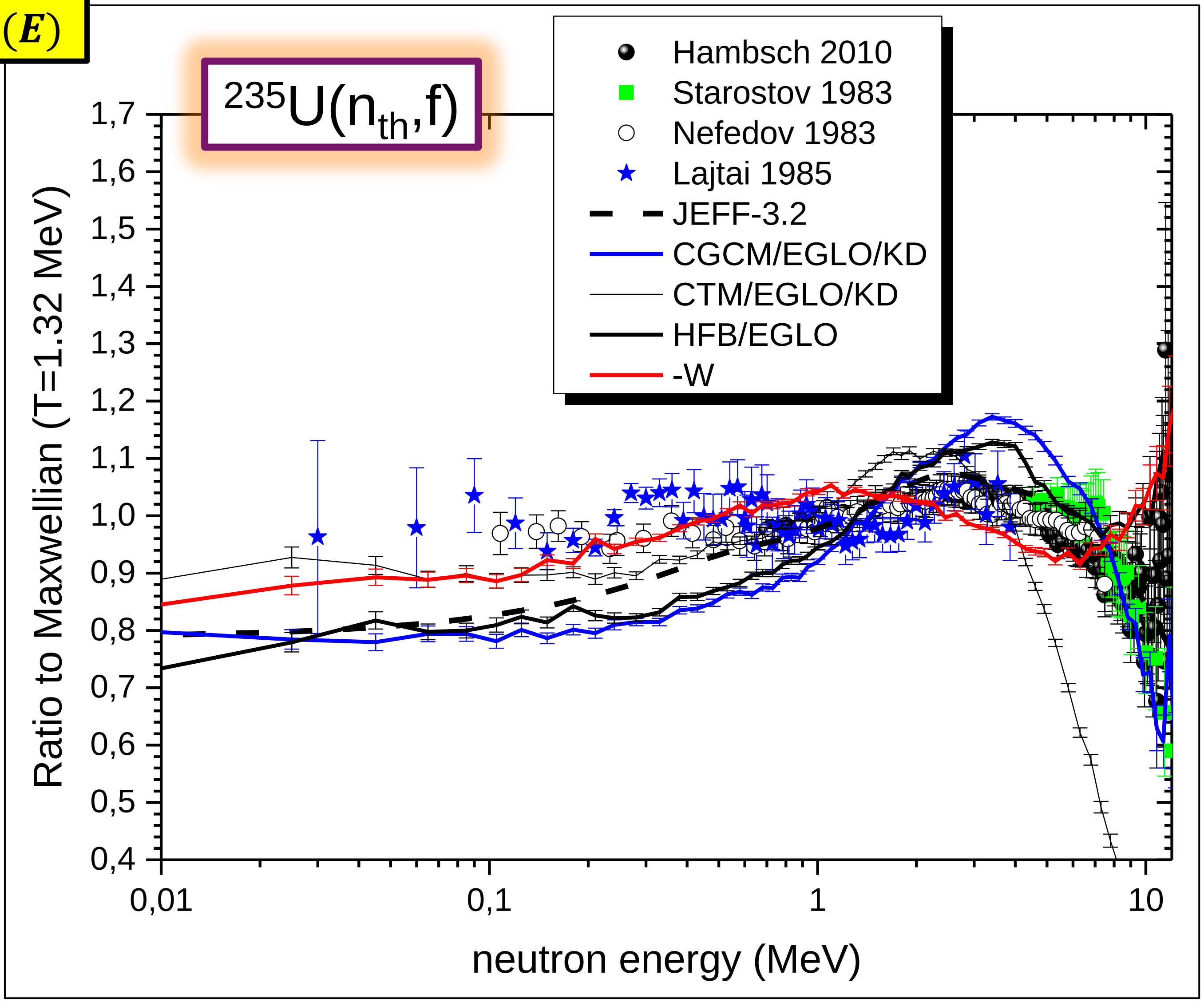
Prompt fission neutron spectrum

FIFRELIN -HF (LDM)	<E> MeV	<ν>
(CGCM)	2.102(2)	2.424(2)
(CTM)	1.891(1)	2.444(1)
(HFB)	2.079(2)	2.397(2)

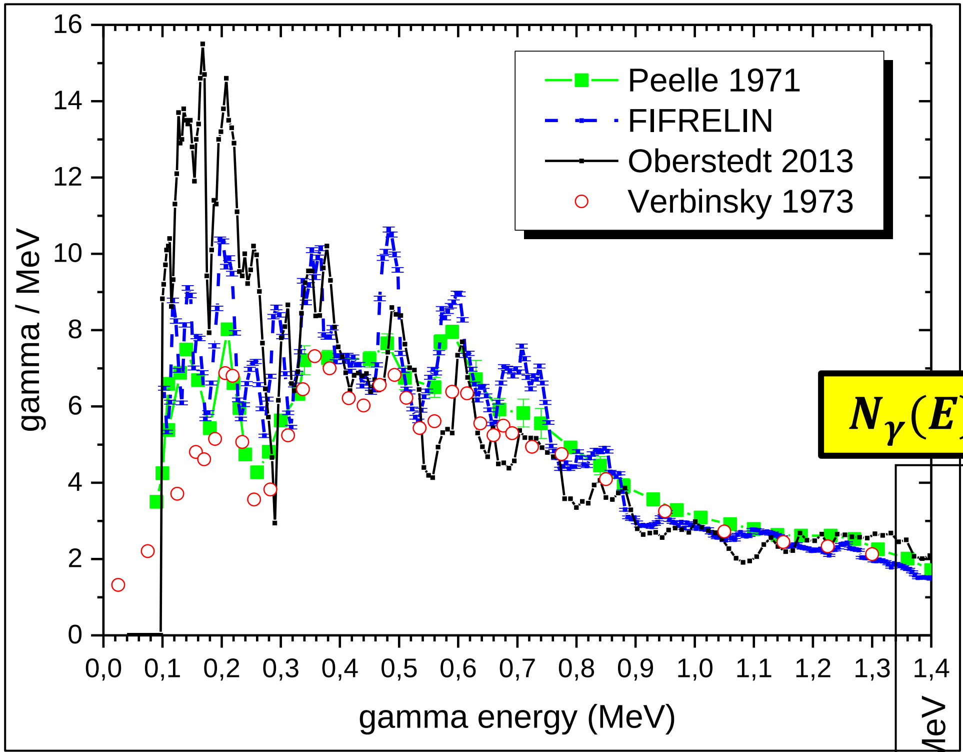
FIFRELIN -W	1.945(2)	2.430(3)
JEFF-3.2	2.03	2.42

Micro data	1.974(2)
Macro data	2.03

$N_\nu(E)$



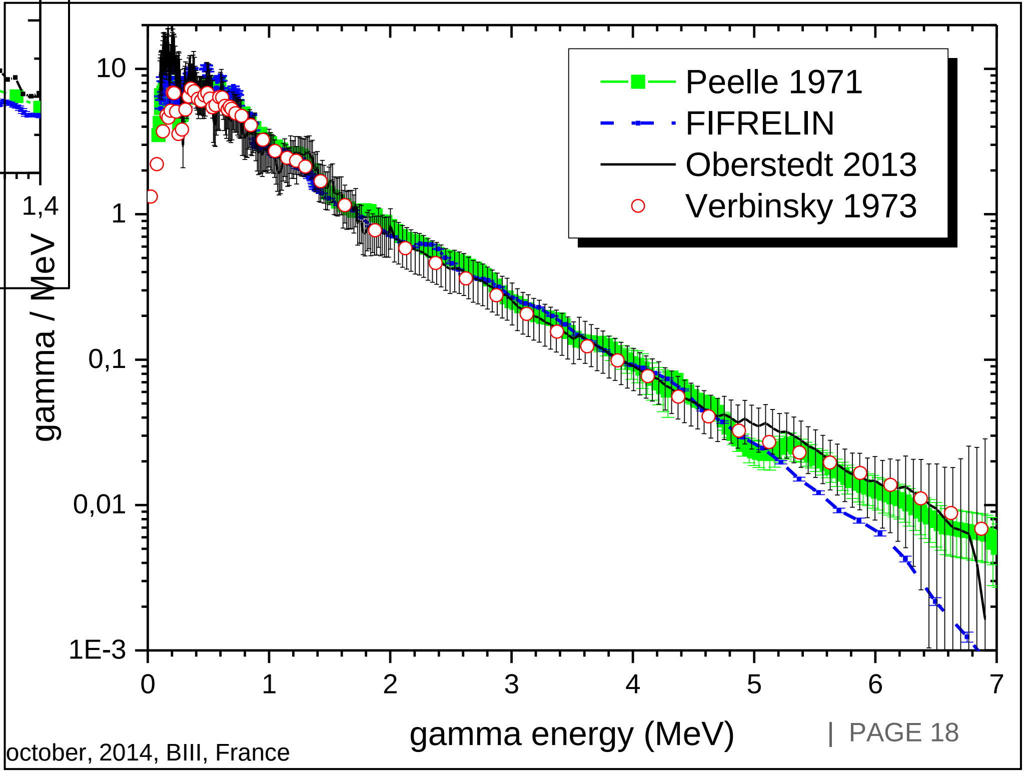
Fission Observables: comparison with experiment



Prompt fission gamma spectrum

$N_\gamma(E)$

- **Lower strength in the calculation above 6 MeV ?**



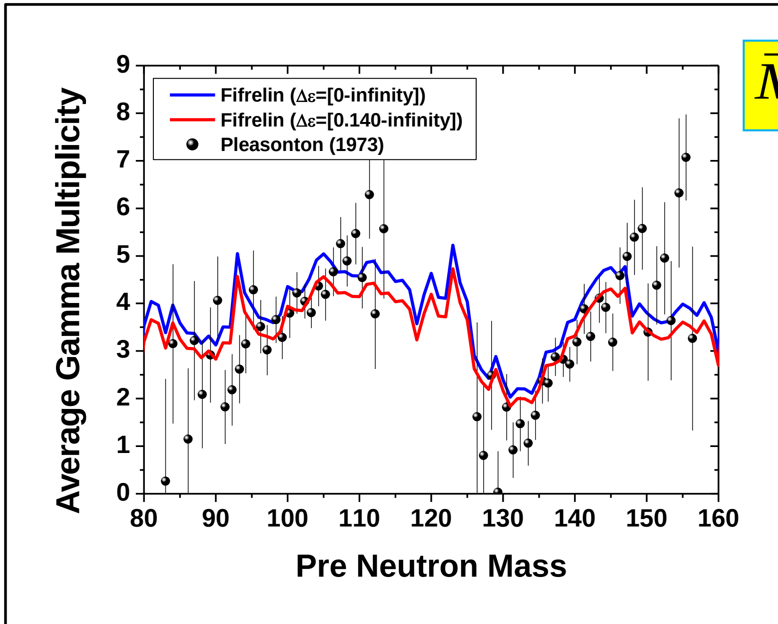
- **Position of the structures at low energy is reproduced by the calculation**

$^{235}U(n_{th},f)$

Fission Observables: comparison with experiment

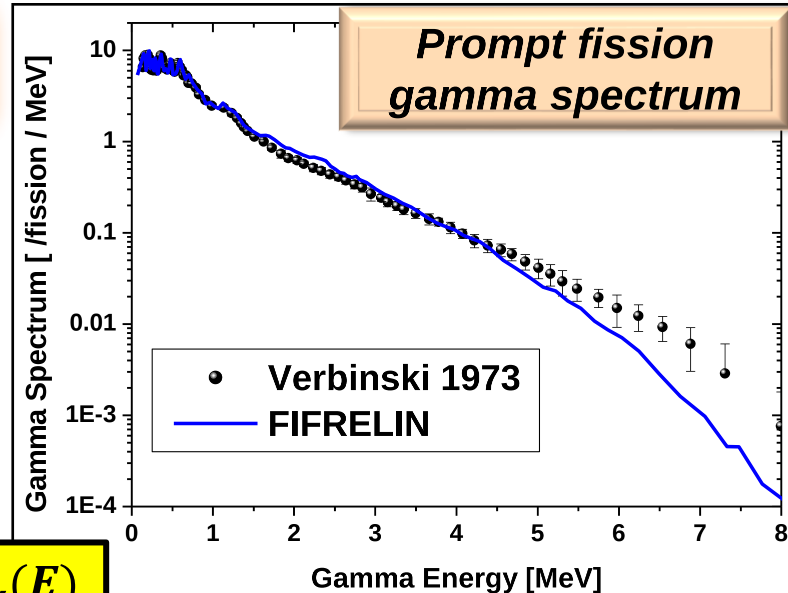
Average prompt gamma multiplicity as a function of pre-neutron fragment mass

$^{239}Pu\ (n_{th},f)$

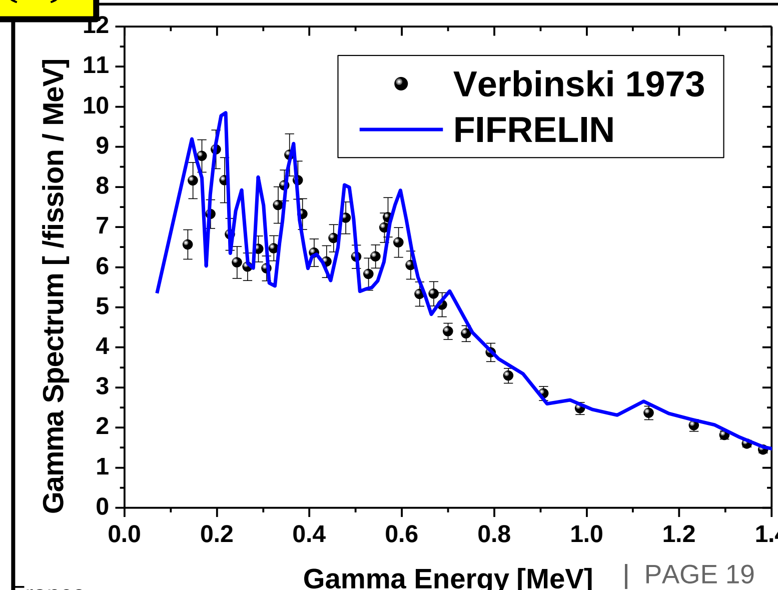


$\overline{M}_\gamma(A)$

Prompt fission gamma spectrum



$N_\gamma(E)$



	Threshold [keV]	ΔT [ns]	M_γ [γ/f]	$<E_\gamma^{tot}>$ [MeV]	$<\varepsilon_\gamma>$ [MeV]
Verbinski 1973	140	10	7.23	6.81 ± 0.03	0.94
FIFRELIN	140	10	7.19	6.81	0.95

O. Serot, O. Litaize, D. Regnier, Workshop Gamma-2, 24-26 sept. 2013

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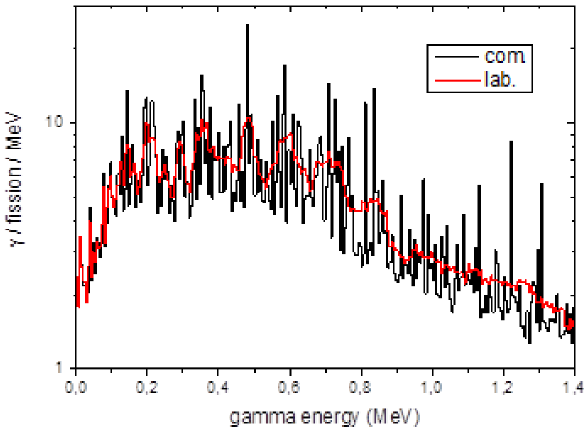
Beyond common observables

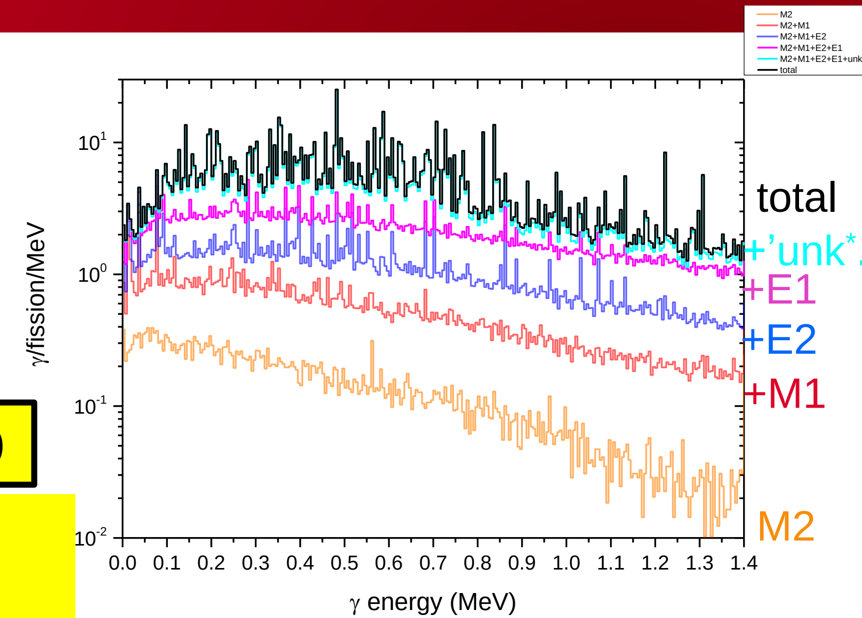


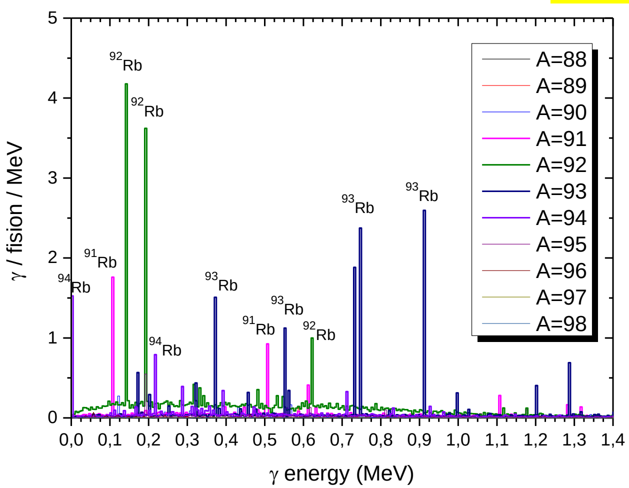
Resolution below 1.4 MeV: 5 keV

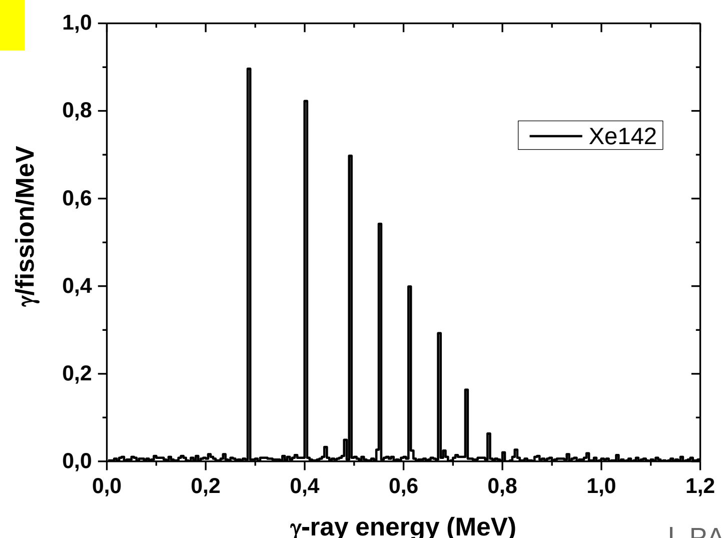
$^{235}U(n_{th},f)$

$$N_\gamma(E|A,Z,XL)$$

Gamma spectra
- ***per mass***
- ***per charge***
- ***per emitting fragment***
- ***per multipolarity***

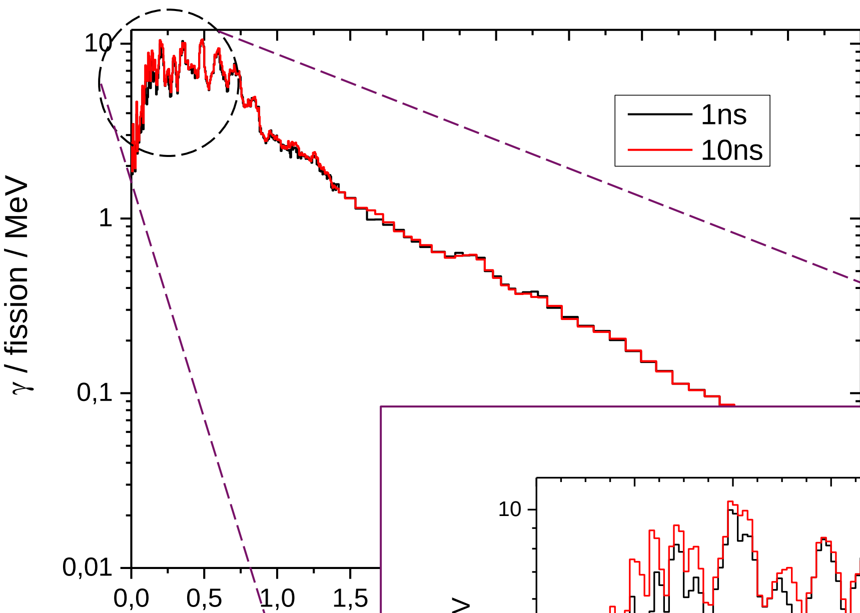


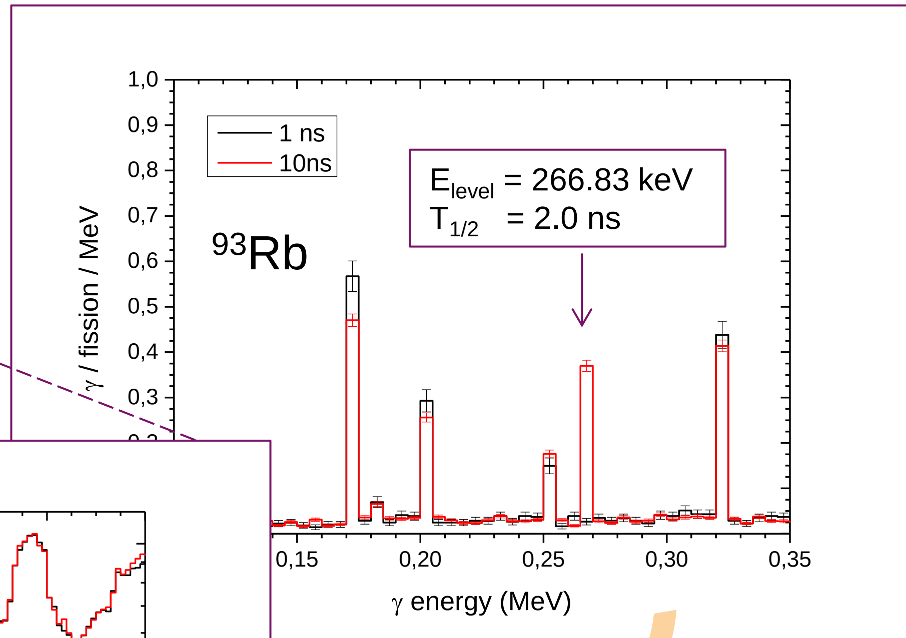


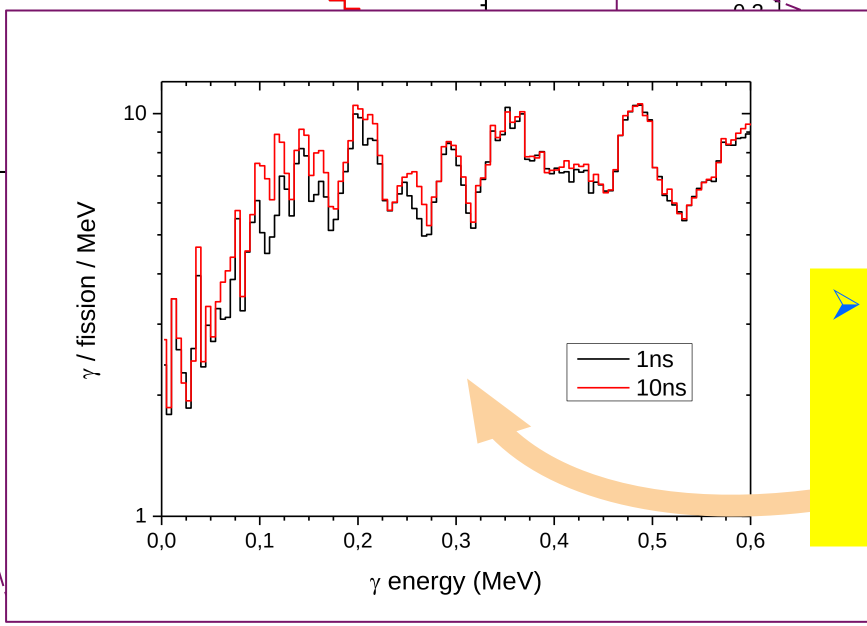


Influence of the maximum half life considered in the simulation

→ **Useful for comparison with experiments (coincidence time window)**





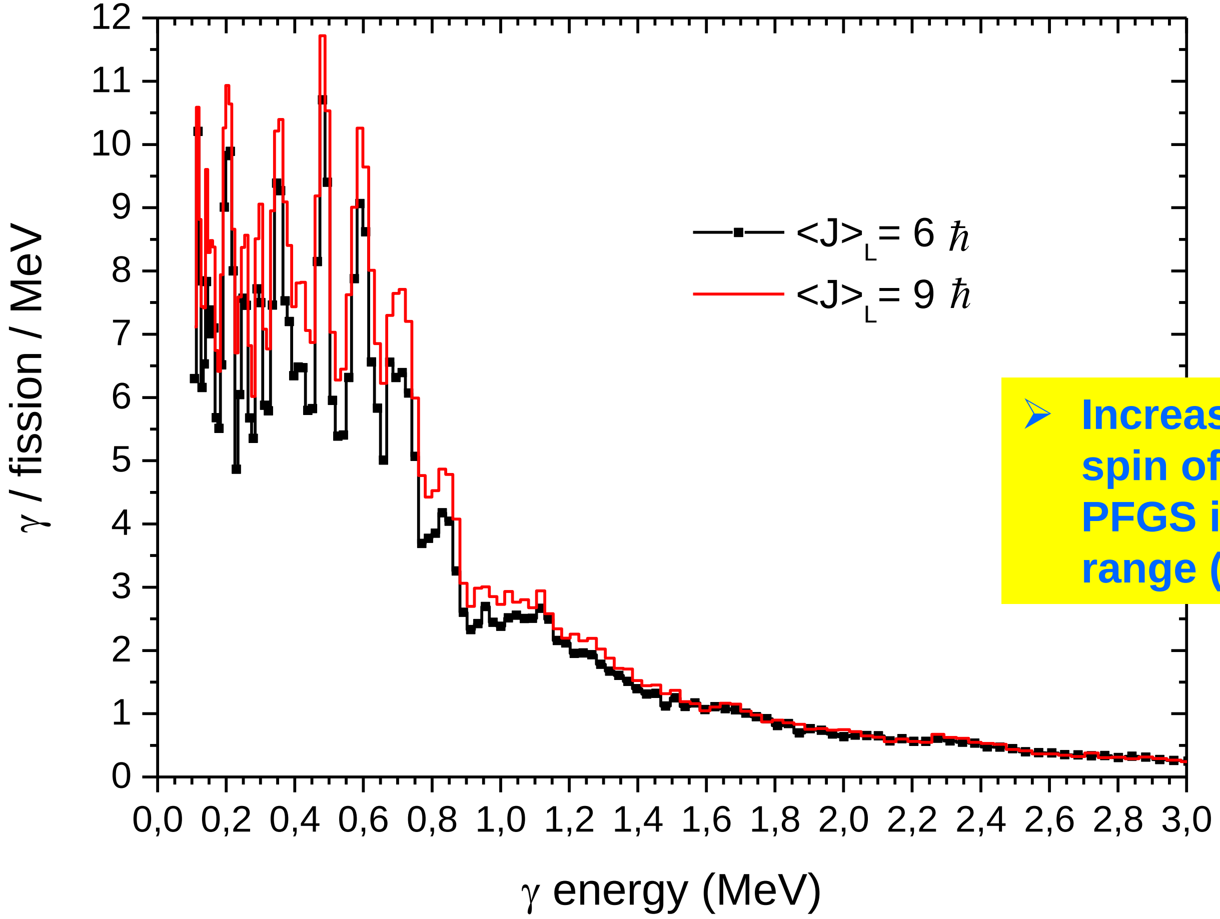


- **Importance of the data available from nuclear structure**

+
+
+

Sensibility of the PFGS to the initial spin distribution

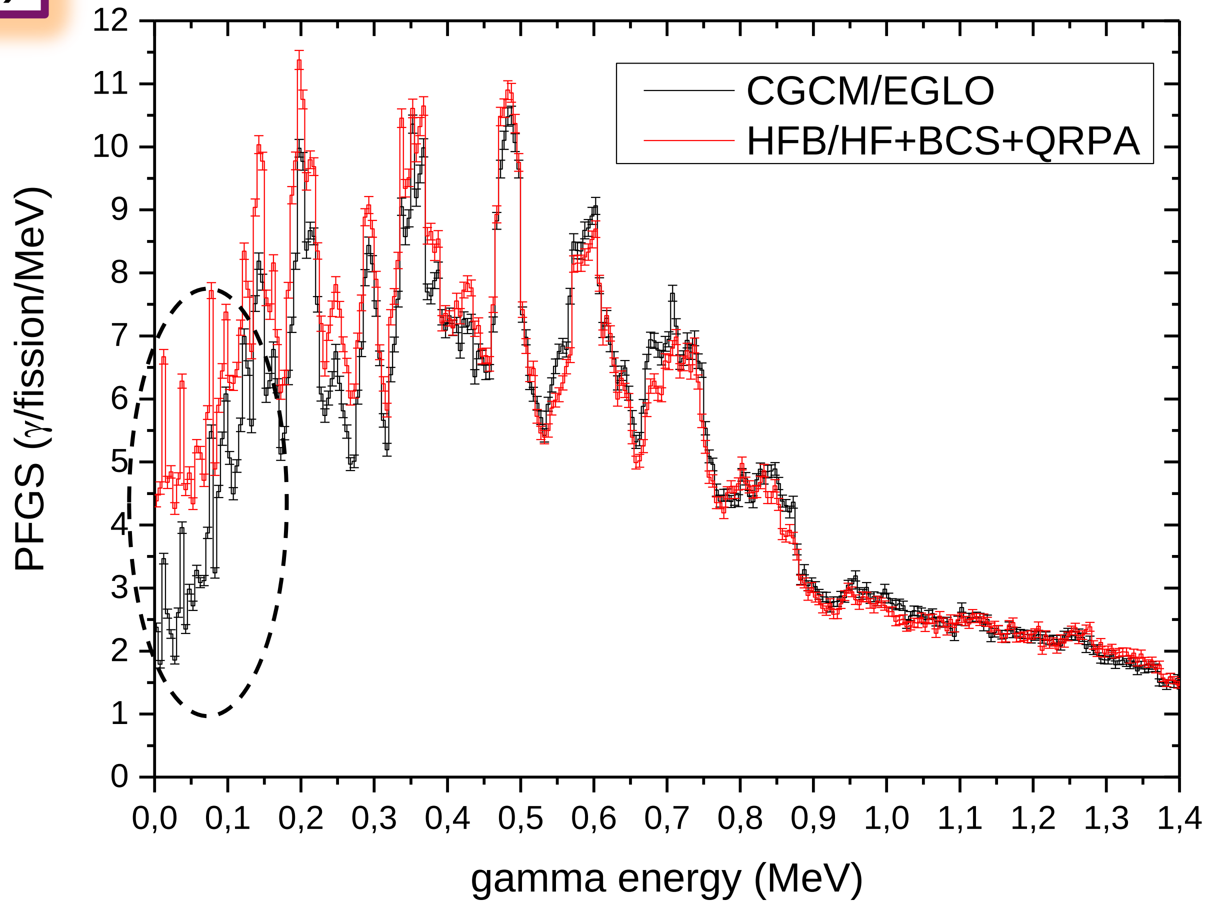
$^{235}U(n_{th},f)$



- **Increasing the initial spin of FF increases the PFGS in the low energy range (below 1 MeV).**

$^{235}U(n_{th},f)$

Differential spectra & multiplicities

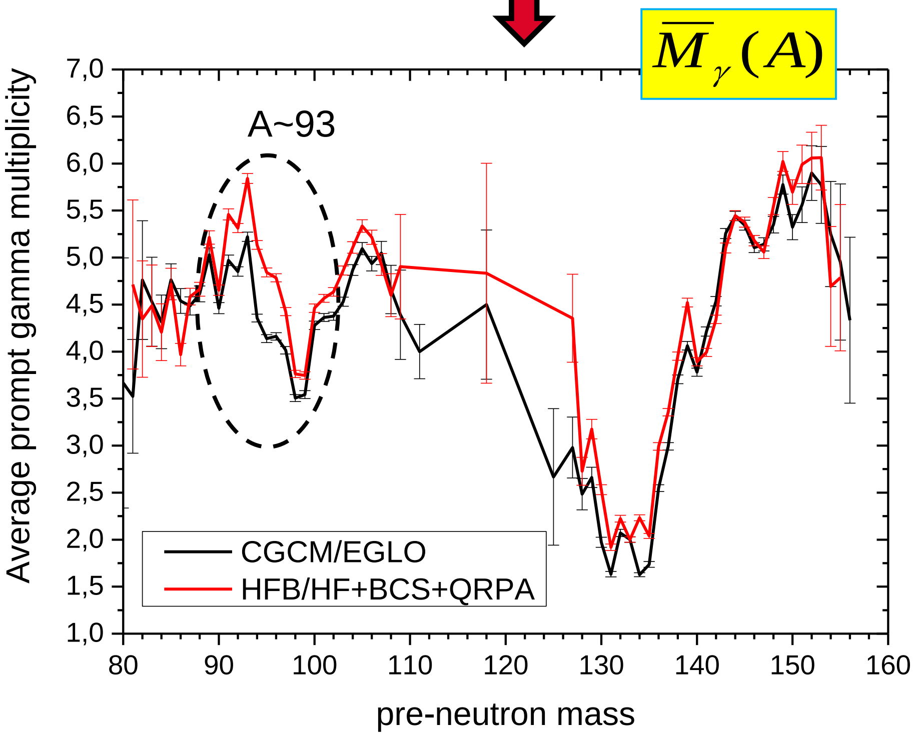


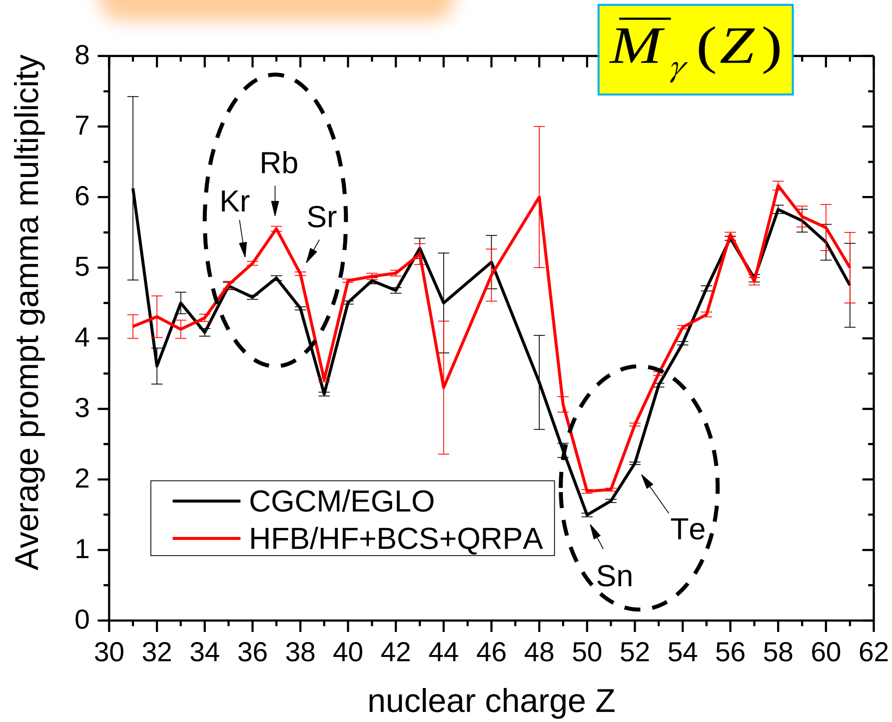
➢ **Noticeable difference observed between two models (among others) below 200 keV…**

Differential spectra & mutiplicities

$^{235}U(n_{th},f)$

➢ **The responsible could have a mass around 93**

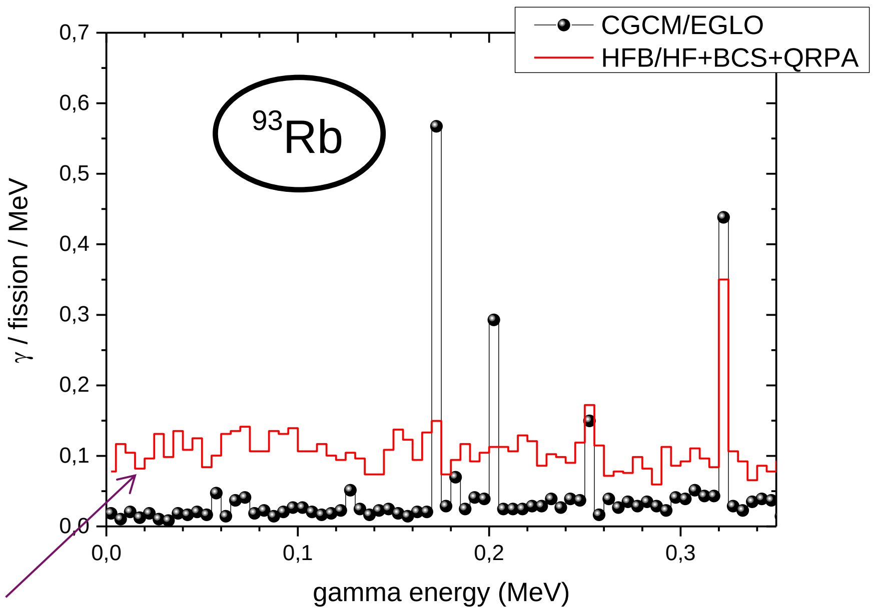


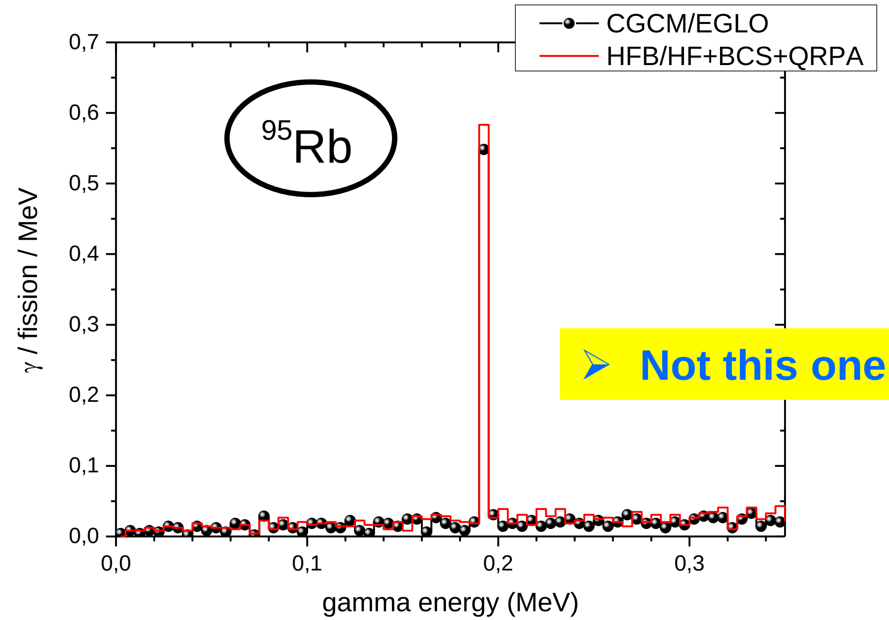


Remember that due to neutron emission, the mass shown here is not the mass of the γ-emitter

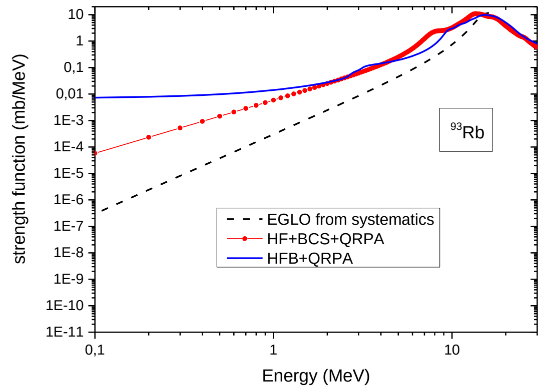
➢ **The responsible could be Kr, Rb or Sr …**

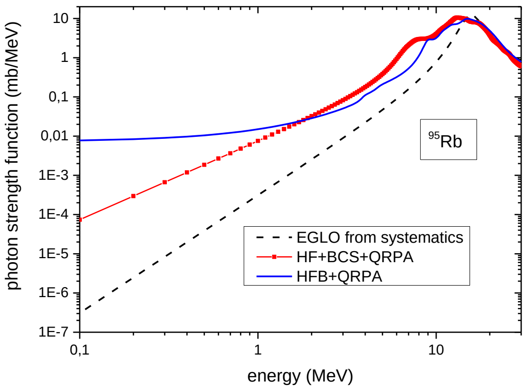
$^{235}U(n_{th},f)$





- **Not this one !**
- **This guy may be potentially guilty**





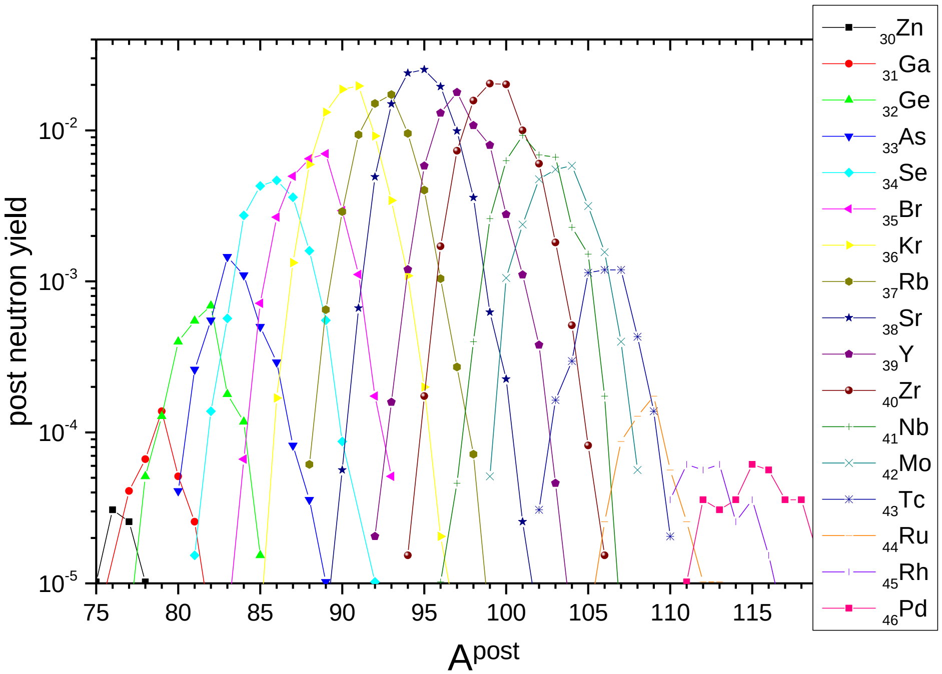
- **PSF: no**
- **LD: yes**

- **Experiment could help to choose between those two models.**
- **Theory could explain why.**

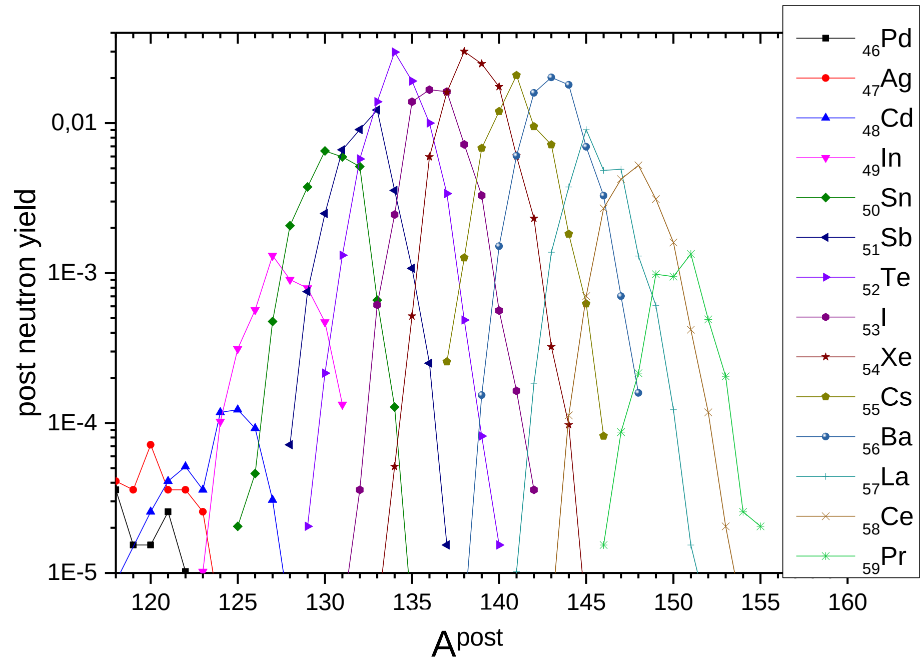
Beyond common observables

Isotopic yields Y(A,Z)

$^{235}U(n_{th},f)$



Light peak



Heavy peak

Around 400 nuclei calculated

- Introduction
- Models in FIFRELIN
- Fission observables: comparison with experiments
- Beyond common observables
- **Perspectives**

Ongoing work

- Fission modes,
- *Excitation energy sharing at scission,*
- *Multiple chance fission,*
- *Scission neutrons,*

Fission

- *Level Density, spin cut-off,*
- *Photon strenght functions,*
- *Neutron transmission coefficients,* **…**

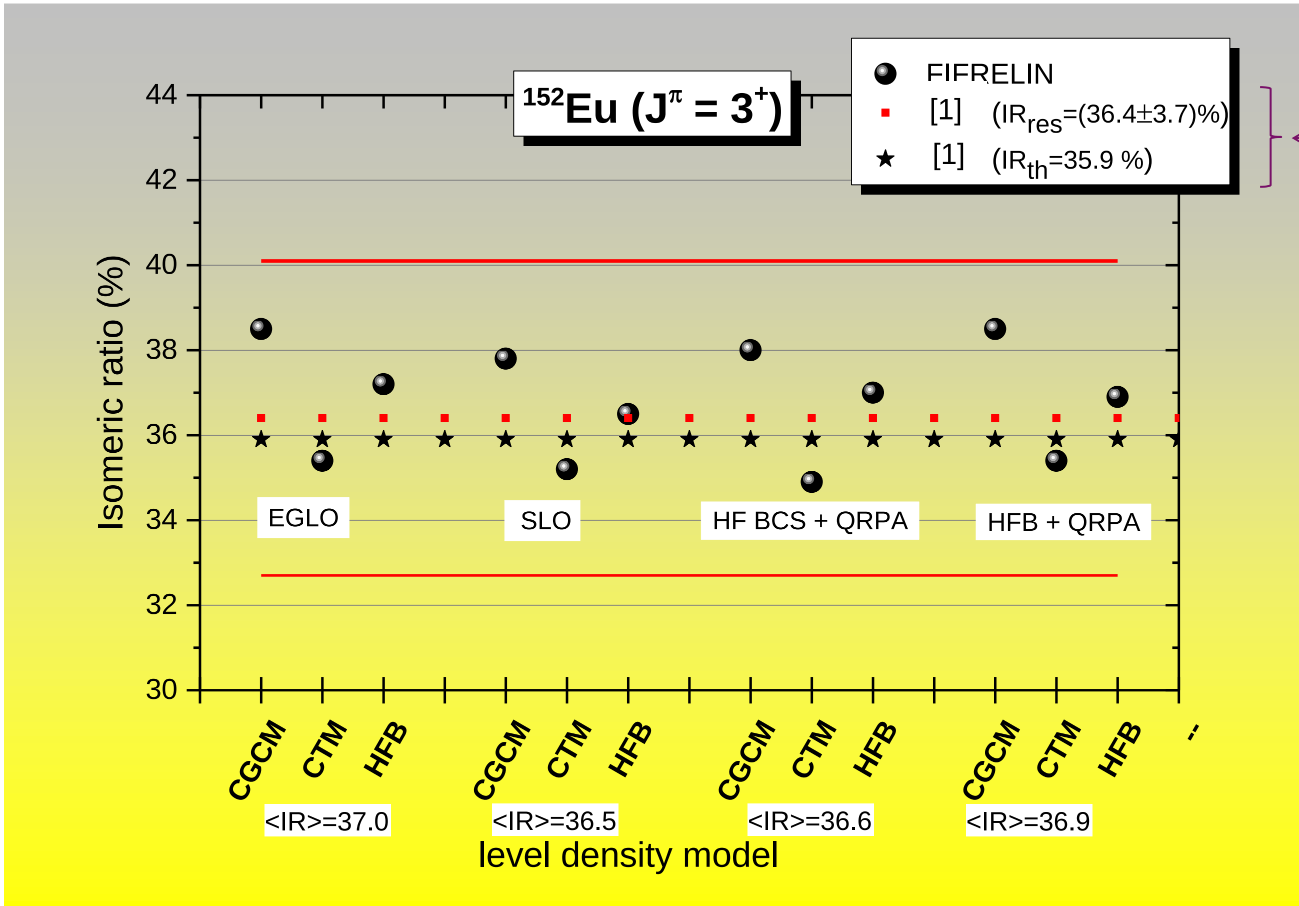
Nuclear structure

Global scope

- *Weisskopf / Hauser-Feshbach deexcitation models,*
- *Parallel computing*
- *Coupling codes, extended application area (detection, transport in reactors, heating, …)*

Isomeric ratio calculations

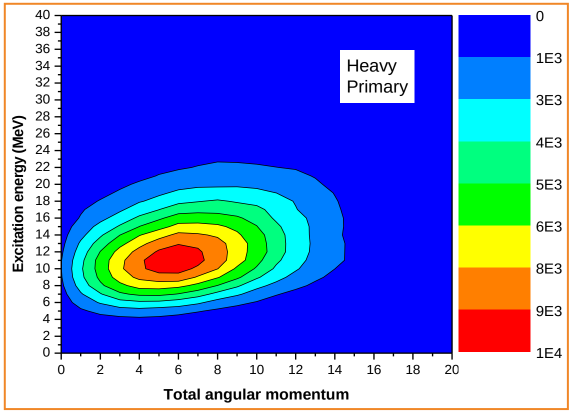
^{152}Eu after thermal neutron capture



[1] X. Ledoux et al., Eur. Phys. J. A 27, 59 (2006)
→ CIRENE measurements
→ Calculation: IR_{th} = 0.21%

- **Experimental precision not sufficient. What about new facilities ?**
- **Less sensitive to PSF**
- **Sensitive to LD**

Isomeric ratio and level population calculations



Calculate a matrix of isomeric ratio in a [J , E*, π] ensemble

Simulation of fission gives Spin distribution after neutron emission P(J) and excitation energy after neutron emission P(E*)

- **Could be used to estimate isomeric ratio in fission and to select the optimal distribution.**
- **Find the best spin distribution that allows to reproduce 'fine' observables:**
  - **Yields of specific fragment pairs (Kr-Ba, …),**
  - **Population of well known 2^+ states of even even nuclei (from EXILL campaign and FIPPS in a near future).**

CEA/DEN - CEA/DSM – CNRS/LPSC collaboration

Improve Modeling

- ❑ Using tabulated 'microscopic' ingredients

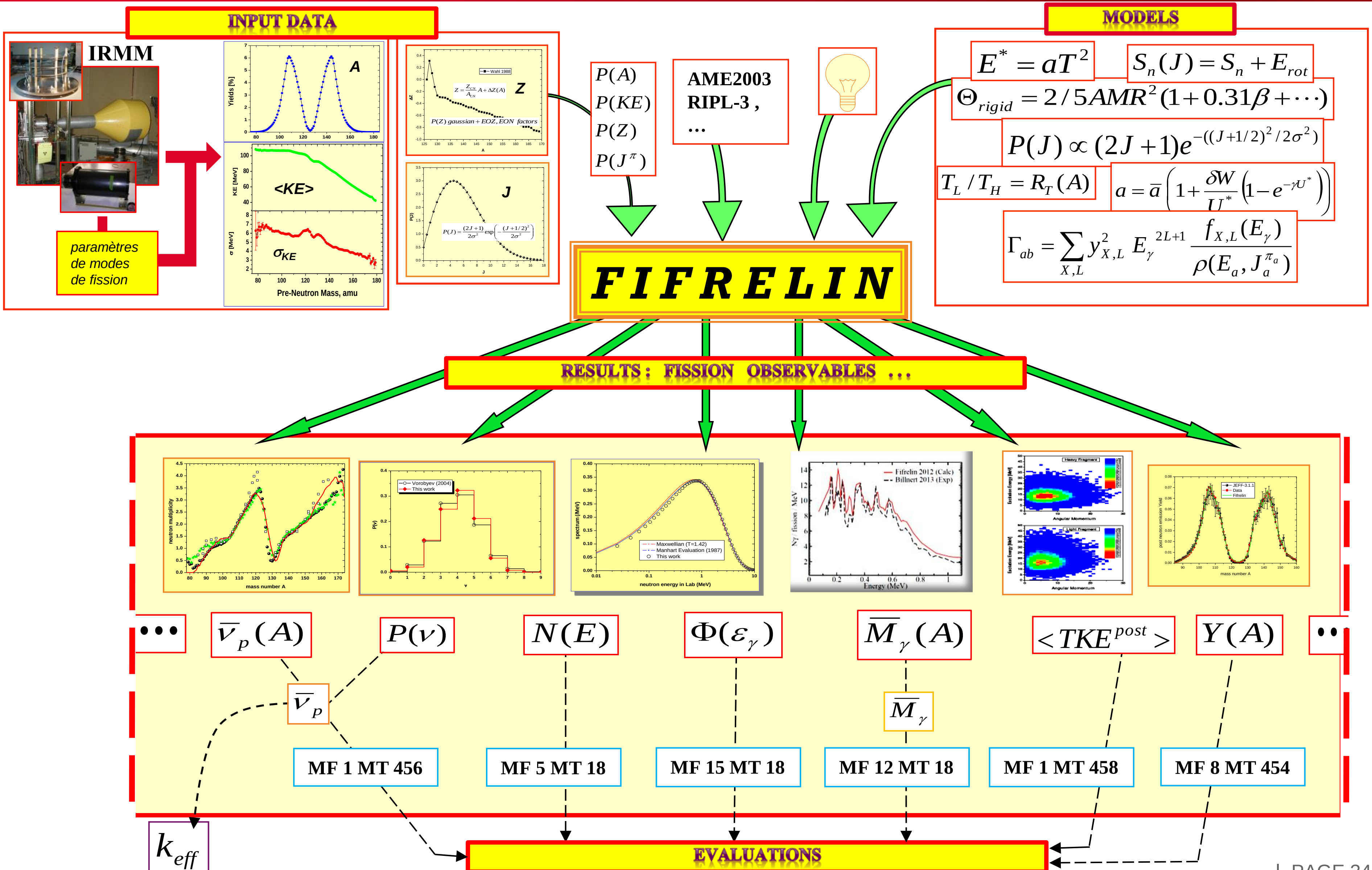
- HFB +QRPA compared to SLO, EGLO, MLO … a clash of clans ? … not sure.

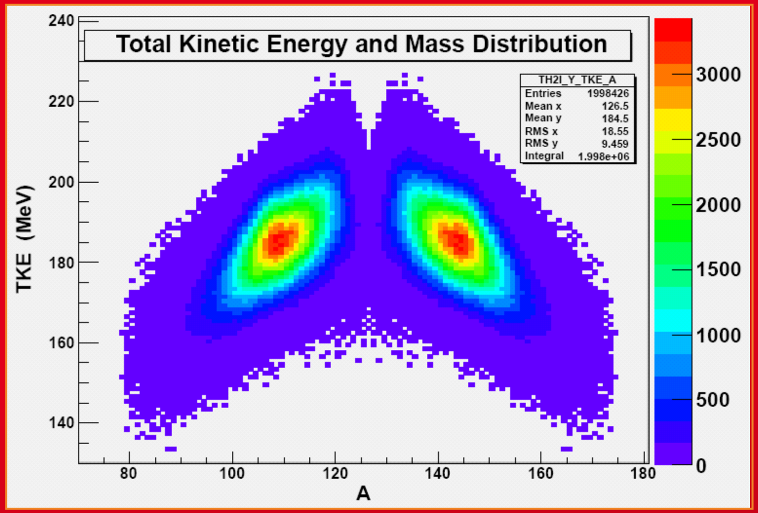
- ❑ Accounting for energy partition at scission from microscopic calculations provided by SPY code (PES + HFB D1S) to estimate the energy available for particle emission

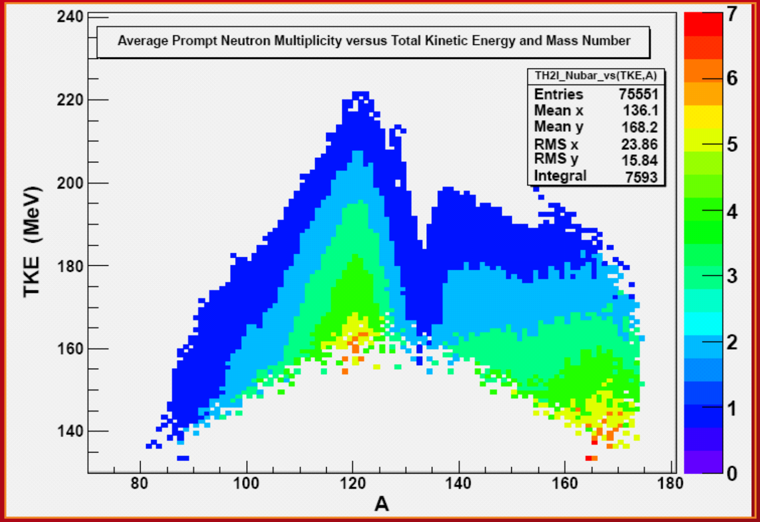
Panebianco et al. , Phys. Rev. C, 064601 (2012).

Input / Output	Today	Next decade ?
Mass and Kinetic Energy distributions before neutron emission	• Reconstructed from experimental post neutron distributions, • Calculated from fission mode parameters	• HFB calculations (CEA/DAM), • Langevin equations (LANL, LLNL), • Provided by GEF code (CENBG), • New experimental facilities
Charge distribution	• UCD+ΔZ+EOZ+EON.	• New experimental facilities (FALSTAFF, FIPPS, SOFIA, SPIDER…).
Spin distribution	• Various spin cut-off formula • Check with PFGS, PFGM	• Check with isomeric ratio • Check with yields of specific fragment pairs (EXILL)
Excitation energy sharing	• $R_T(A)$	• HFB from SPY code (CEA/DAM/DSM) • Influence of scission neutrons
De-exciation process	• CGCM-CTM/EGLO-SLO/KD	• CGCM-CTM/EGLO-SLO/KD + HFB/QRPA, deformed OMP, …
Observables	• Yield, spectrum, multiplicity from estimators	• Same + other from 'root tree', angular correlations, …

Thank you for your attention …







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