LA-UR-13-28858

CGMF and CoH3
Nuclear Reaction Codes

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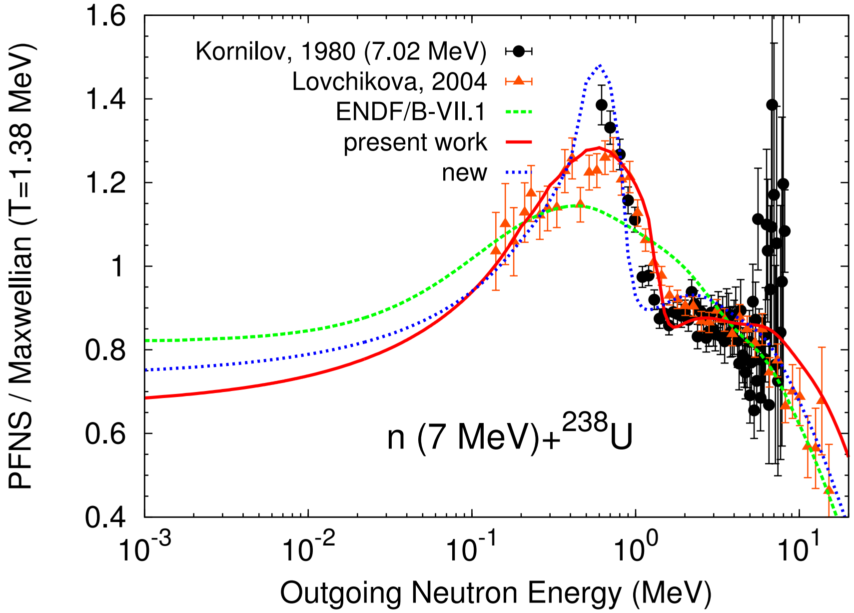
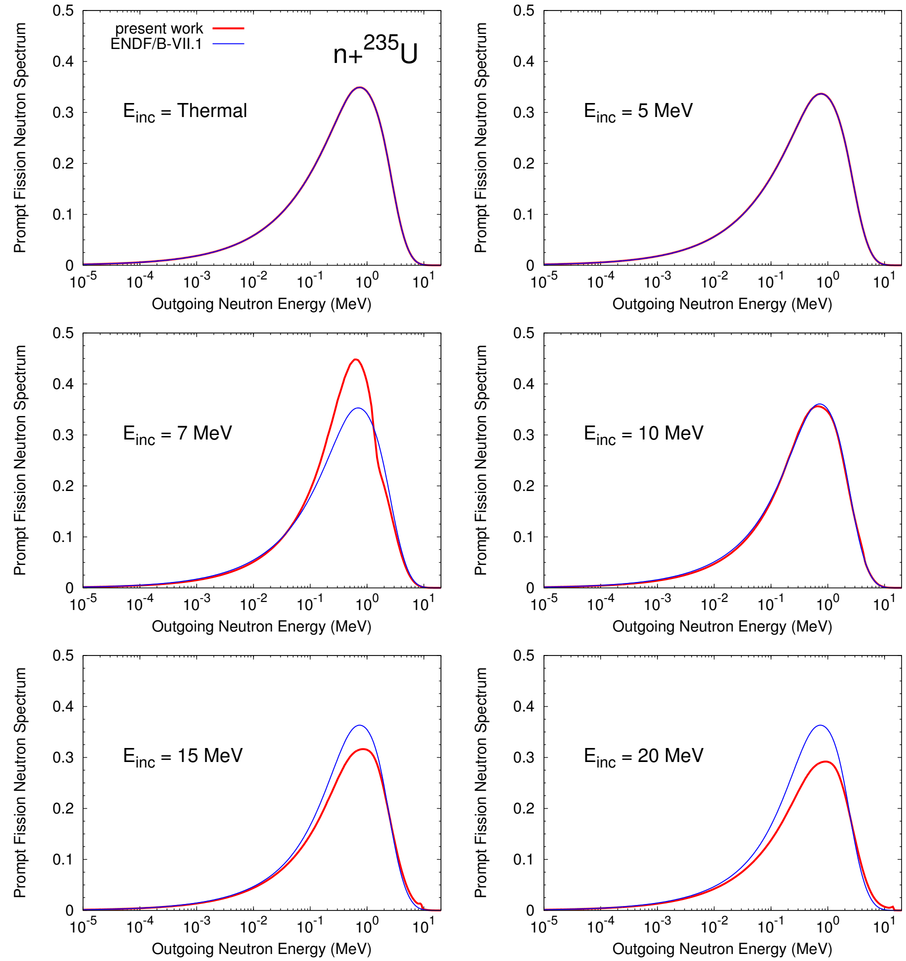
CoH3

- **What is it?**
  - Optical model and coupled-channels calculations (spherical and deformed)
  - Exciton pre-equilibrium model
  - Direct and semi-direct capture model
  - Hauser-Feshbach statistical model
  - Calculates nuclear reaction cross sections for medium and heavy targets
  - keV and MeV energy regions
- **Written in C++**
- **Input files** or… "super-lazy mode": coh –z 26 –a 56 -e 10.0
- **Newest addition:**
  - **prompt fission neutron spectrum** calculated with the Los Alamos model equations.
  - Pre-fission neutrons included

CoH3 calculations of PFNS

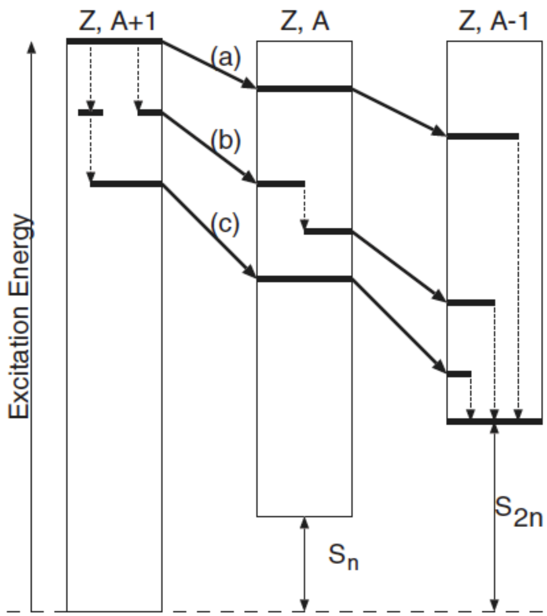
n+^{235}U





CGM
Cascading Gamma Multiplicities

- T.Kawano, P.Talou, M.B.Chadwick and T.Watanabe, "Monte Carlo Simulation for Particle and γ-Ray Emissions in Statistical Hauser-Feshbach Model," J. Nucl. Sci. Tech. 47, 462 (2010).
- **Monte Carlo Hauser-Feshbach code**



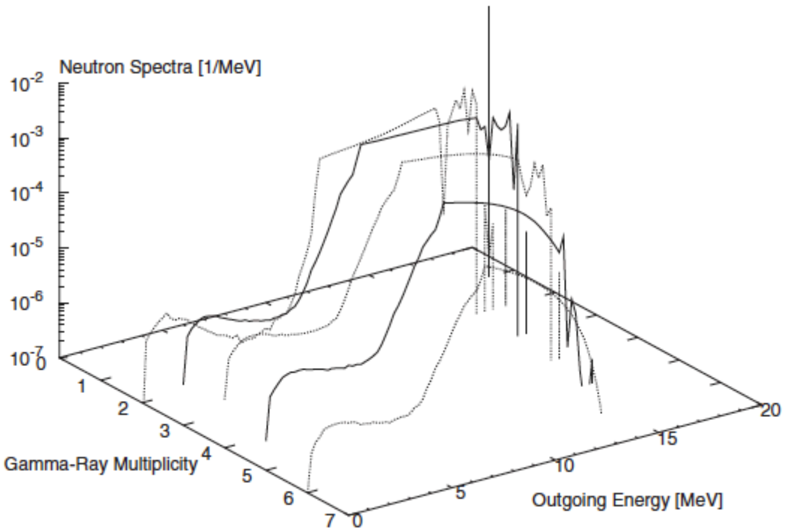
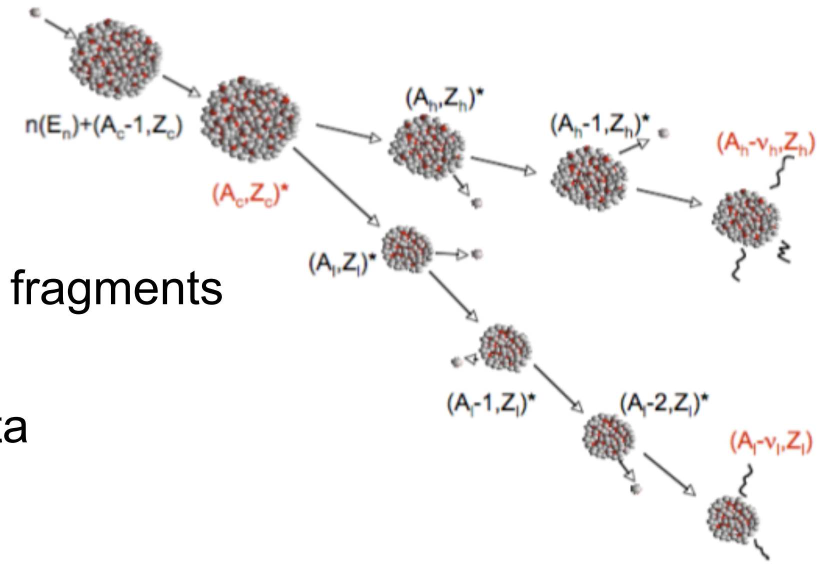
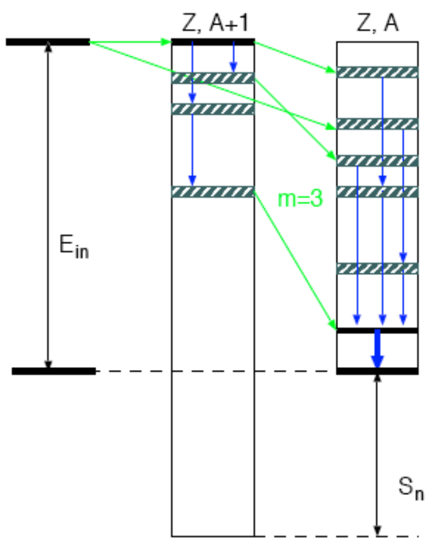


Fig. 6 Inelastic scattering neutron energy spectra from ^{56}Fe by 20-MeV incident neutron. The outgoing neutrons are virtually gated by a γ-ray transition from 847 keV 2^+ state to the 0^+ ground state, as well as a fixed number of γ-ray multiplicities. The spectra are shown alternately by solid and dotted lines.

CGMF
CGM in Fission

- Perform CGM calculations for all fission fragments
- Event-by-event
- Correlations, distributions, exclusive data
- MPI parallel options included





✧ CGMF –i 98252 –e 0.0 –n 100000 ➔ output: history file:

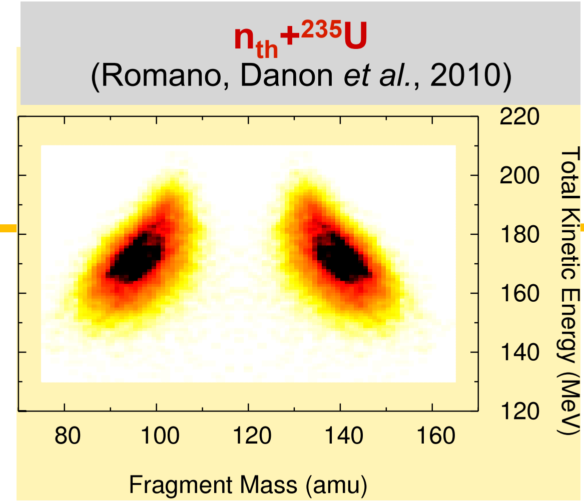
```
43 107 18.6565 5.5 1 104.368 2 6 0 0 0 1 1 1 2 3 3
4.382 0.410 0.242 2.450
0.819 1.890 0.801 1.946 0.275 1.622 0.423 1.827 0.160 2.905 0.077 0.766
55 145 14.7974 9.5 -1 77.0161 2 5 0 0 0 1 2 3 3 3
1.126 1.597 0.900 0.989
0.635 0.359 0.637 2.227 0.810 0.750 0.282 1.098 0.090 1.332
```

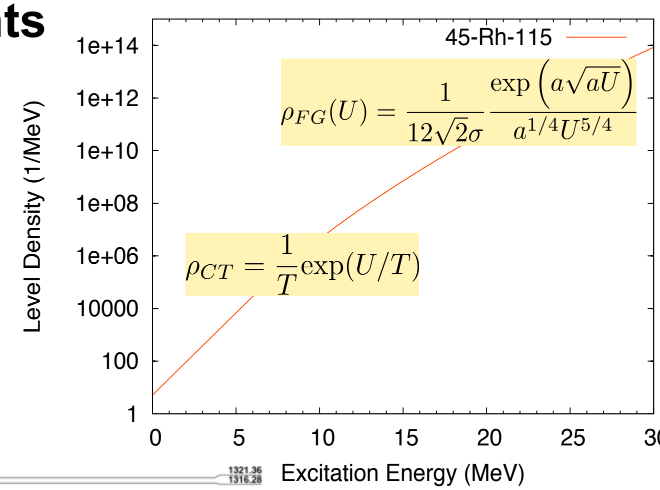
Z, A, U_i, J_i, π_i, KE_i, N_ν, N_γ, …
Neutrons: ε^1_{cm}, θ^1_{cm}, E^1_{lab}, θ^1_{lab}, ε^2_{cm}, θ^2_{cm}, E^2_{lab}, θ^2_{lab},…
Gammas: ε^1_{cm}, θ^1_{cm}, E^1_{lab}, θ^1_{lab}, ε^2_{cm}, θ^2_{cm}, E^2_{lab}, θ^2_{lab}, …

times 100,000 times 2, in this case

CGMF
Complications due to Fission

- **Initial conditions of the fission fragments**
  - Yields in mass, charge, and kinetic energy
  - Initial excitation energies
  - Initial spin and parity distributions
- **Limited information on neutron-rich fragments**
  - Low-lying levels
  - Level density representations
  - Ground-state deformations



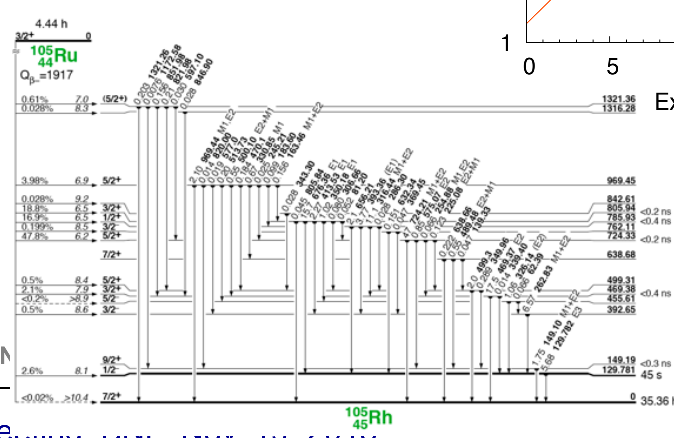


Most probable fission fragment for A=115

(7/2+) 0.99 s

$^{115}_{45}Rh$ β–

Stable isotope ^{105}Rh ?



Fission Fragment Initial Conditions in **Excitation Energy** and **Angular Momentum**

- **Initial Excitation Energies**
  - For a given fragment pair $TXE = Q - TKE = \left(E^*_{int} + E^*_{def} + E^*_{\perp}\right)_{L,H}$
  - Sharing of TXE between light and heavy fragments → $\boxed{R_T} = T_L/T_H$

- **Initial Angular Momentum Distributions**
  - Total angular momentum conservation $\vec{J}_{tot} = \vec{J}_L + \vec{J}_H + \vec{l}$
  - Initial distribution in fragments:

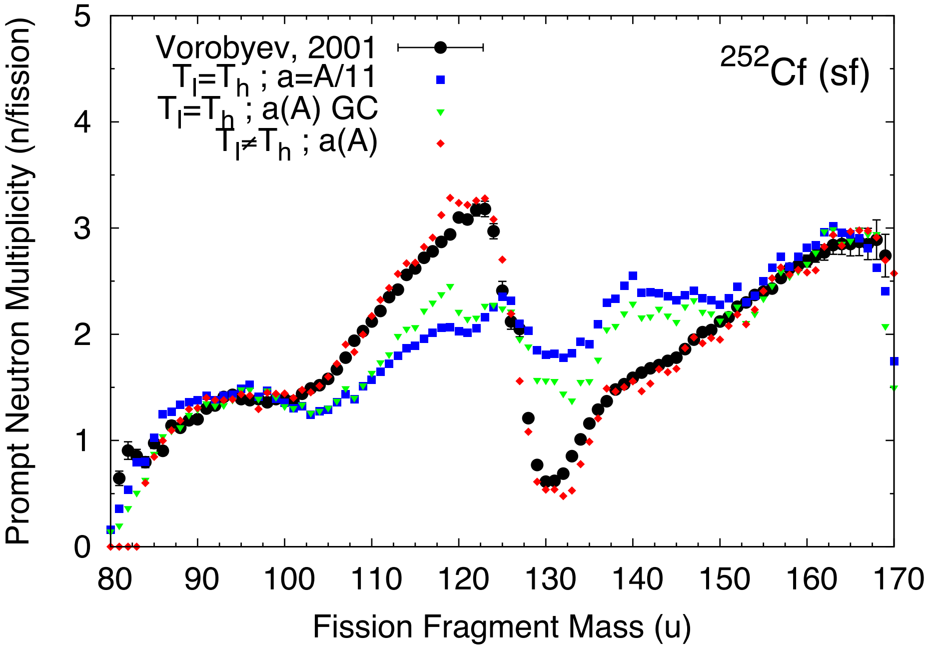
$$P(J) \propto (2J+1)\exp\left[-\frac{J(J+1)}{2B^2(Z,A,T)}\right]$$

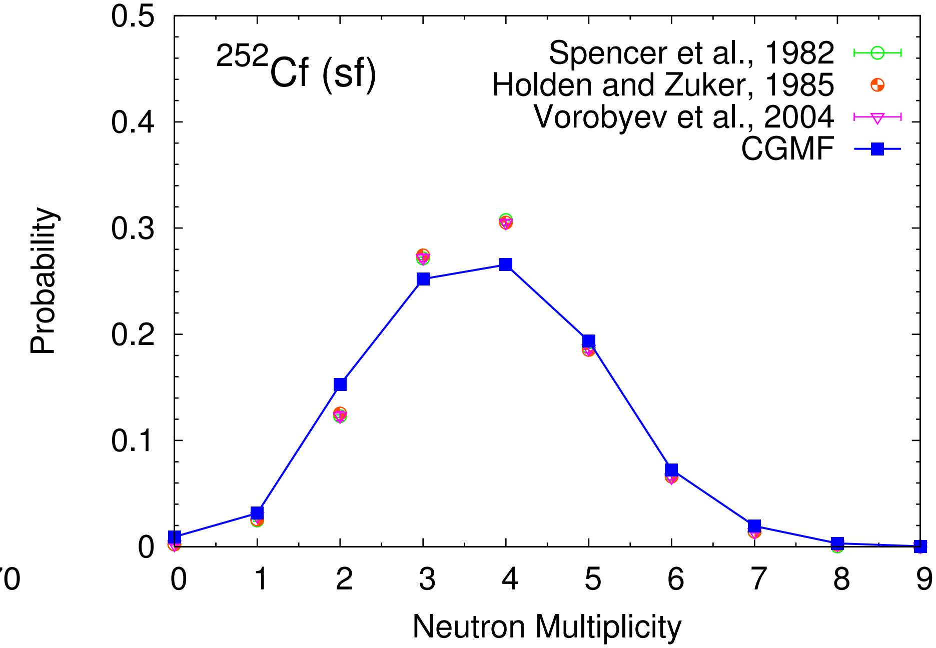
with $B^2(Z,A,T) = \boxed{\alpha}\frac{\mathcal{I}_0(A,Z)T}{\hbar^2}$

I_0 is the moment of inertia of the fragment (A,Z) in its ground-state.

Prompt Neutron Multiplicity <ν>(A) and P(ν)

Example of ^{252}Cf (sf)

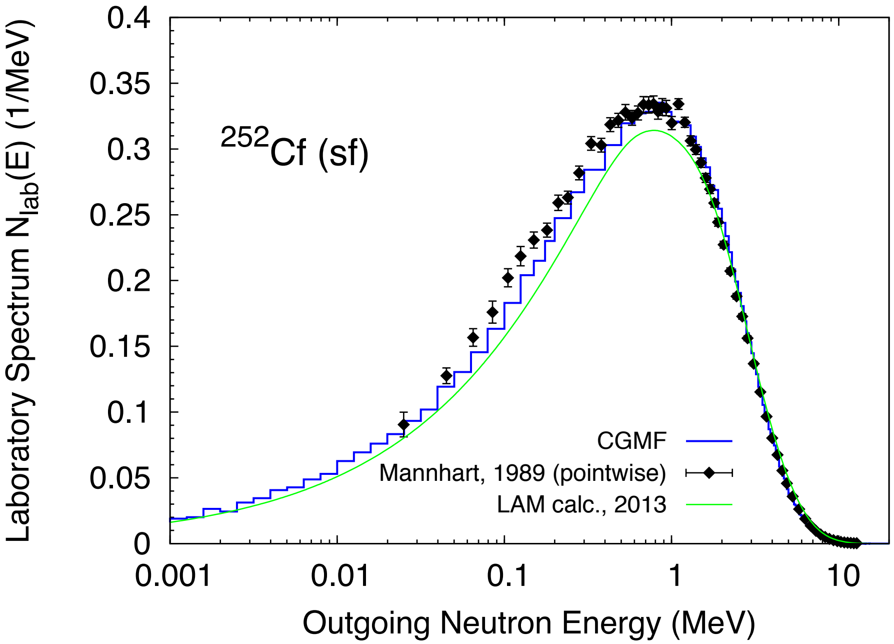


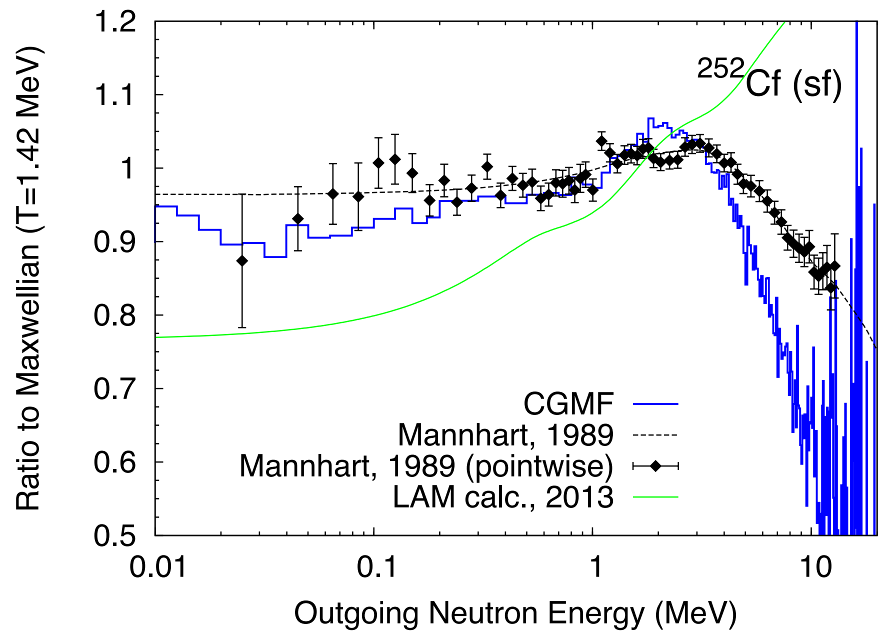


$<\nu>_{calc}=3.78$ vs. $<\nu>_{std}=3.7606$

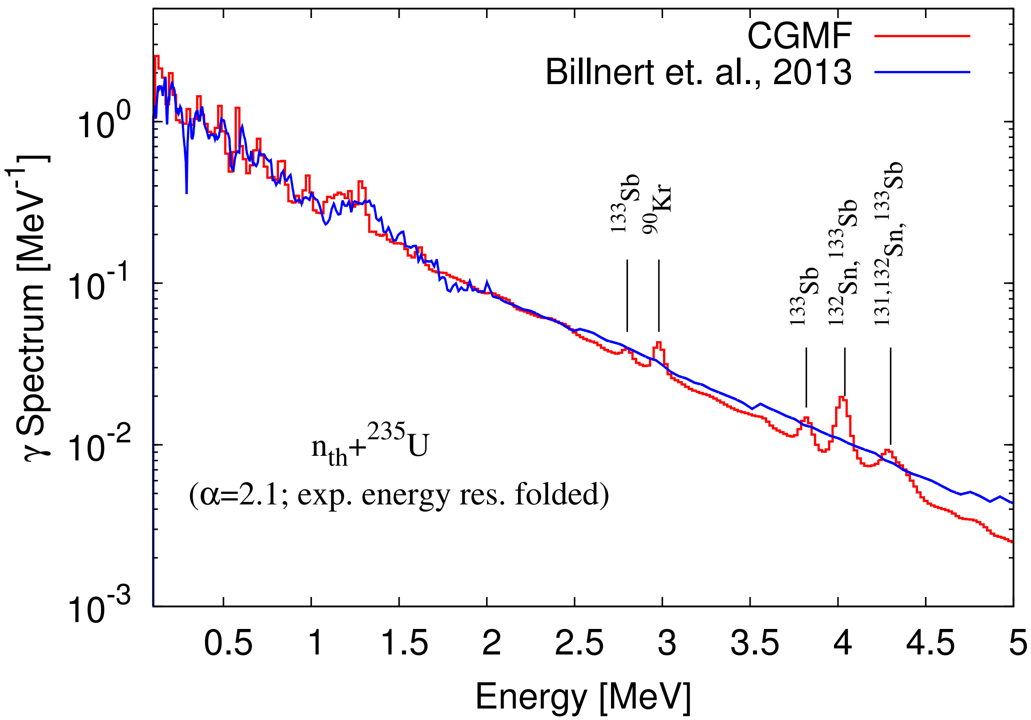
Average Prompt Fission Neutron Spectrum

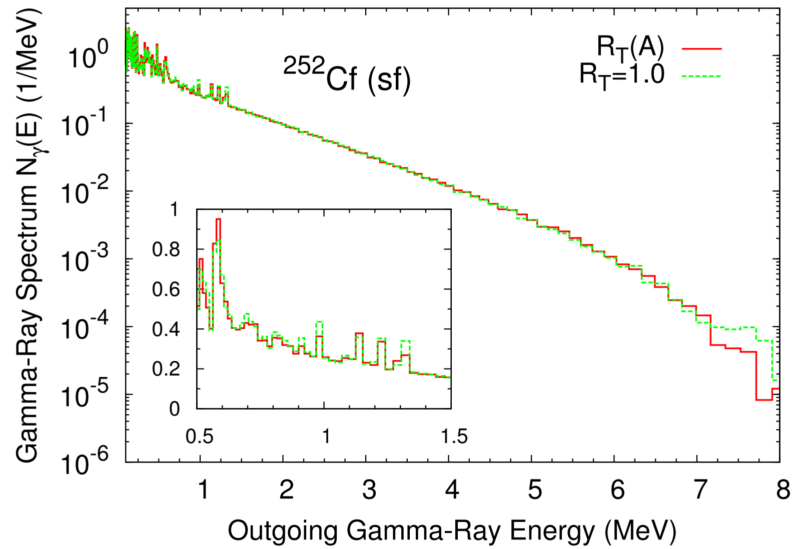
- ^{252}Cf (sf) PFNS is a "**standard**" (Mannhart, 1989)
- Difficulty to reproduce low-outgoing energy tail
- CGMF calculations better at low-energy but too soft at high energies

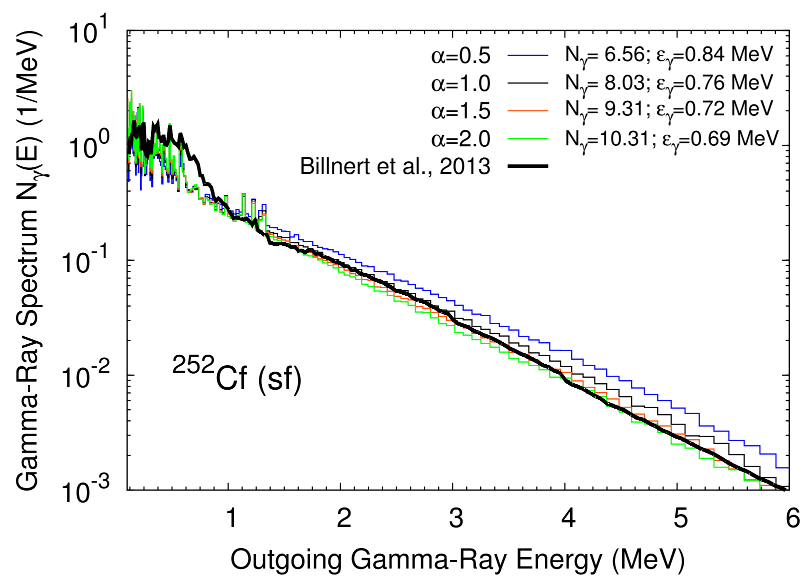




Prompt Photon Spectrum

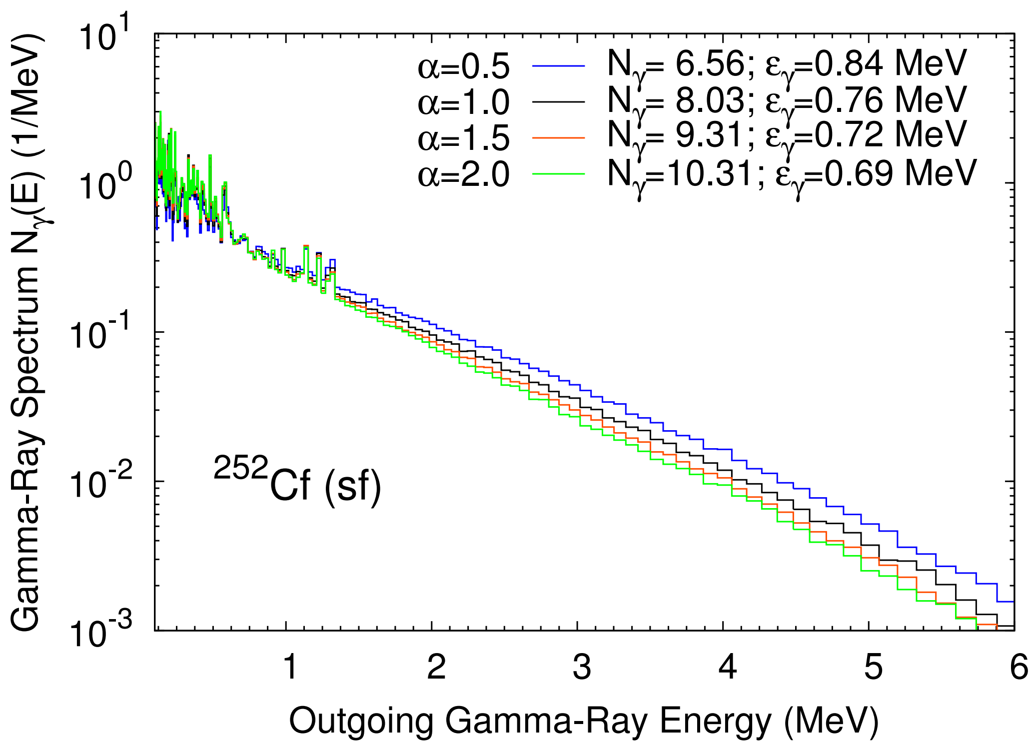


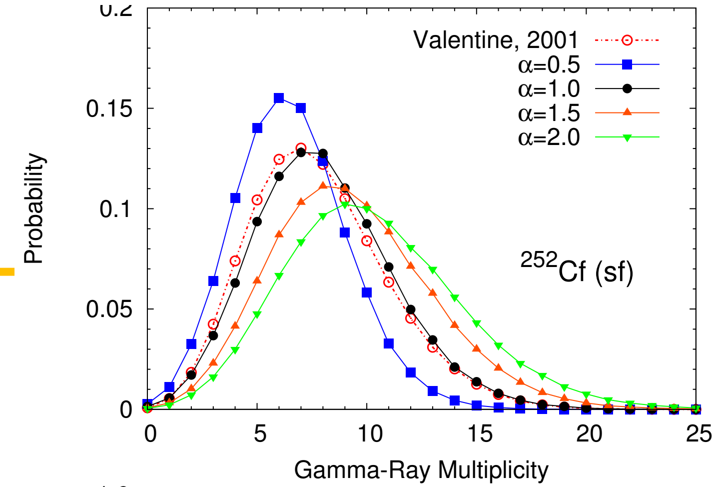


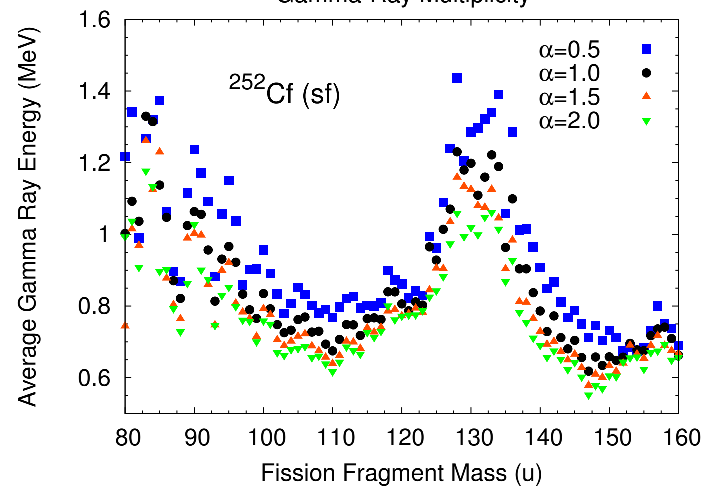


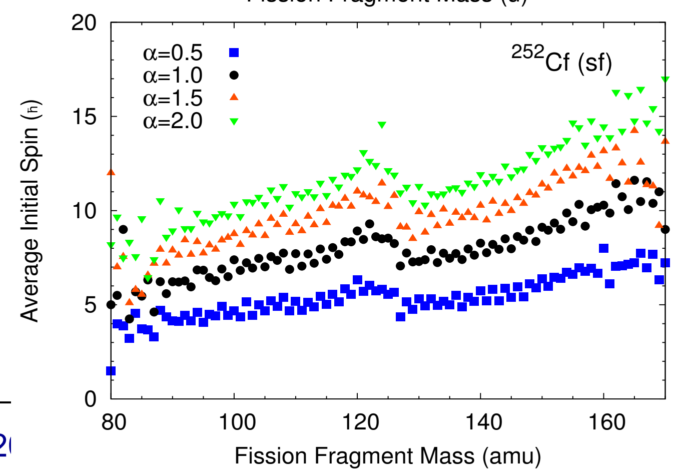
Impact of α (<J_i>)

- **The α-parameter impacts directly the spin-dependent initial population of the fragments.**

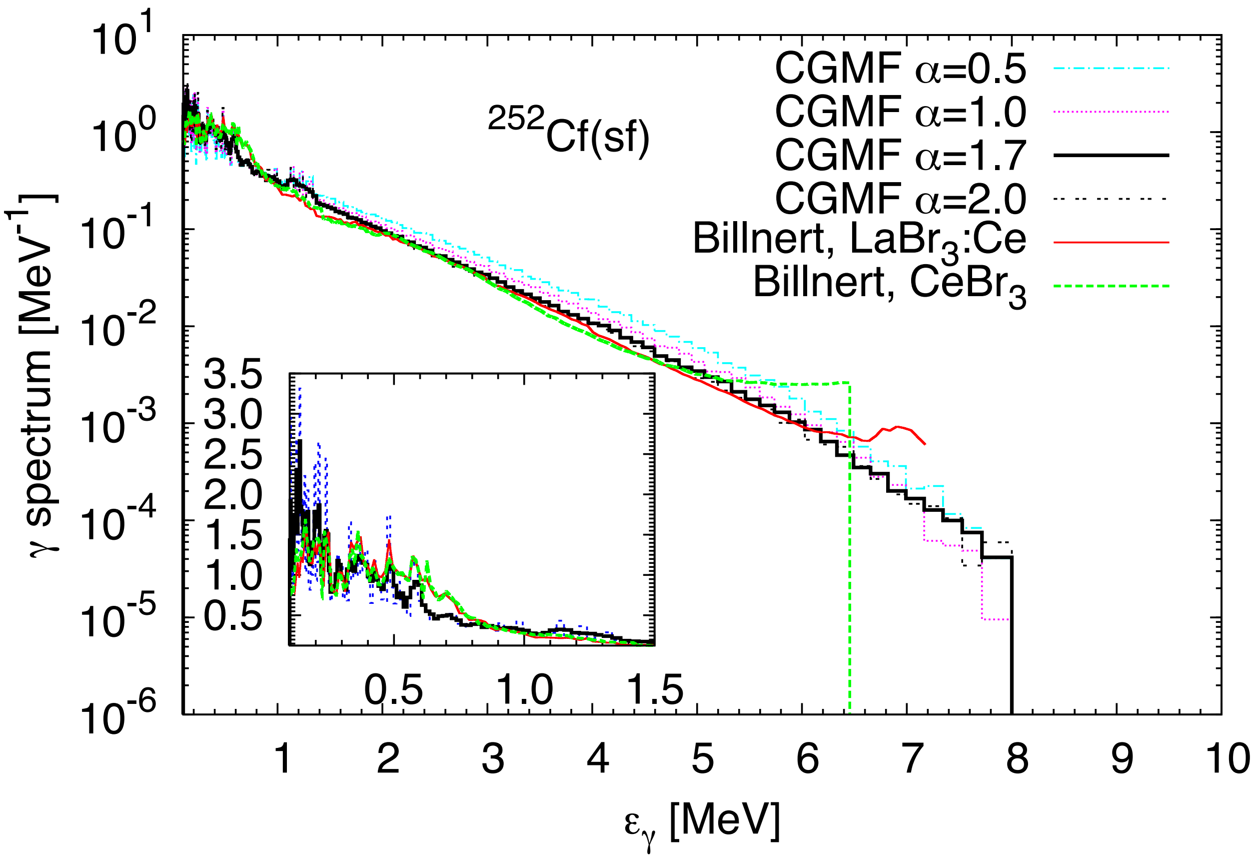






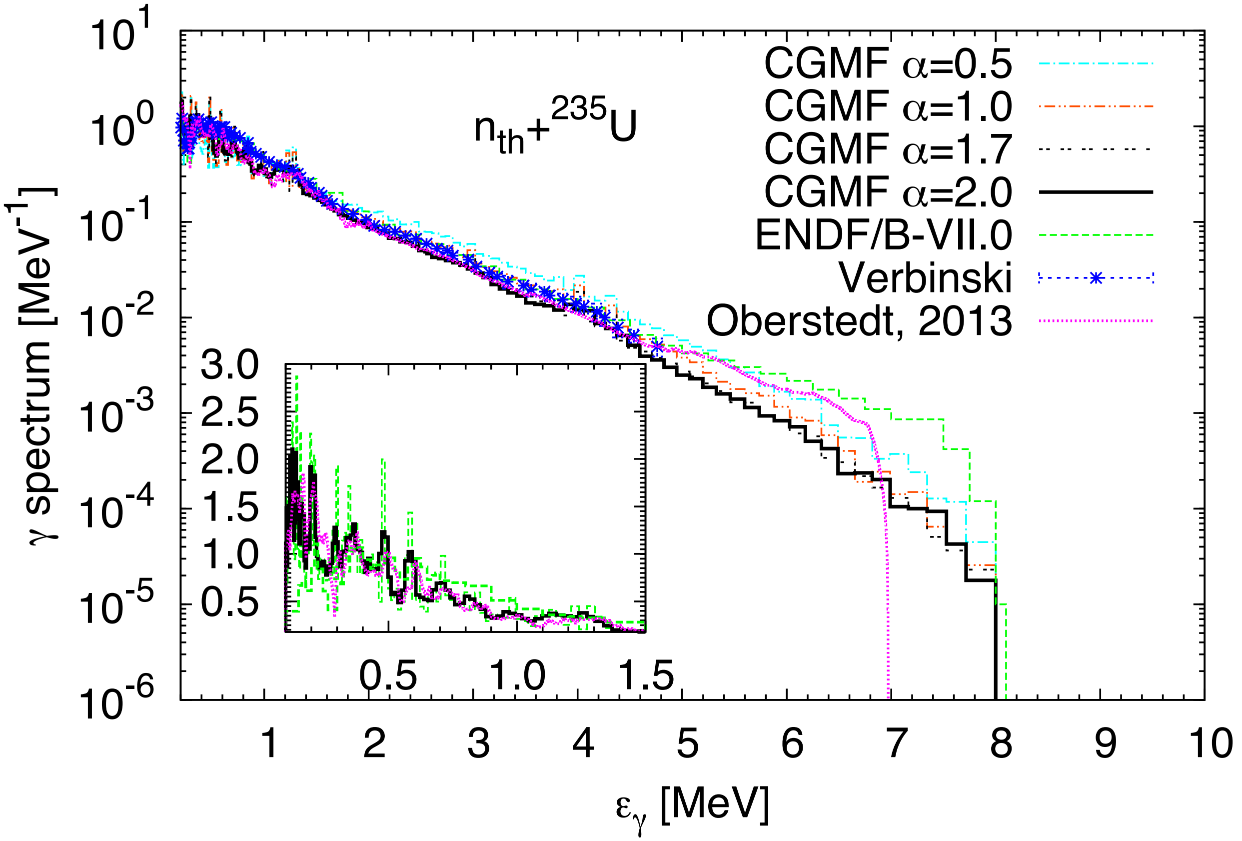


^{252}Cf (sf)



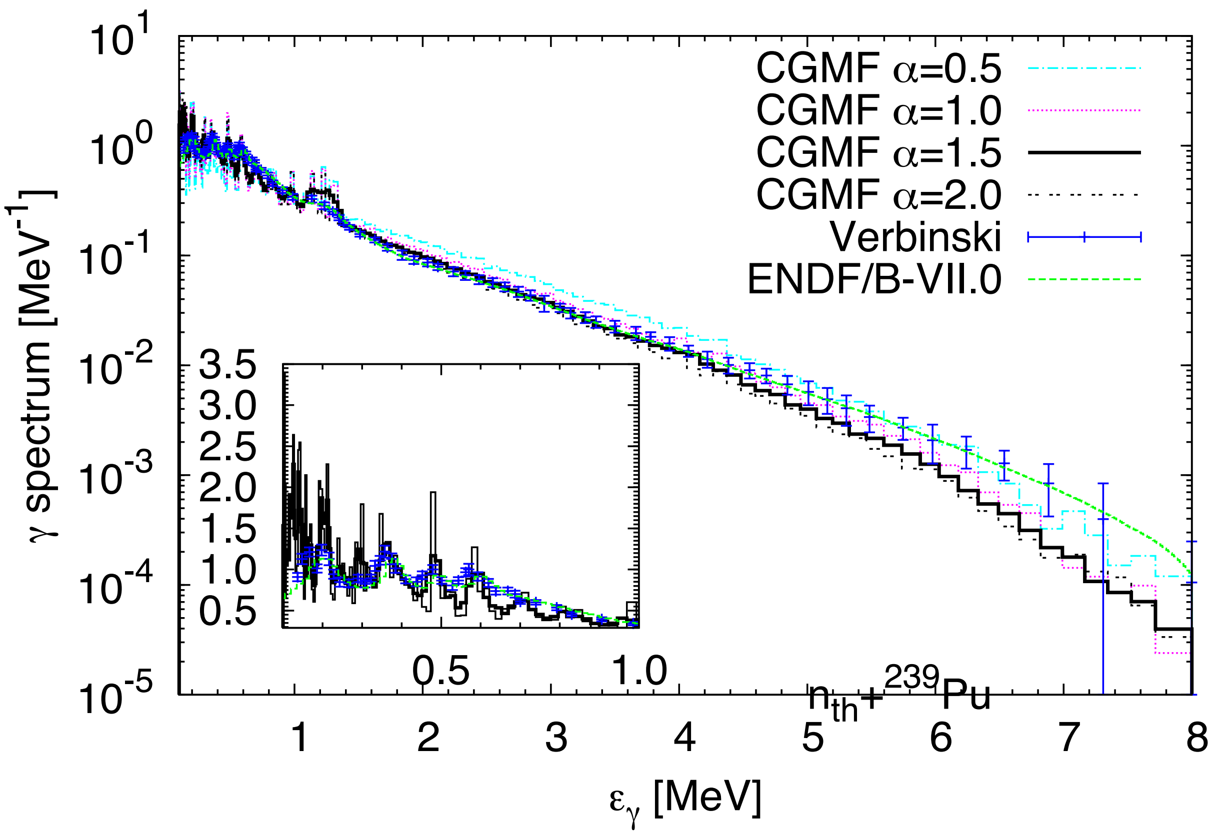
	$<N_\gamma>$	$<\varepsilon_\gamma>$
CGMF (α=1.7)	8.33	0.82
Billnert (2013)	8.30(8)	0.80(1)
ENDF/B-VII.1*	7.48	0.94

n_{th}+^{235}U



	$\langle N_\gamma \rangle$	$\langle \varepsilon_\gamma \rangle$
CGMF (α=2.0)	8.29	0.83
Oberstedt (2013)	8.25(17)	0.84(17)
ENDF/B-VII.1	7.78	0.87

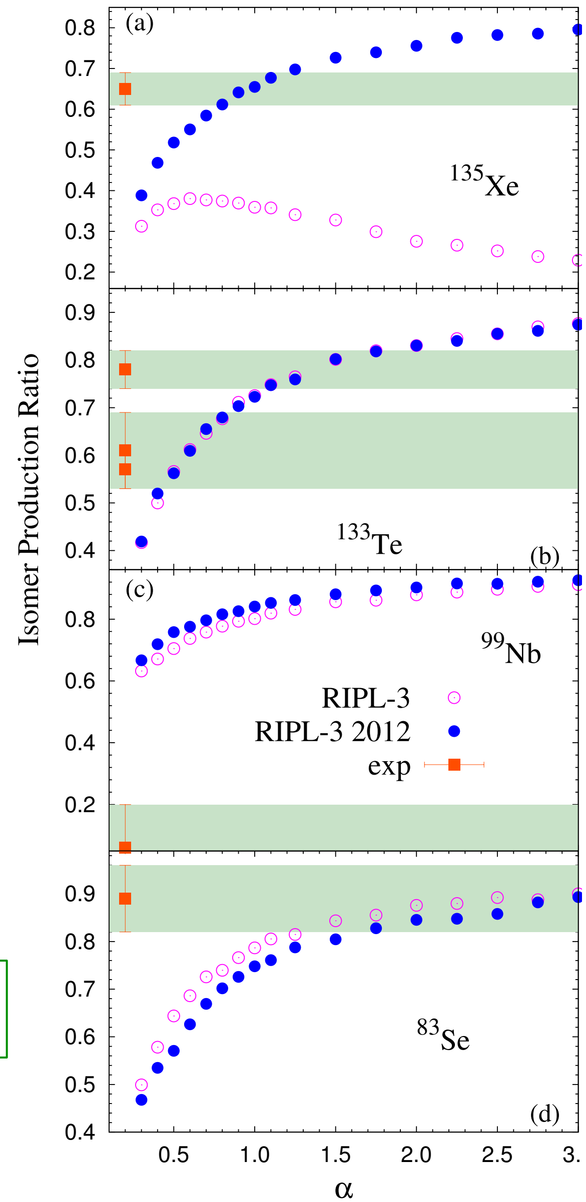
$n_{th}+^{239}Pu$

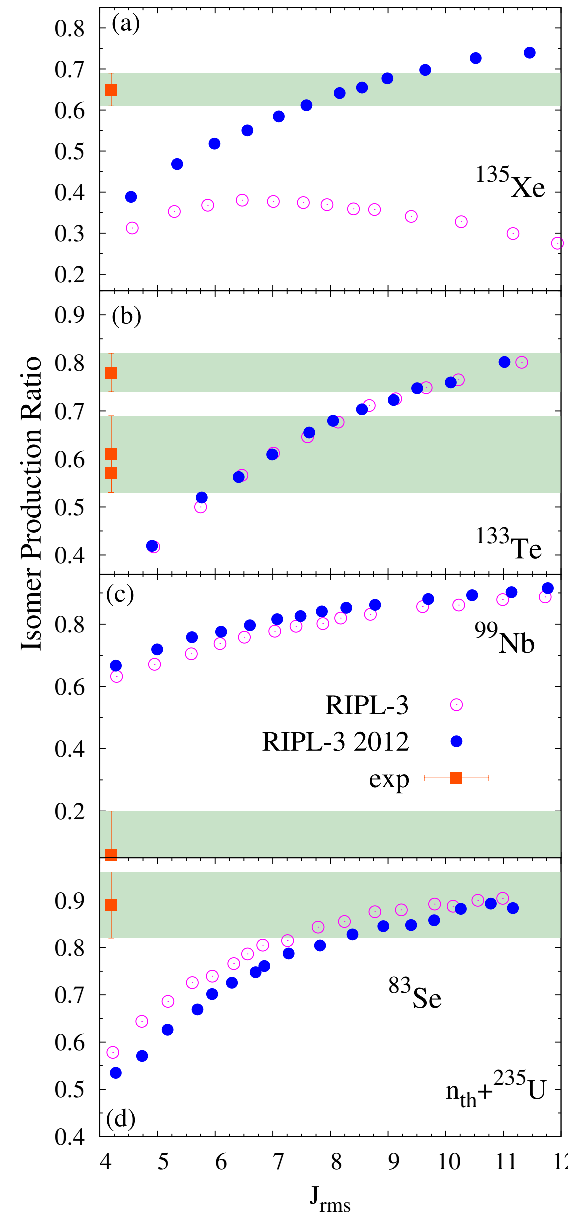


	$<N_\gamma>$	$<\varepsilon_\gamma>$
CGMF (α=1.5)	7.91	0.83
ENDF/B-VII.1	7.048	0.87

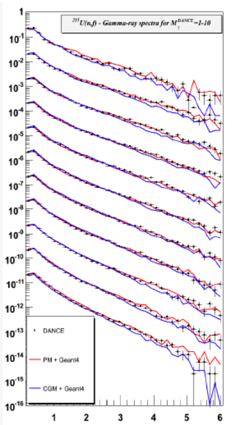
Isomeric Ratios

- Using measured ratios of isomer to ground-state to infer initial J_{rms}
- Very mixed results
- Very sensitive to (often unknown) detailed nuclear structure



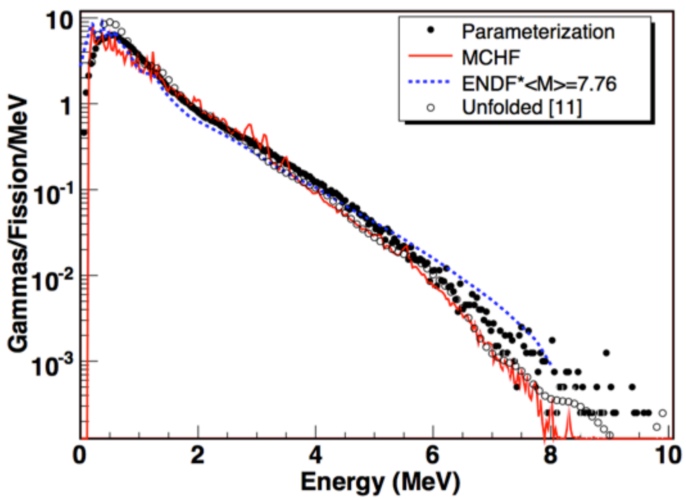


I. Stetcu, P. Talou, T. Kawano, M. Jandel, Phys. Rev. C **88**, 044603 (2013)

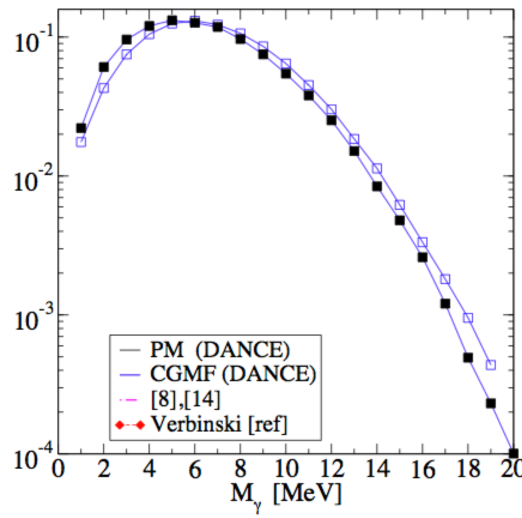


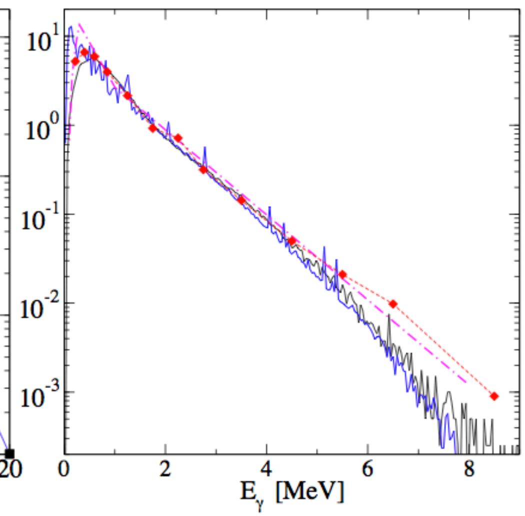
Prompt γ Rays in DANCE

^{239}Pu (n,f)



^{235}U (n,f)





J.Ullmann *et al.*,
"Prompt Gamma-Ray Production in Neutron-Induced Fission of 239Pu", Phys. Rev. C **87**, 044607 (2013).

M.Jandel *et al.*,
"Prompt Gamma-Ray Emission in Neutron-Induced Fission of 235U," to be submitted to PRC.

CGMF Future Work

- **Extensions to**
  - Higher incident energies
  - Other isotopes
    - → Need for pre-neutron fission fragment yields Y(A,Z,KE)
- **User manual**
- **Web interface**
- **Integration with MCNP6**
  (NA-22 funded project starting FY14)