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Title: Fission modeling at LANL

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LA-UR-17-xxxx

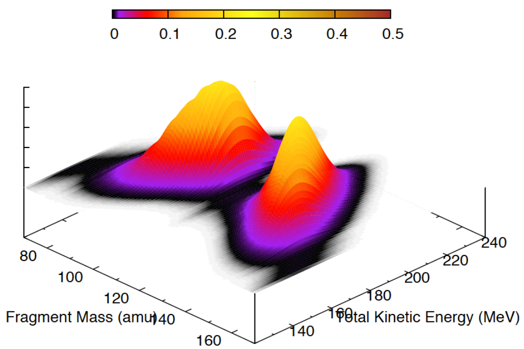
Fission Modeling at LANL

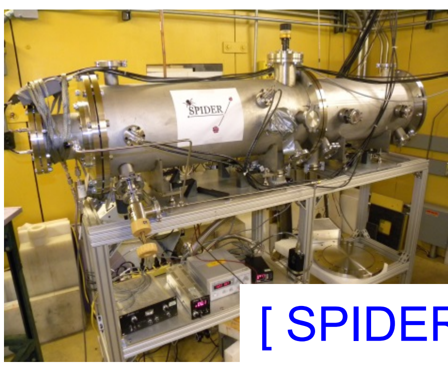
Ionel Stetcu

Theoretical Division, Los Alamos National Laboratory

A Comprehensive Understanding of Fission?

Fission Fragment Yields





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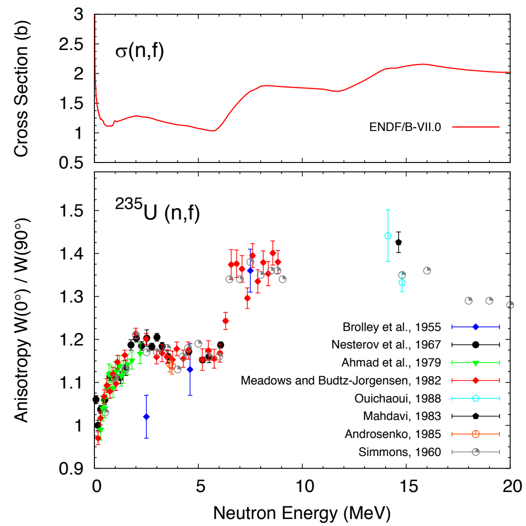
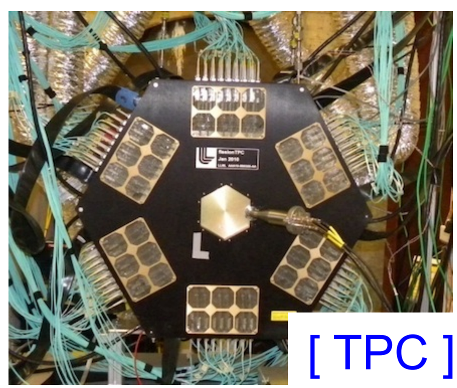
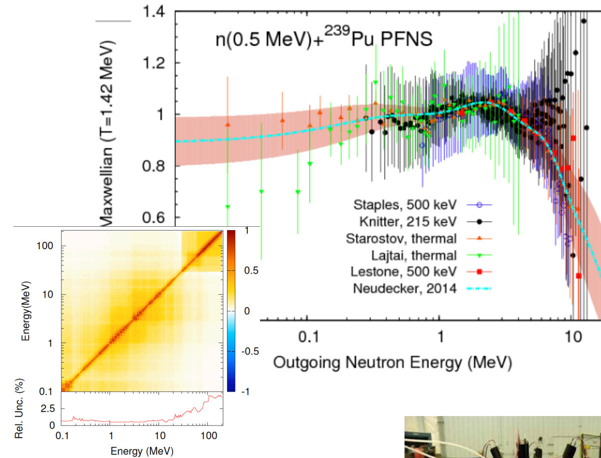
Fission Cross Sections & Fission Fragment Angular Distributions

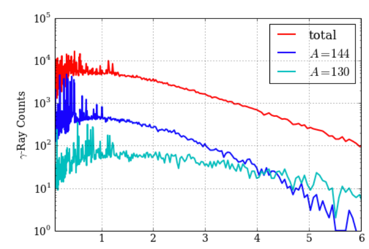


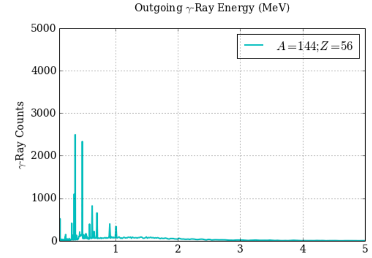


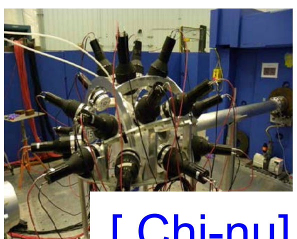
[TPC]

Prompt Fission Neutrons & Photons









[Chi-nu]

[DANCE]

T-2 Nuclear Physics Group, Theoretical Division, LANL

T-2 group
(working on nuclear fission)

- Toshihiko Kawano
- Patrick Jaffke (postdoc)
- Skip Kahler*
- Eric J. Lynn (consultant)
- Peter Möller*
- Denise Neudecker (XCP-3)
- Arnie Sierk*
- Ionel Stetcu
- Patrick Talou

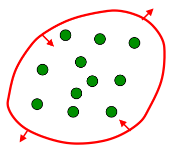
Selected Fission Topics

- (n,f), (γ,f), (t,pf), etc. cross sections
- Fission fragment yields Y(A,Z,TKE)
- Fragment angular distributions
- The (n,γf) process
- Prompt fission neutron spectrum
- Correlations in prompt fission data
- Prompt fission γ rays
- Benchmarking (not just fission) and evaluations

Fission Fragment yields

Fission Fragment Yields

(slide borrowed from Peter Möller & J. Randrup)



Brownian shape motion

Nuclear deformation energy: $E_{\text{def}}(i,j,k,l,m)$

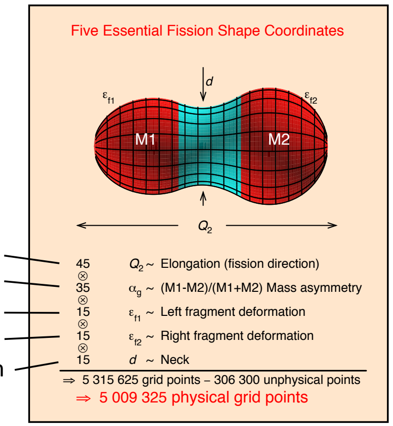
Bias potential: $V_{\text{bias}}(i) = V_0\,(Q_0/Q_2)^2$

Level density parameter: $a_A = A/(8\text{ MeV})$

Temperature T: $E^* - E_{\text{def}} = a_A T^2$

$$\boxed{\Rightarrow\ V(\chi) = E_{\text{def}} + V_{\text{bias}}}$$

χ { i, j, k, l, m



P. Möller *et al*, Nature 409 (2001) 785

Metropolis walk:

N. Metropolis *et al*, J Chem Phys 26 (1953) 1087

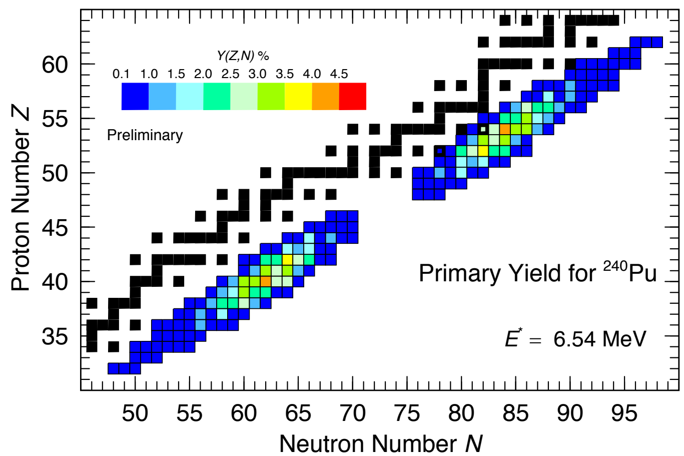
Change shape: $\chi \rightarrow \chi'$?

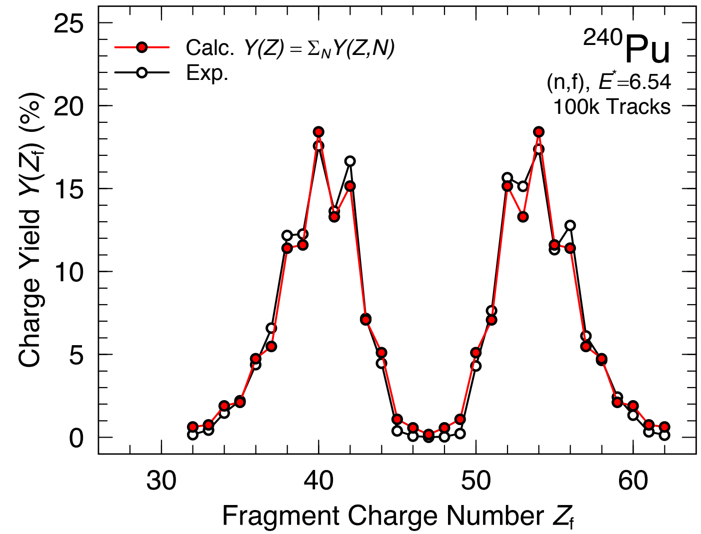
$$\begin{cases} V(\chi') < V(\chi):\ \text{move with } P = 1 \\ V(\chi') > V(\chi):\ \text{move with } P = \exp(-\Delta V/T) \end{cases}$$

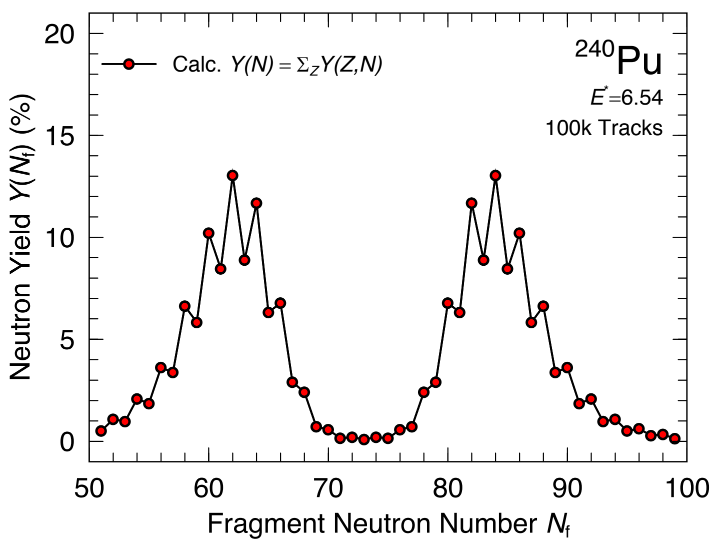
Scission: Critical neck radius $c_0 \approx 2.5$ fm

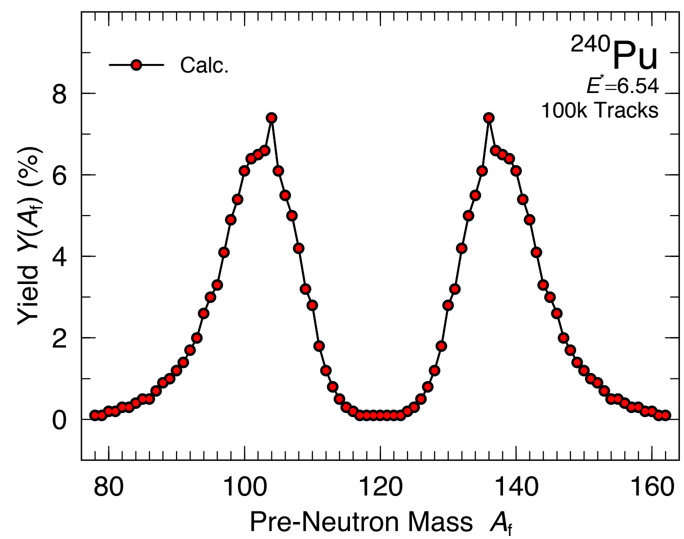
JR: NPF 2010

Selected results









P. Möller

Fission Fragment Yields

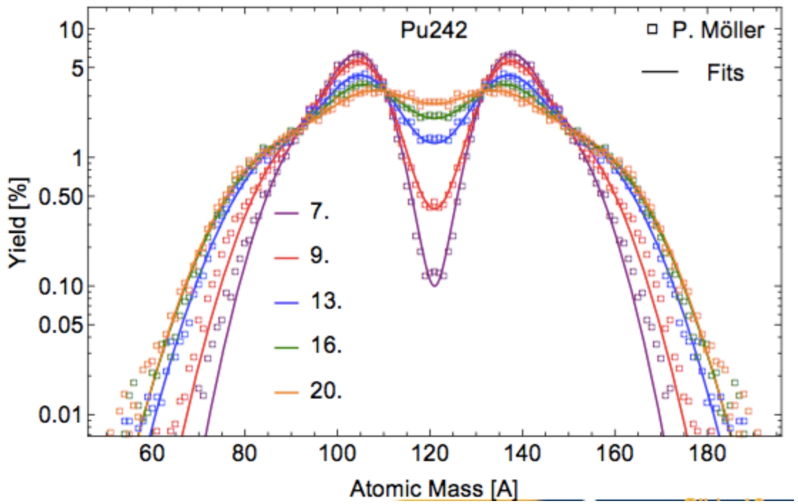
- Results are very promising
  P. Möller and C. Schmitt, EPJA 53, 7 (2017)

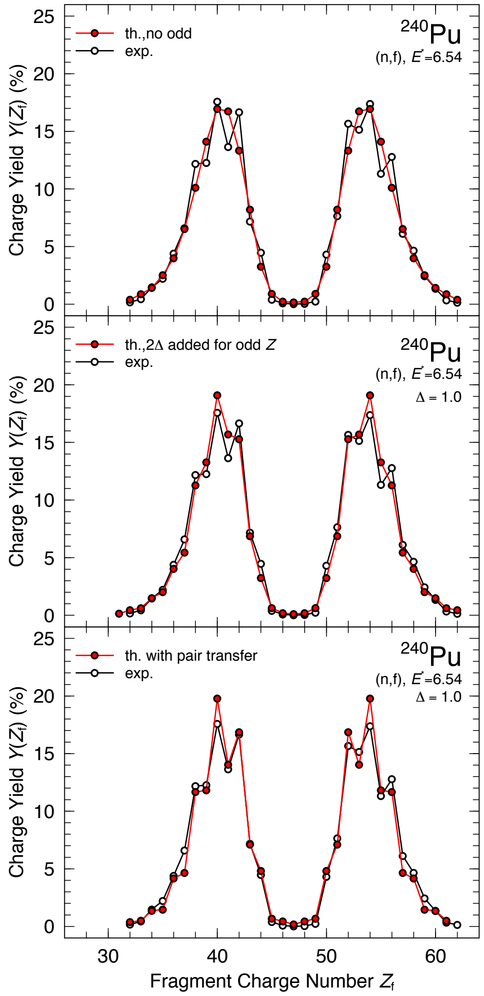
- E*-dependent yields parameterized by 5 Gaussians – Patrick Jaffke (postdoc)

$$Y_i(A, E^*) = \frac{W_i(E^*)}{\sqrt{2\pi\sigma_i^2(E^*)}} exp\left[-\frac{(A-\mu_i(E^*))^2}{2\sigma_i^2(E^*)}\right]$$

Fermi-function fits

Quadratic fits





→ Working on Pu, U and Np series

Langevin model calculations

- Classical dissipative system with fluctuating damping forces

Nuclear shape coordinates

Inertia tensor

$$\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j} = \frac{\partial (K+V)}{\partial p_j} = \frac{\frac{1}{2} M^{-1}_{jk} p_j p_k}{\partial p_j} = M^{-1}_{jk} p_k$$

Stochastic function

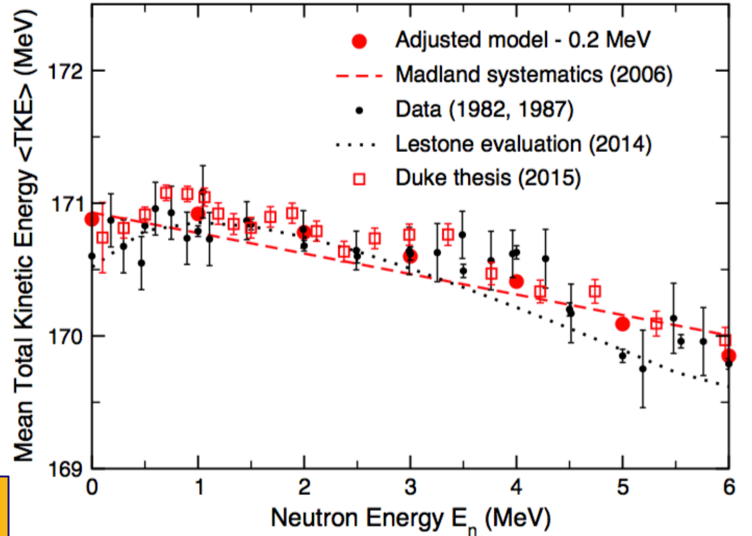
$$\frac{dp_j}{dt} = \frac{\partial H}{\partial q_j} = -\frac{\partial V}{\partial q_j} \dot{q}_k \dot{q}_l - \eta_{jk} \dot{q}_k + \sqrt{\frac{2T}{\Delta t}} \gamma_{jk} \Theta_k(t)$$

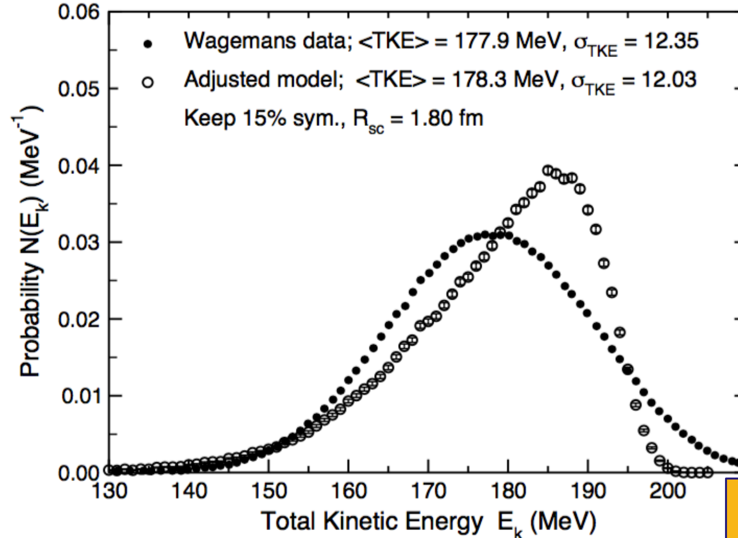
Dissipation tensor

Nuclear temperature

A. J. Sierk

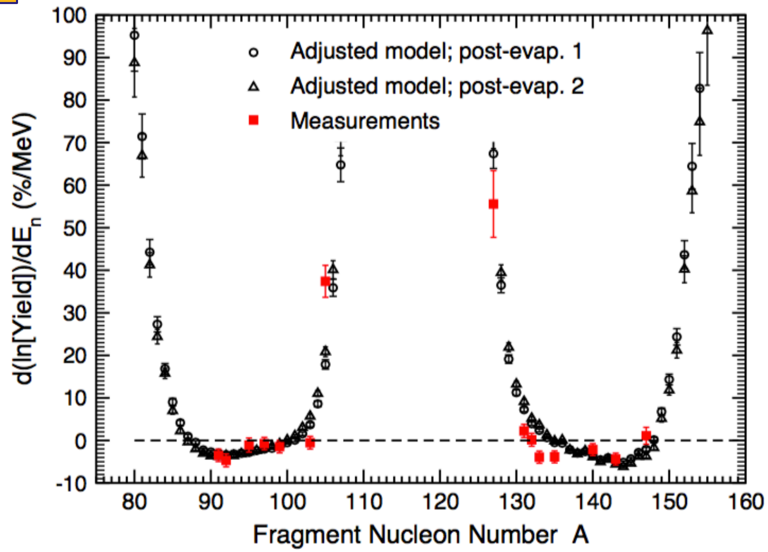
Some results with the Langevin model

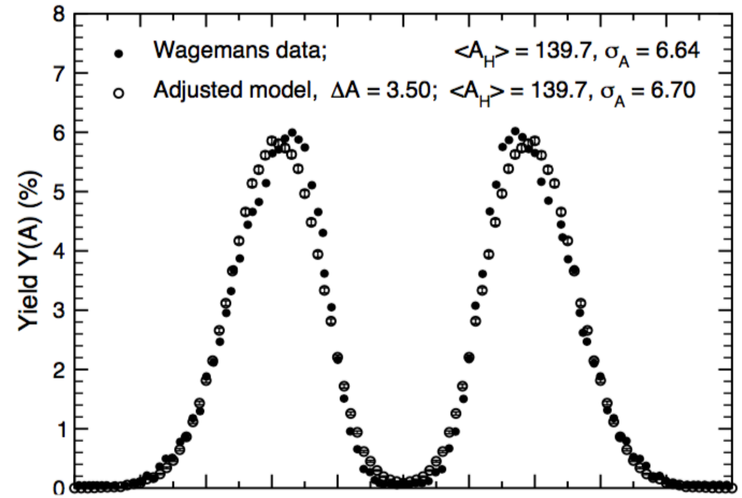




^{235}U

^{239}Pu





Fission Fragment properties within TD-SLDA

Highlight from first microscopic calculation of ^{240}Pu fission:

- ***Fully unrestricted 3D calculation with full nuclear energy density functional***
- ***Long evolution times from outer fission saddle to full scission***
- ***TKE predicted within 3% of expected values***
- ***Light fission fragment heavily deformed, heavy fission fragment spherical (as expected)***
- ***Demonstrated the essential role played by pairing correlations in nuclear shape evolution***

Time-Dependent Density Functional Theory with Nuclear Energy Density Functional a la Skyrme

↓

Construct constrained initial state near the outer fission barrier

↓

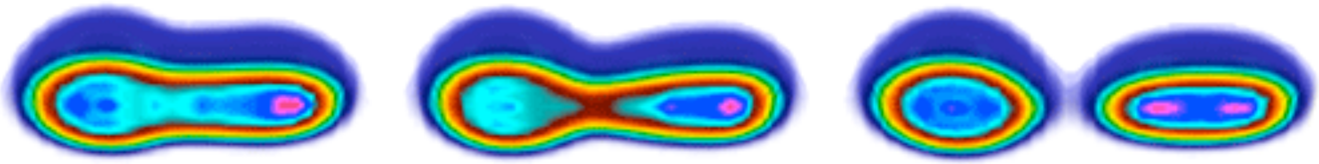
Evolve in time beyond the scission point

↓

Full characterization of fission fragment properties as a function of initial excitation energy of the fissioning nucleus (neutron incident energy):

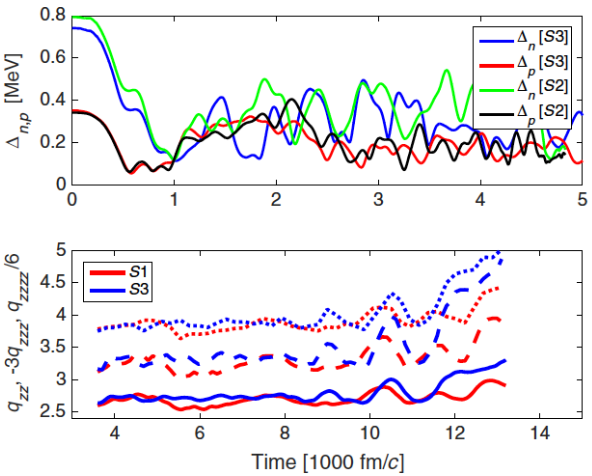
- Average mass, charge, excitation energy, and angular momentum
- TKE of fission fragments

Bulgac et. al, PRL **116**, 122504 (2016)



I. Stetcu

Average fission fragment properties



- Significant amount of collective shape and pairing oscillations
- Time from saddle to fission is sensitive to the functional

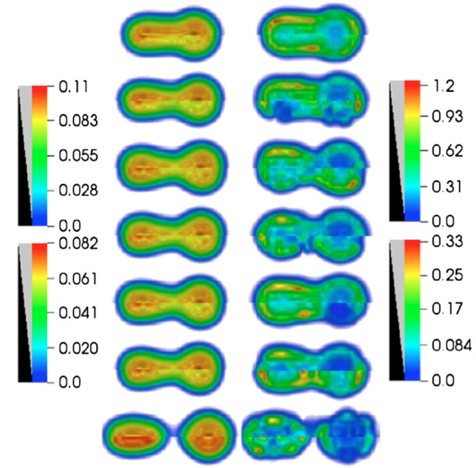
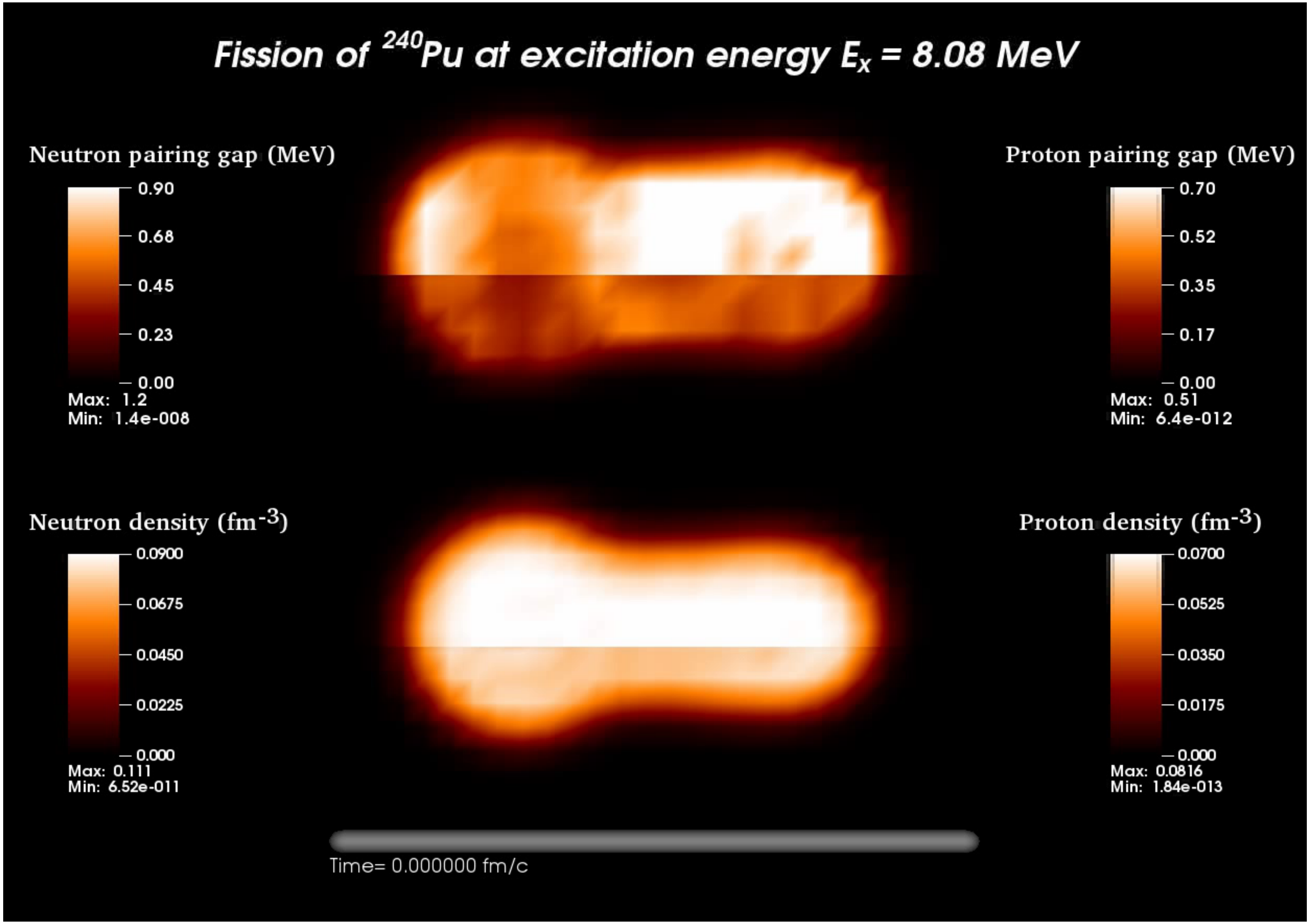


TABLE I. The simulation number, the pairing parameter η, the excitation energy (E^*) of $^{240}_{94}\mathrm{Pu}_{146}$ and of the fission fragments [$E^*_{H,L} = E_{H,L}(t_{SS}) - E_{gs}(N_{H,L}, Z_{H,L})$], the equivalent neutron incident energy (E_n), the scaled initial mass moments $q_{20}(0)$ and $q_{30}(0)$, the "saddle-to-scission" time t_{SS}, TKE evaluated as in Ref. [71], TKE, atomic (A_L^{syst}), neutron (N_L^{syst}), and proton (Z_L^{syst}) extracted from data [72] using Wahl's charge systematics [73] and the corresponding numbers obtained in simulations, and the number of postscission neutrons for the heavy and light fragments ($\nu_{H,L}$), estimated using a Hauser-Feshbach approach and experimental neutron separation energies [8,74,75]. Units are in MeV, fm^2, fm^3, fm/c as appropriate.

S no.	η	E^*	E_n	q_{zz}	q_{zzz}	t_{SS}	TKE$^{\mathrm{syst}}$	TKE	A_L^{syst}	A_L	N_L^{syst}	N_L	Z_L^{syst}	Z_L	E_H^*	E_L^*	ν_H	ν_L
S1	0.75	8.05	1.52	1.78	−0.742	14 419	177.27	182	100.55	104.0	61.10	62.8	39.45	41.2	5.26	17.78	0	1.9
S2	0.5	7.91	1.38	1.78	−0.737	4360	177.32	183	100.56	106.3	60.78	64.0	39.78	42.3	9.94	11.57	1	1
S3	0	8.08	1.55	1.78	−0.737	14 010	177.26	180	100.55	105.5	60.69	63.6	39.81	41.9	3.35	29.73	0	2.9
S4	0	6.17	−0.36	2.05	−0.956	12 751	177.92	181		103.9		62.6		41.3	7.85	9.59	1	1

Bulgac et. al, PRL **116**, 122504 (2016)

Fission Dynamics



Modeling of prompt fission neutron and gamma properties

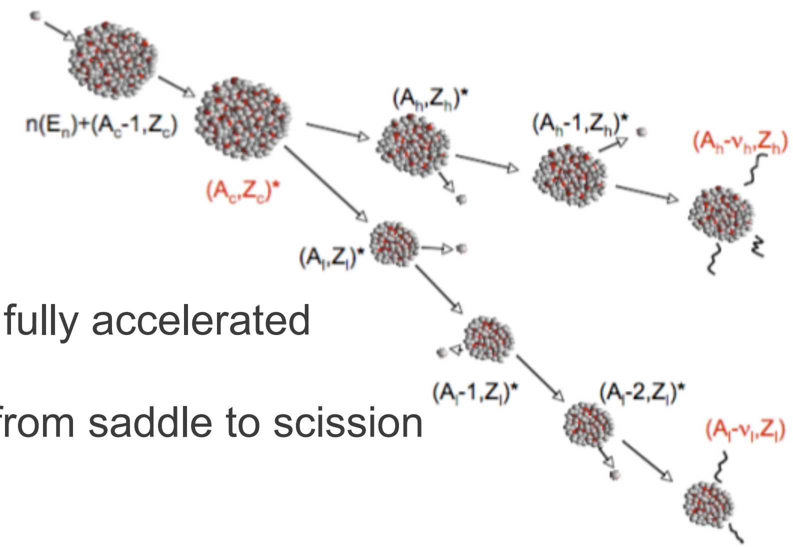
CGMF

- CGM
  - Monte-Carlo implementation of the de-excitation of compound nuclei using the Hauser-Feshbach model
  - Full treatment of neutron-gamma competition
  - Phenomenological approach, many parameters from experiment or systematics

- F
  - Monte-Carlo sampling of fission fragment yields
  - (Monte-Carlo sampling of pre-fission neutrons)
  - Parameterization of
    1. fission yields (mass, charge, TKE)
    2. TXE sharing between FFs
    3. FF angular momenta

$$Y(A, Z, TKE, J, \pi; E_n) \approx Y(A; E_n)Y(Z|A)Y(TKE|A; E_n)P(J)P(\pi)$$

Fission simulation



- Assumptions:
  - prompt fission products emitted from the fully accelerated fragments
  - no emission occurs during the evolution from saddle to scission
  - no emission at the neck rupture

- Model:
  - Consider fission fragments compound nuclei
  - Model neutron and gamma emissions in Hauser-Feshbach formalism
  - Monte-Carlo: access to more quantities (e.g. average multiplicities), correlations

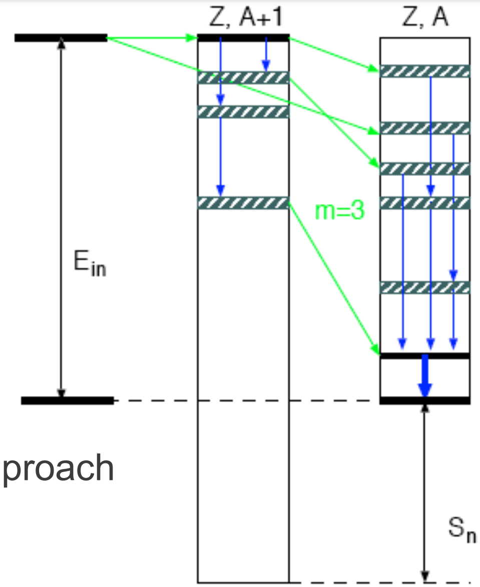
PHYSICAL REVIEW C **87**, 014617 (2013)

Monte Carlo Hauser-Feshbach predictions of prompt fission γ rays: Application to $n_{th}+{}^{235}$U, $n_{th}+{}^{239}$Pu, and ^{252}Cf (sf)

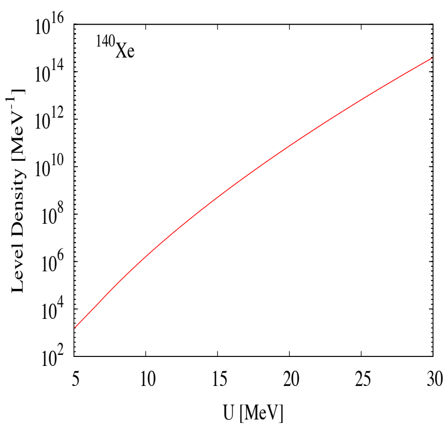
B. Becker,[1] P. Talou,[2,*] T. Kawano,[2] Y. Danon,[1] and I. Stetcu[2]
[1]*Gaerttner LINAC Laboratory, Rensselaer Polytechnic Institute, New York 12180, USA*
[2]*T-2 Nuclear Theory Group, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

Hauser-Feshbach formalism

initial conditions play an important role



MC approach



Neutron emission probability:

$$P(\epsilon_n)dE \propto T_n(\epsilon_n)\rho(Z, A-1, E-\epsilon_n - S_n)$$

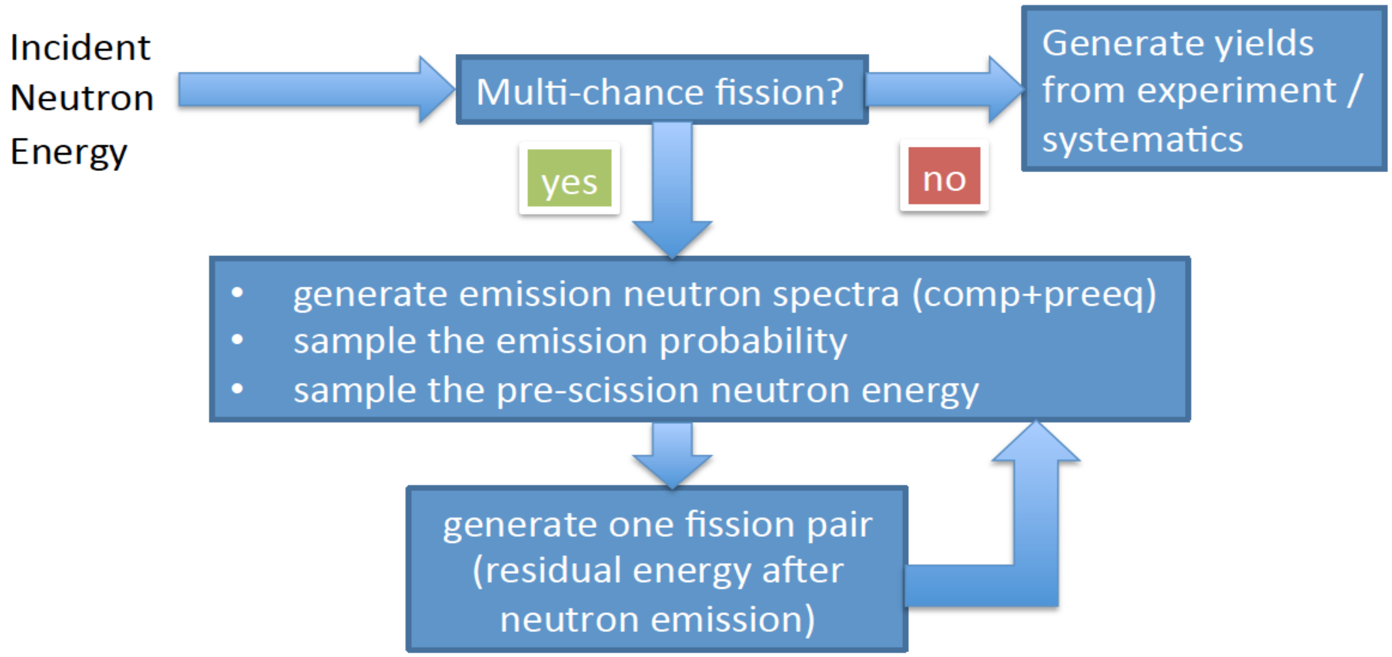
- ✓ Transmission coefficients computed using an optical model
- ✓ Density of states

Gamma emission probability:

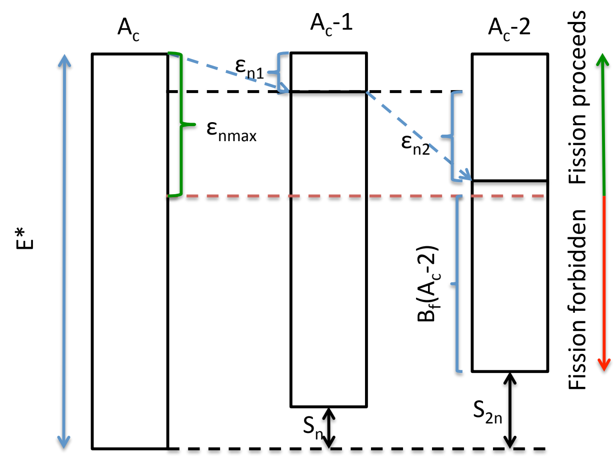
$$P(\epsilon_\gamma)dE \propto T_\gamma(\epsilon_\gamma)\rho(Z, A, E-\epsilon_\gamma)$$

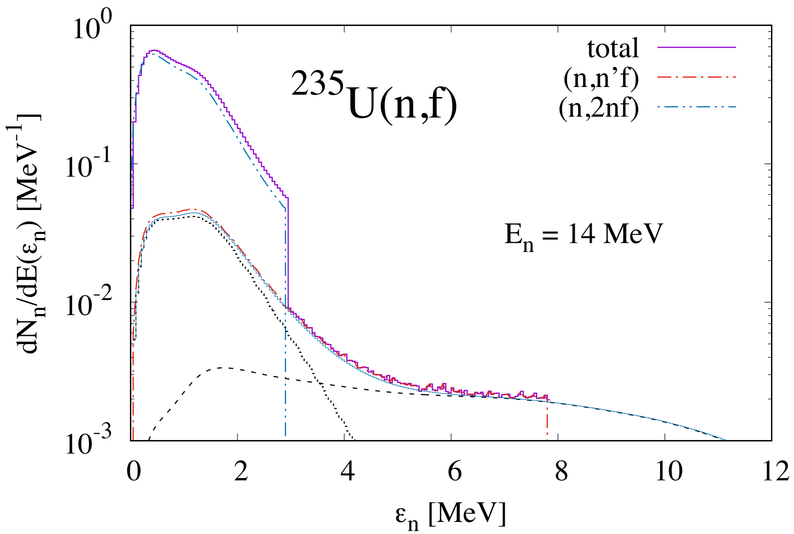
- ✓ Transmission coefficients calculated from the gamma strength function (Brink-Axel hypothesis)
- ✓ Density of states
- ✓ Discrete levels
- ✓ Branching ratios

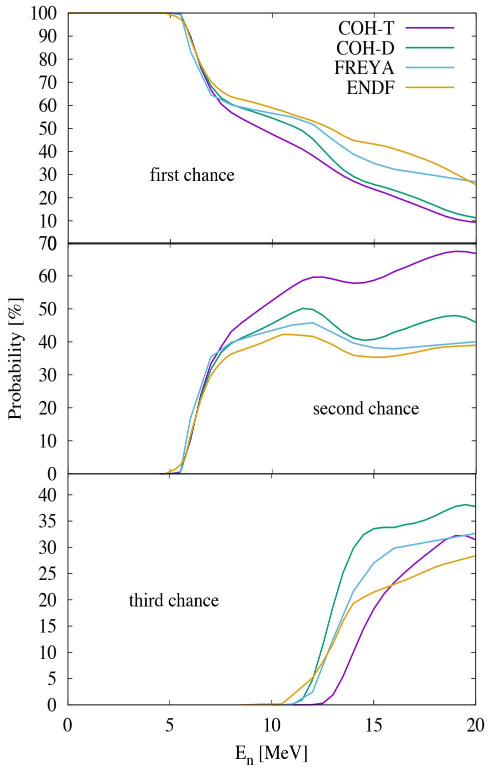
Neutron-induced fission schematics



Multi-chance fission





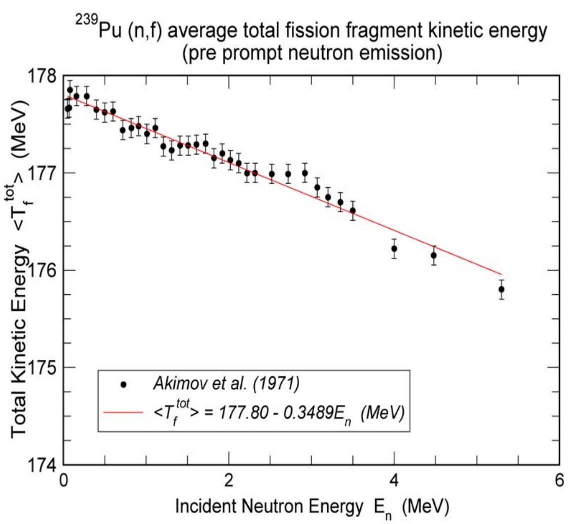


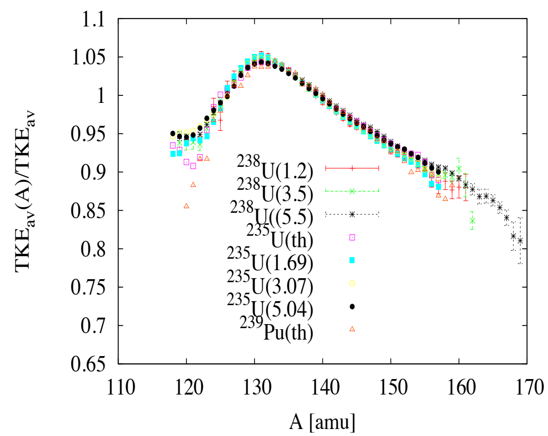
- Double-hump fission barrier penetrability calculations
- Fission probabilities/barrier not observables
- Other fission observables sensitive to the fission probabilities?

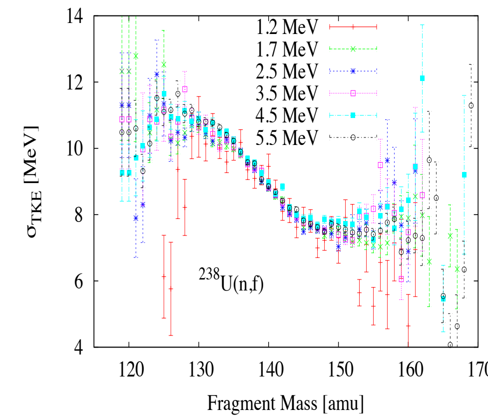
TKE distribution

For each FF mass, assume a Gaussian distribution* given by TKE(A) and $\sigma_{TKE}(A)$

$$Y(A|TKE) = \frac{1}{\sqrt{2\pi}\sigma_{\mathrm{TKE}}(A)} \exp\left(-\frac{(TKE - \overline{\mathrm{TKE}}(A))^2}{2\sigma^2_{\mathrm{TKE}}(A)} \right)$$







- ❖ use TKE(A) at thermal, rescaled to obtain TKE(E_n) from Madland
- ❖ assume the slope fit by Madland holds for all fissioning systems (for a particular initial isotope)
- ❖ TKE(n_{th}) fitted within reasonable values to reproduce ν; for other systems use systematics
- ❖ use $\sigma_{TKE}(A)$ at thermal for all fissioning systems

* Needs corrections because of the Q value

Mass and charge yields

Vogt et. al., PRC **85**, 024608 (2012)

$$Y(A;E_n) = S_L(A;E_n) + \sum_{i=1,2} S_i(A;E_n)$$

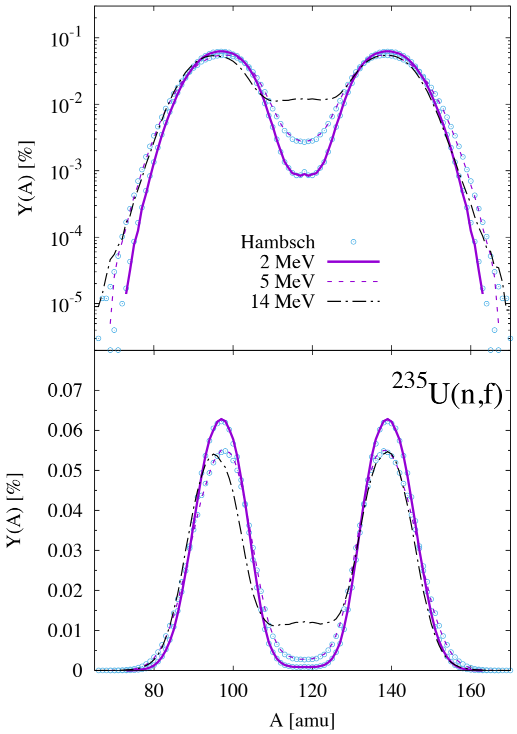
exponential energy dependence

$$S_i(A;E_n) = \frac{N_i(E_n)}{\sqrt{2\pi}\sigma_i(E_n)}\left[\exp\left(-\frac{(A-\bar{A}-D_i(E_n))^2}{2\sigma_i^2(E_n)}\right) + \exp\left(-\frac{(A-\bar{A}+D_i(E_n))^2}{2\sigma_i^2(E_n)}\right)\right]$$

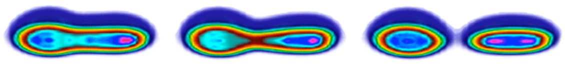
$$S_L(A;E_n) = \frac{N_L(E_n)}{\sqrt{2\pi}\sigma_L}\exp\left(-\frac{(A-\bar{A})^2}{2\sigma_L^2}\right)$$

Quadratic energy dependence

$$2N_1 + 2N_2 + N_L = 2$$



In the future we plan to use data from model simulations (Moller/Sierk/Bulgac)



Charge distribution:

$$Z_p = A_h\frac{Z_c}{A_c} + \Delta Z$$

(Wahl Systematics)

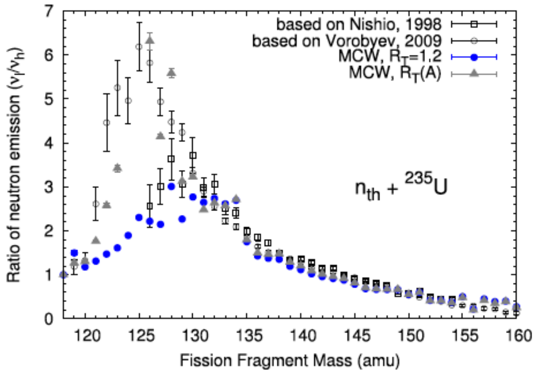
TXE sharing and angular momenta

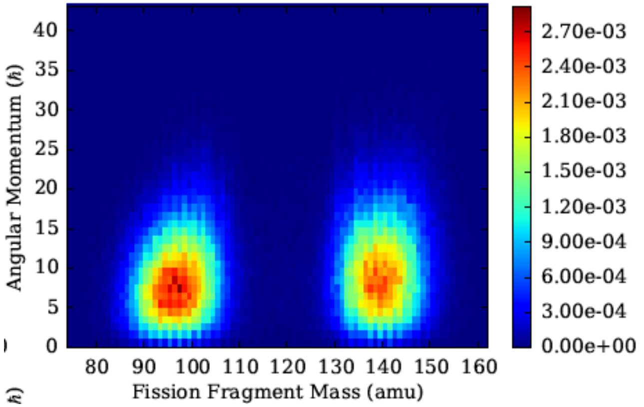
$$TXE = Q_f(A_l, Z_l; A_h, Z_h; A_c, Z_c) - TKE$$
$$= M_l + M_h - M_c + E_{inc} + B_n(A_c, Z_c) - TKE$$

$$R_T = \frac{T_l}{T_h}$$

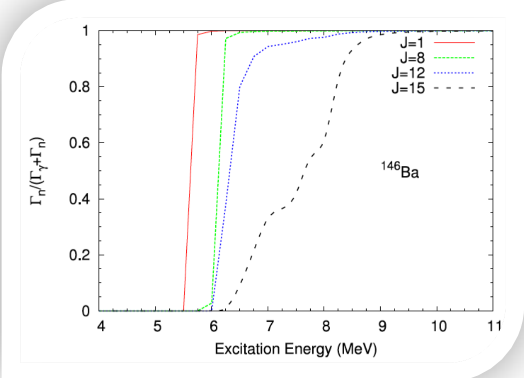
$$P(J) \propto (2J+1)\exp\left(-J(J+1)/(2B^2)\right)$$

$$B^2 = \frac{\mathcal{I}T}{\hbar^2} \quad \mathcal{I} = \alpha \mathcal{I}^0_{rig}(Z, A, \beta)$$





$R_T(A)$ kept constant at all energies



- α fitted to fine tune nubar below 2nd chance fission
- energy dependence extended to 20 MeV

Forward propagation of detector response

$$\begin{pmatrix} \tilde{O}_1 \\ \tilde{O}_2 \\ \vdots \\ \tilde{O}_m \end{pmatrix} = \hat{R} \begin{pmatrix} O_1 \\ O_2 \\ \vdots \\ O_m \end{pmatrix}$$

Bypass the complicated problem of inverting the detector response function

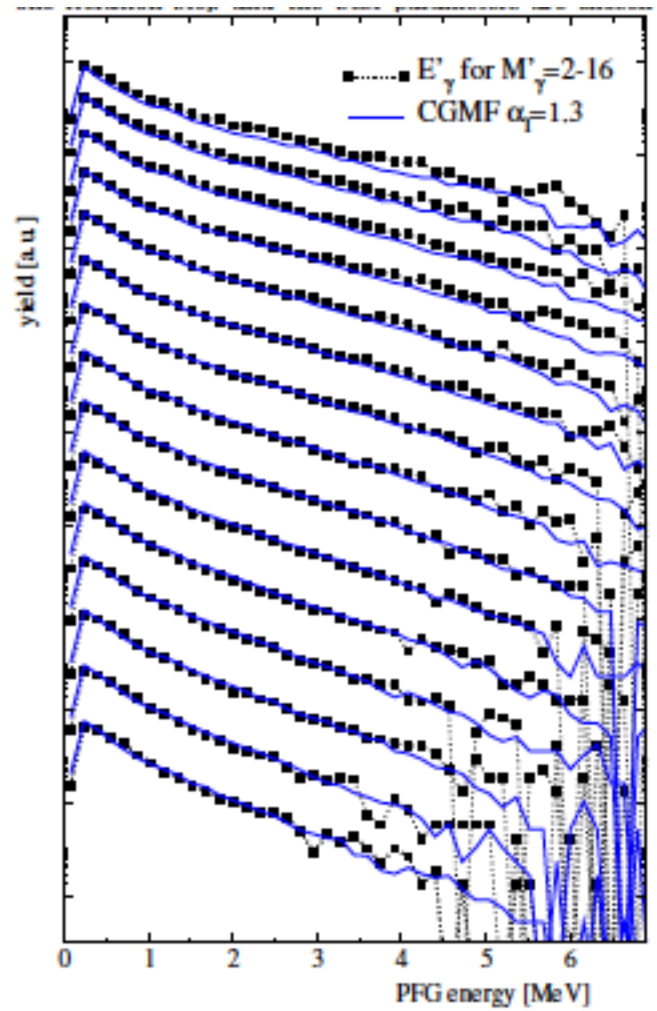
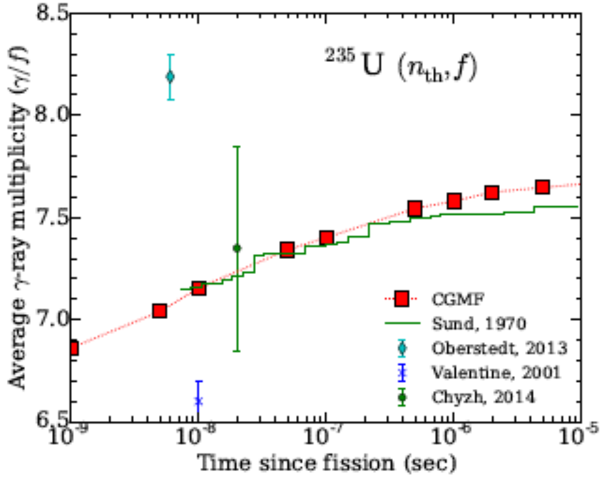
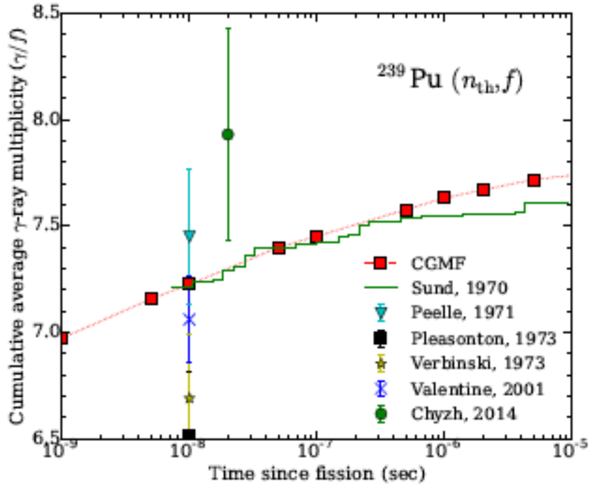
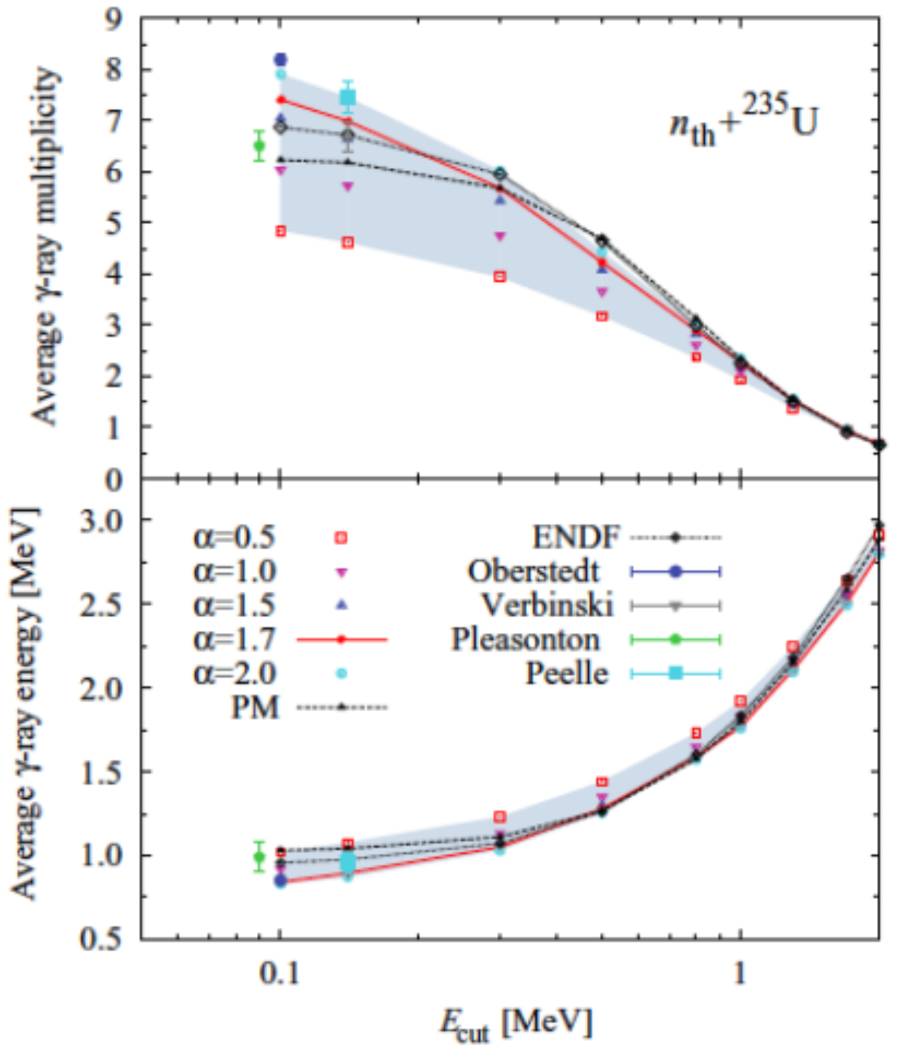


FIG. 16. PFG energy spectra E'_γ for the different multiplicities M'_γ, starting from 2 (top) to 16 (bottom). The measured spectra at DANCE (black markers/lines) are compared to CGMF results (blue solid lines) with α_I=1.3.

Important considerations for γ rays



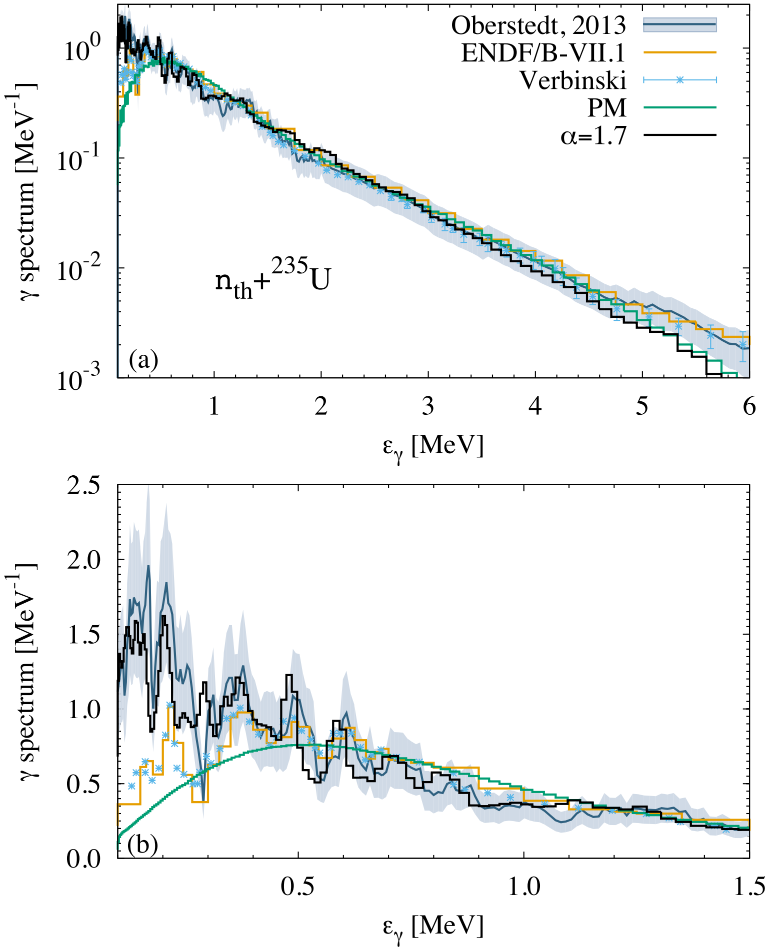


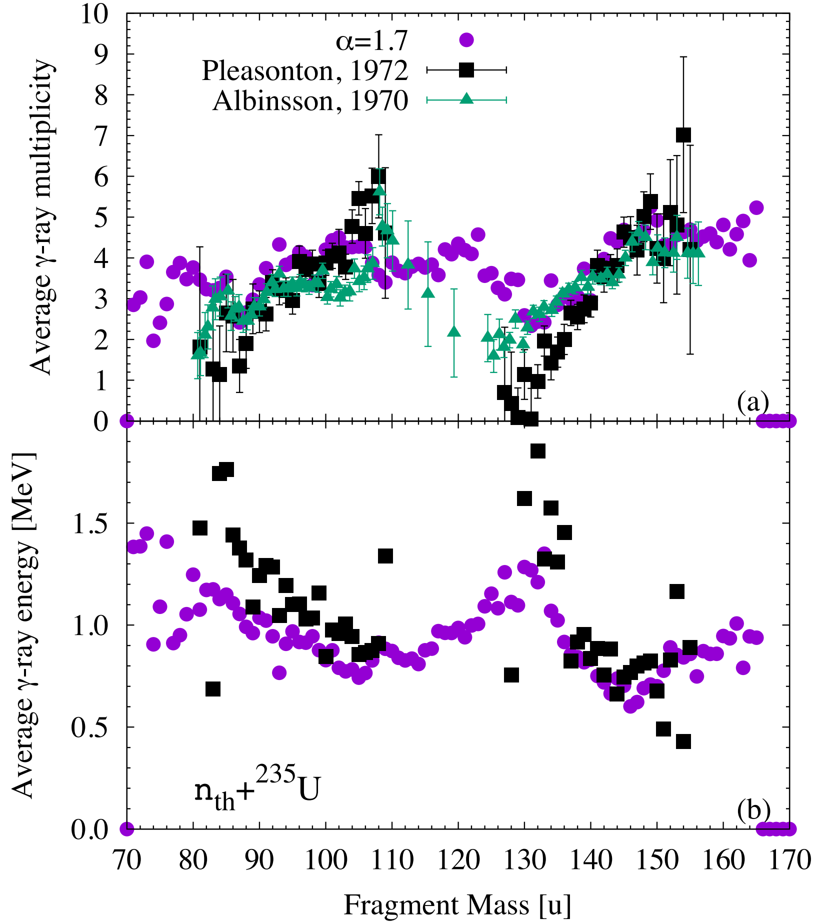


Experimental time coincidence window

Energy detection threshold

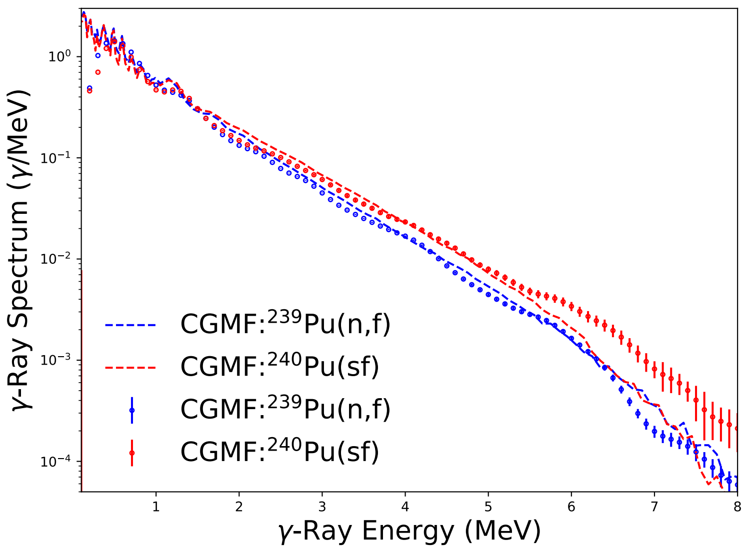
Selected gamma observables

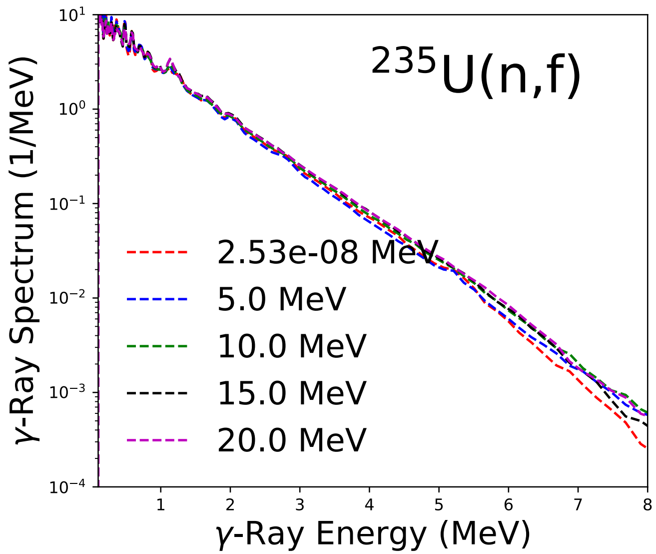


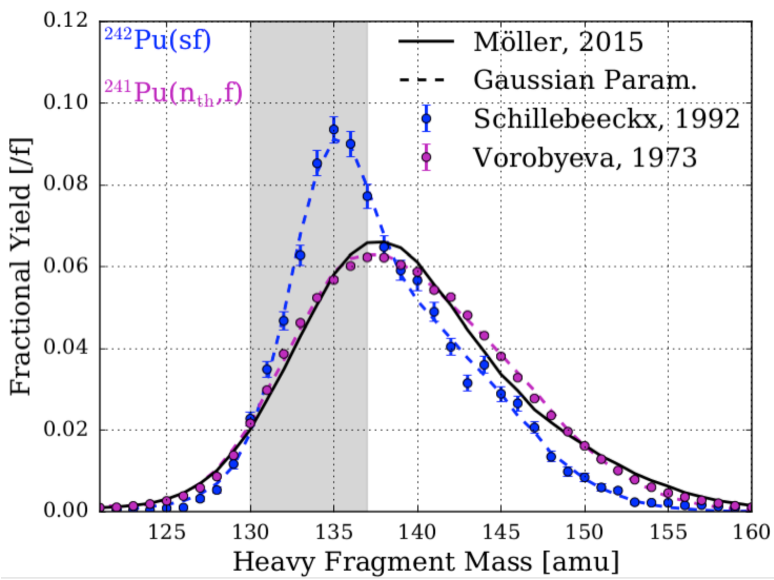


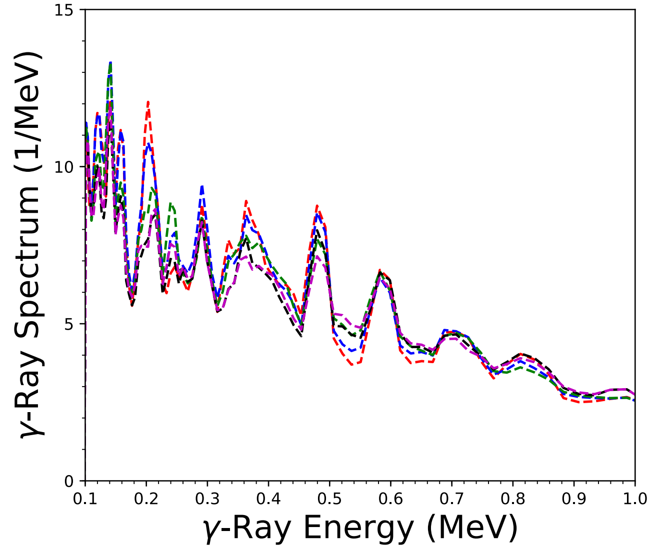
Position of the peaks is determined by available nuclear structure information

Entrance channel dependence



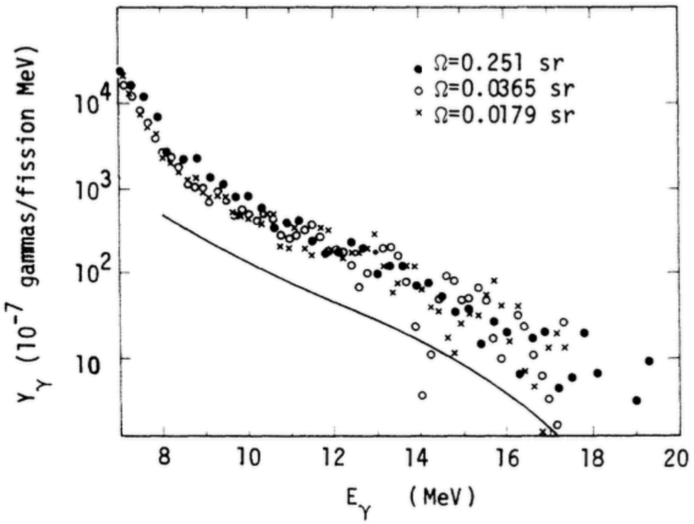




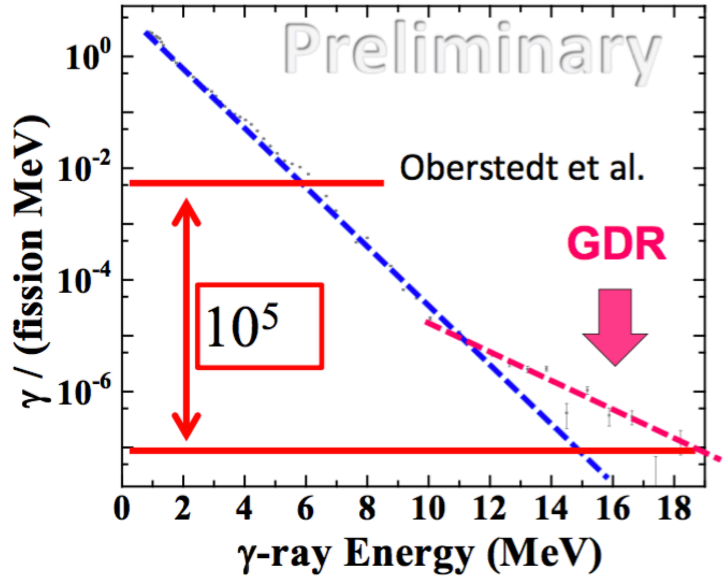


High-energy γ rays (> 8 MeV)

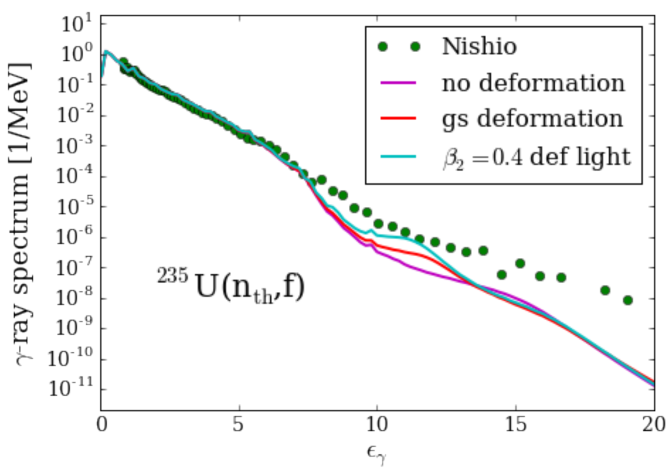
- Impact of GDR in $T_\gamma(\varepsilon_\gamma)$ in FF
- Constraints on CGMF input parameters



Dietrich, Browne et al, PRC **10**, 795 (1974)

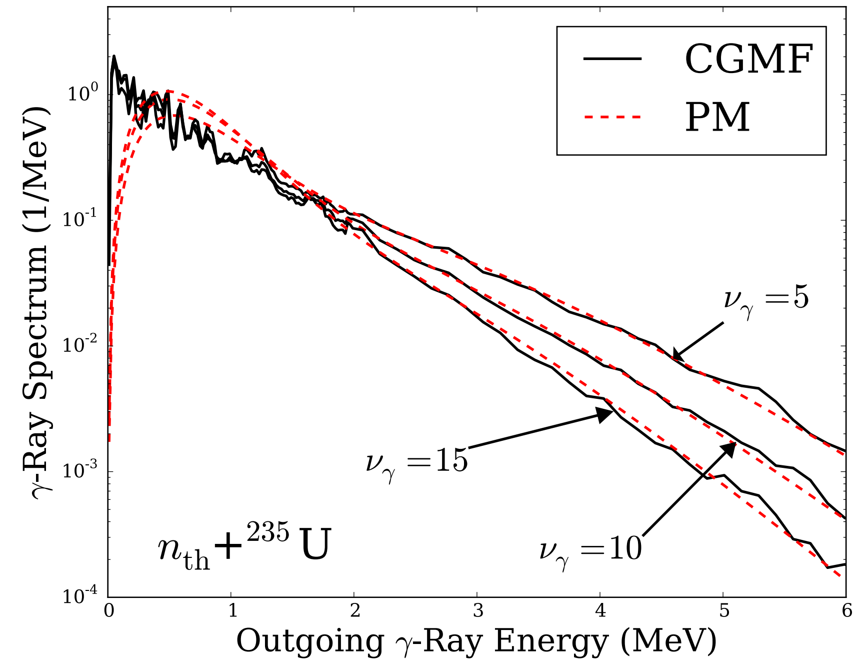


Makii, Nishio et al, ND2016

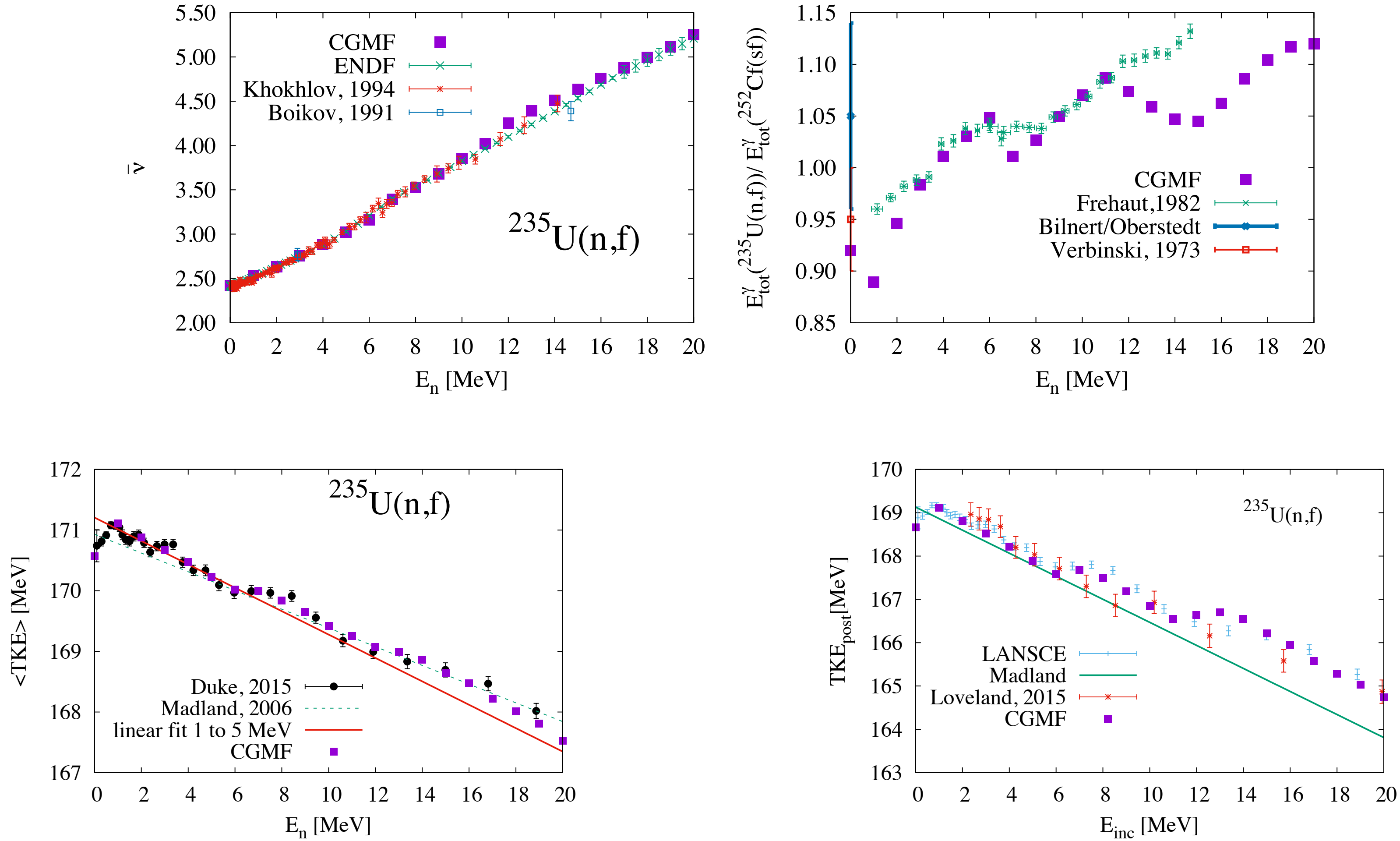


- Similar trend as in experiment between 3-8 MeV
- Sensitivity to γ strength function
- Sensitivity to level densities

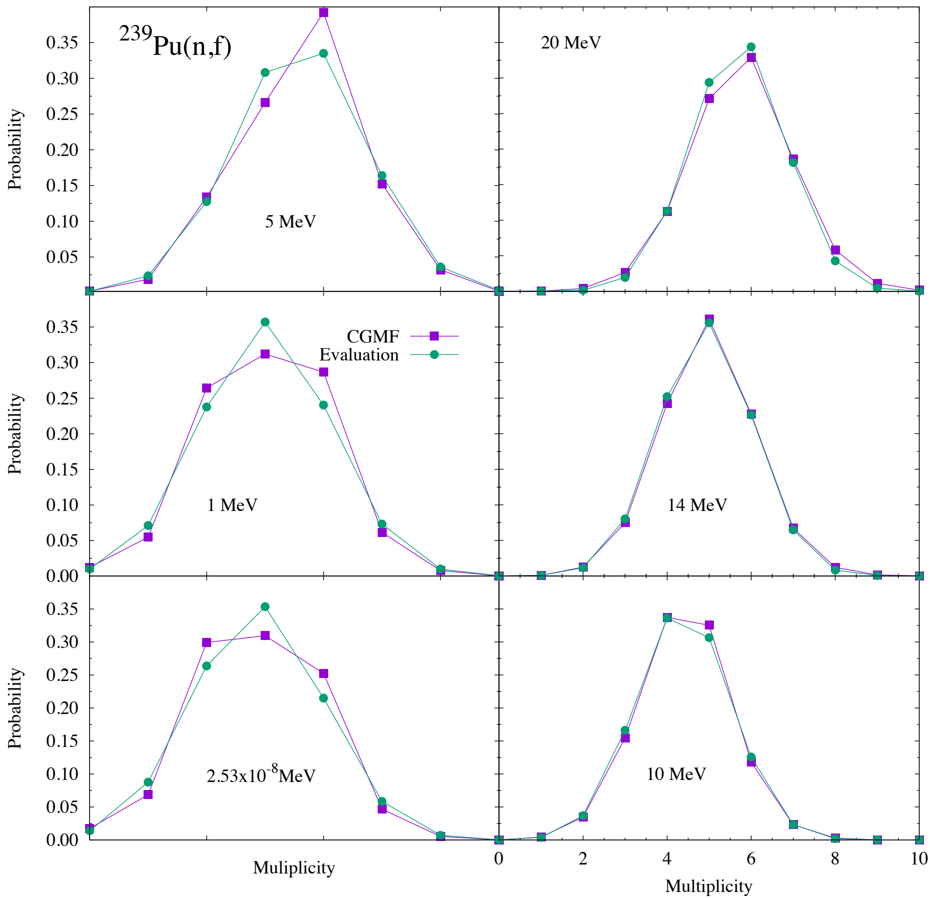
Multiplicity-dependent spectra

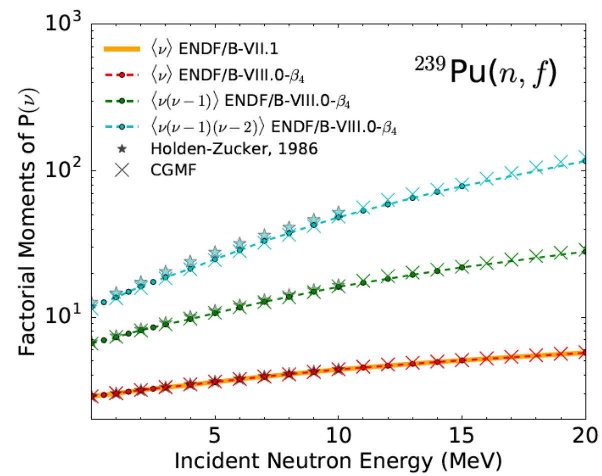


Selected observables vs. incident energy



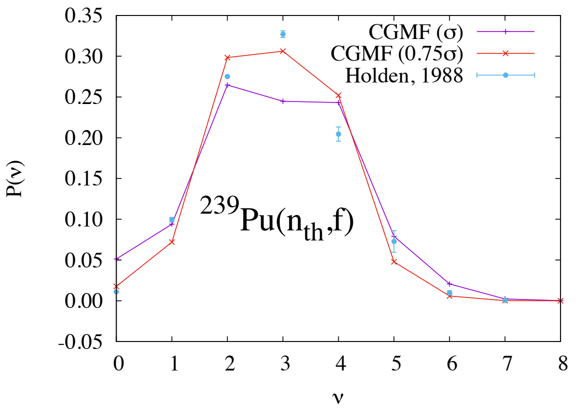
Neutron multiplicity probability



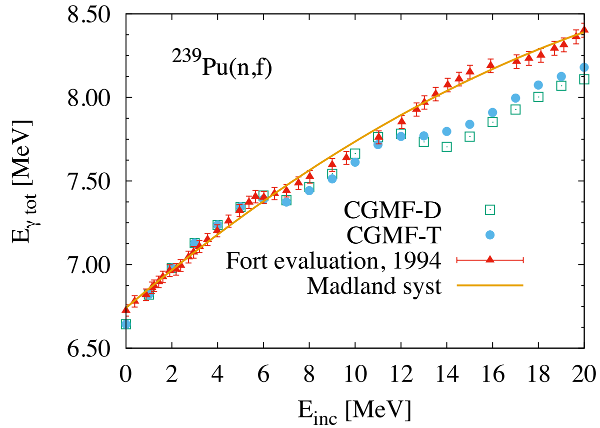


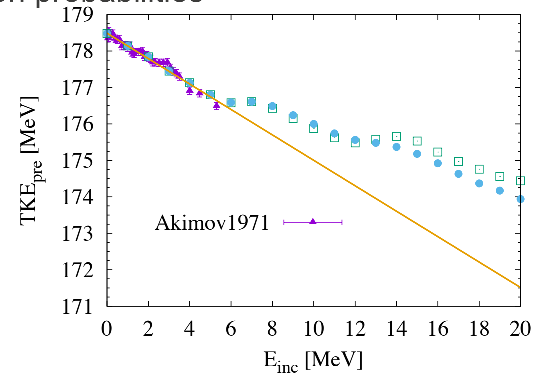
Sensitivity to select parameters

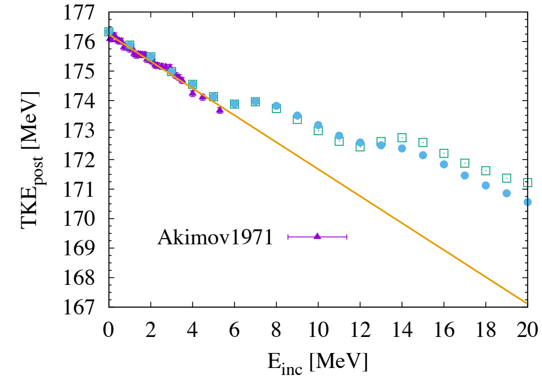
Sensitivity to multi-chance fission probabilities

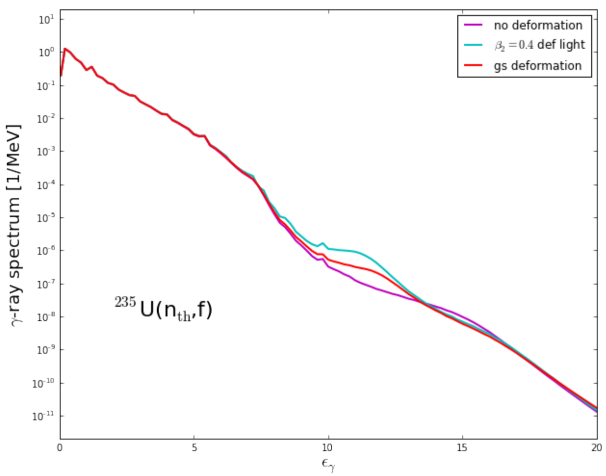


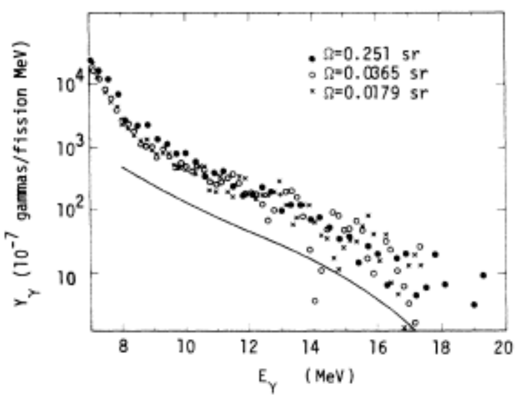
Sensitivity to $\sigma_{TKE}(A)$









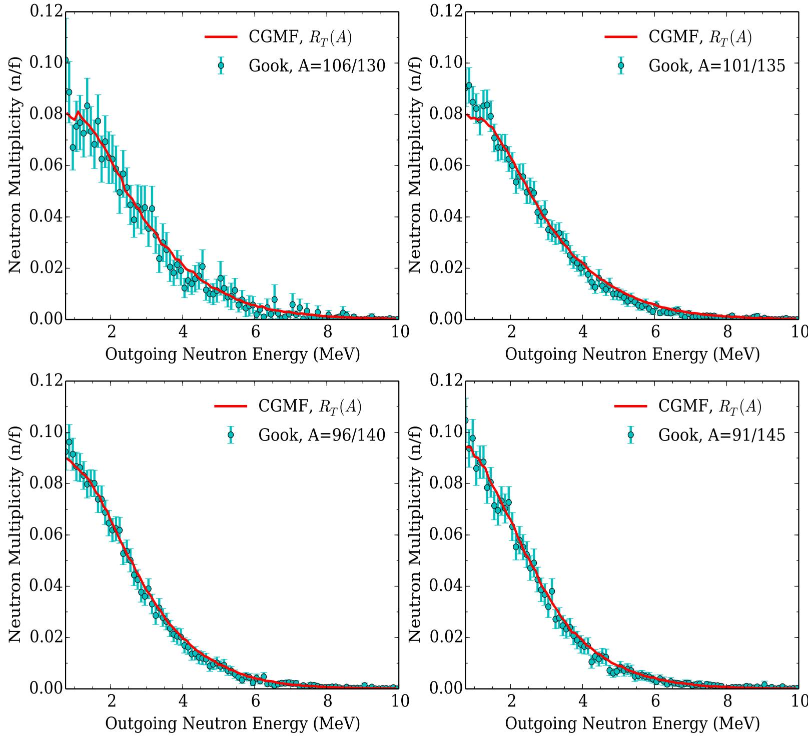


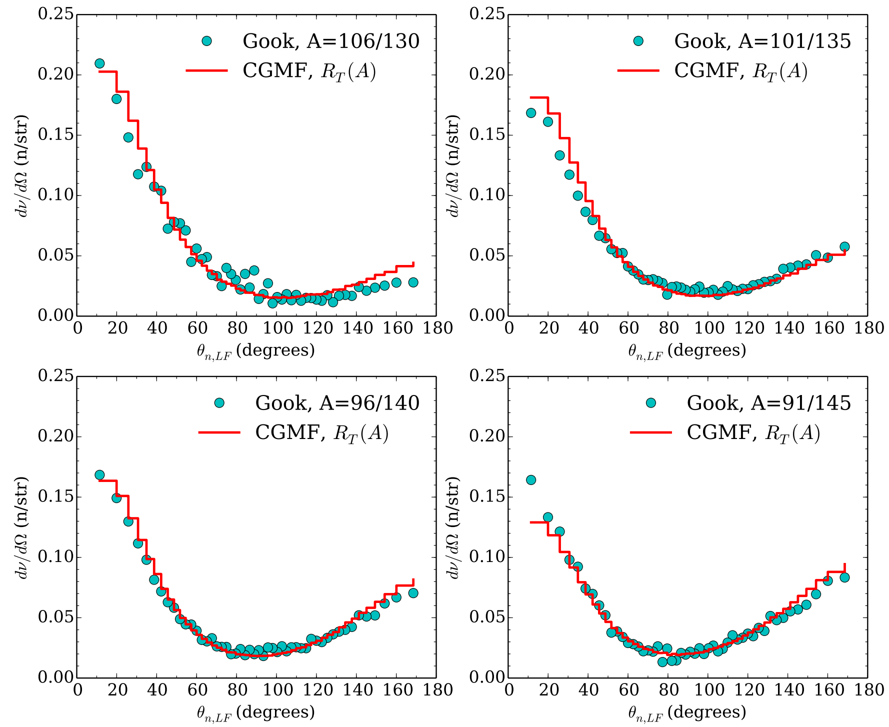
Sensitivity to the deformation

n_{th}+U-235

PFNS (A)

$\Omega_{n\text{-}LF}(A)$



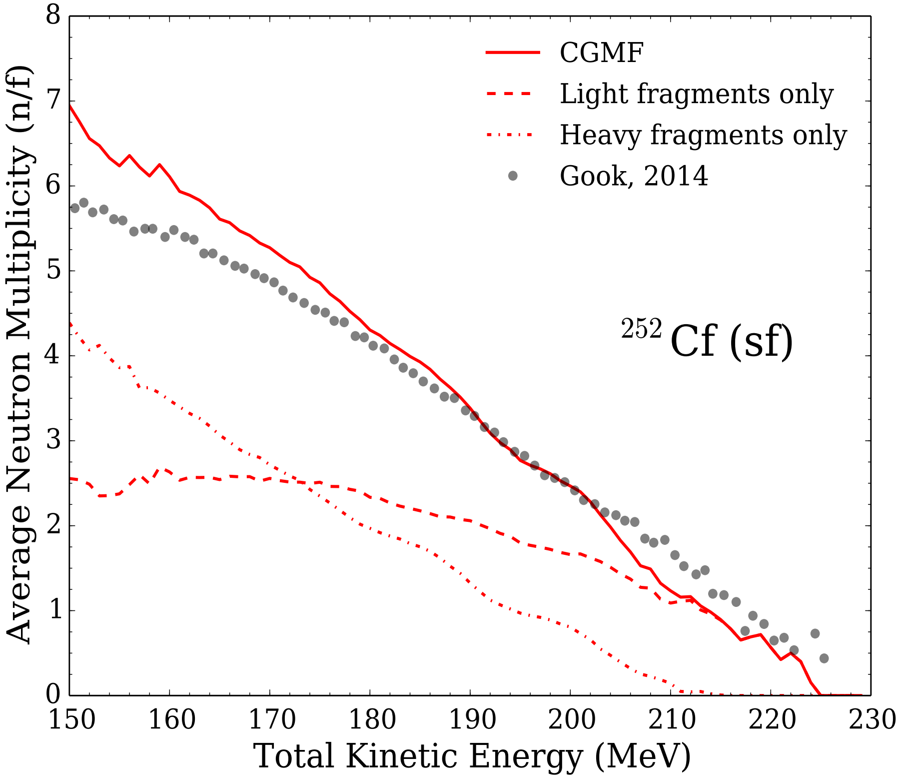


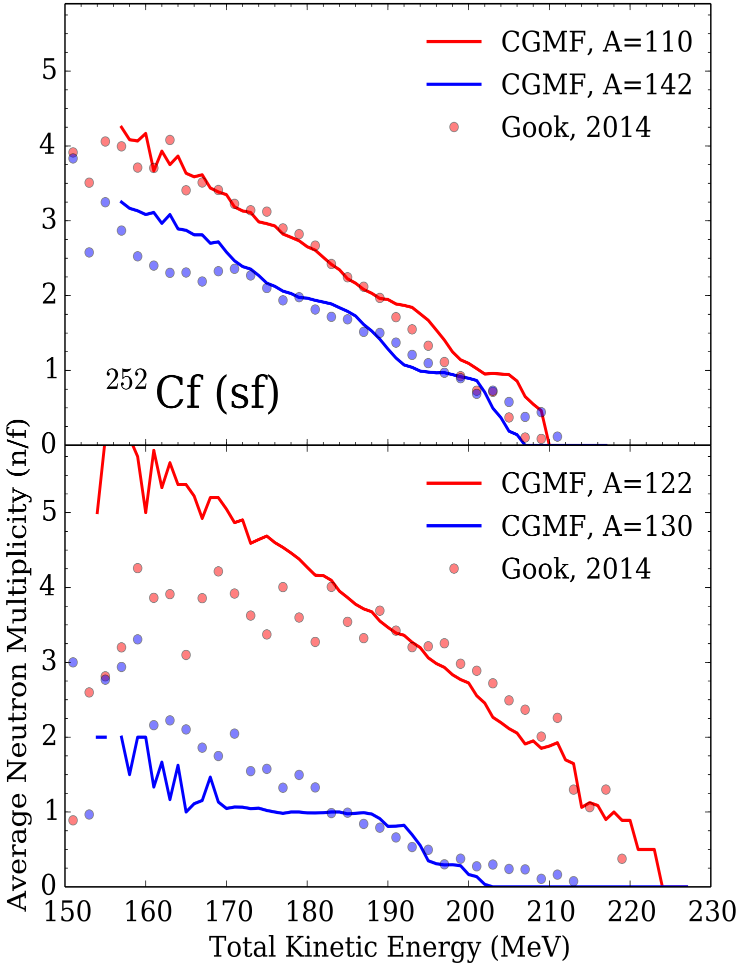
Exp. data by Göök, Hambsch, PRC **90**, 064611 (2014)

Correlated fission data

<ν>(TKE)

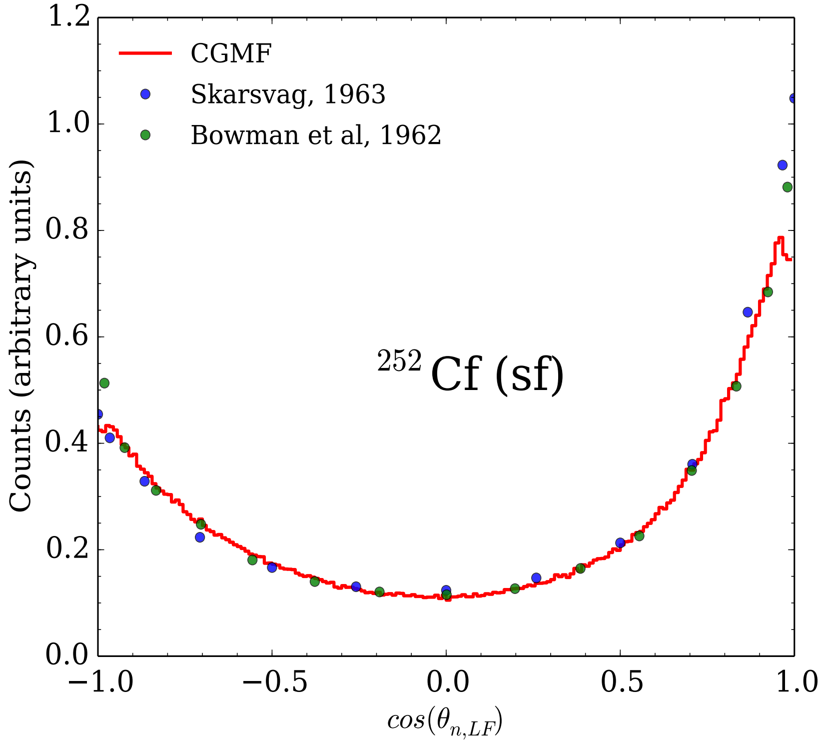
- How much energy does it cost the fragment to emit a neutron?

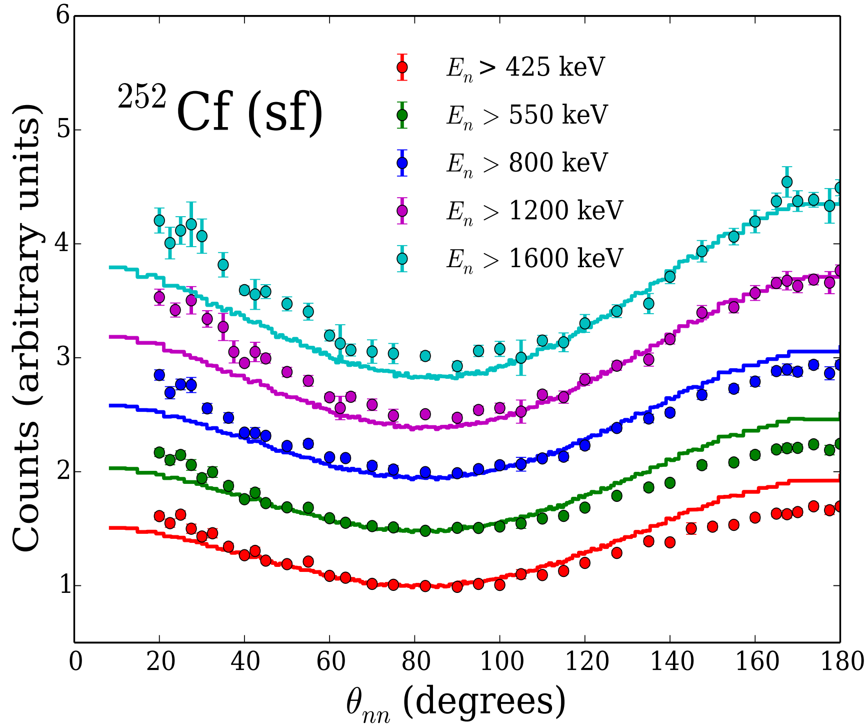




Neutron Angular Distributions

- Neutrons are focused along the fission
-





(No detector response folded.)

Summary

- Theoretical approaches to fission fragment yields:
  - Brownian motion
  - Langevin model
  - TD-SLDA

- Emission of prompt fission neutrons and gammas/ correlations (CGMF):
  - De-excitation of fission fragments described within the Monte-Carlo Hauser-Feshbach formalism
  - Spontaneous (^{252}Cf, ^{240}Pu, ^{242}Pu) and neutron-induced fission up to 20 MeV (^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu)
  - Simple model for TKE and spin as a function of incident energy
  - Reasonable description of experimental data, but not everything
  - Incorporate input from models (Moller, Sierk, Bulgac)
  - Incorporated into transport simulations (part of MCNP)