Detailed Modeling of Fission

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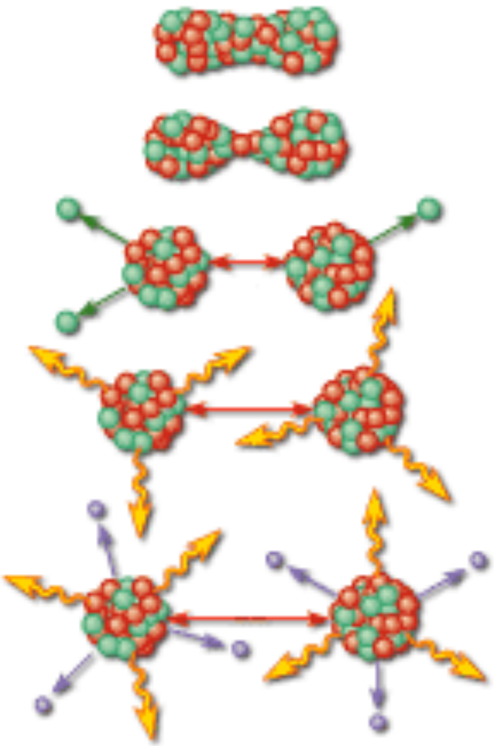
Fission Nomenclature

- Compound nucleus: created from n + A, mass $A_0 = A + 1$, charge Z_0
- Scission: when the neck connecting the pre-fragments snaps
- Fragments: the two excited nuclei immediately after scission,

$A_H + A_L = A_0$, $Z_H + Z_L = Z_0$ assuming binary fission, in general A_f and Z_f

- Products: two types
  - Fission products: after initial neutron emission (detected in fission experiments)
  - Cumulative products: after both prompt and delayed emission has occurred
- Prompt emission: in the first 10^{-13} s, neutrons emitted first, followed by photon emission during initial de-excitation, only A_f changes (is reduced), not Z_f, as fragments become products
- Delayed emission: late in time, after prompt emission products can still emit neutrons and photons (small compared to prompt emission) and can beta decay, emitting neutrinos and electrons (A_f reduced by delayed neutron emission, Z_f can increase by beta decay, $n \rightarrow p + e^- + \nu_e$)



More Nomenclature

- Total Kinetic Energy, TKE: kinetic energies of the two fragments
- Excitation energy, E^*: excitation energy of fragments during prompt emission
- Neutron separation energy, S_n: energy needed to remove one neutron,

if $E^* > S_n$, a neutron can be emitted, if $E^* < S_n$, it can't and photons emitted preferentially

- Rotational energy, E_R: energy in spinning fragments
- Fission Fragment Yields, $Y(A_f,Z_f,TKE)$: probabilities for fragment

production in fission events, normalized to 2 fragments

- Fission Product Yields: probabilities after prompt emission
- Neutron multiplicity: number of neutrons per fission event,

expressed as ν, average multiplicity as $\overline{\nu}$, can be presented as average, as a function of A or TKE, or as probability $P(\nu)$

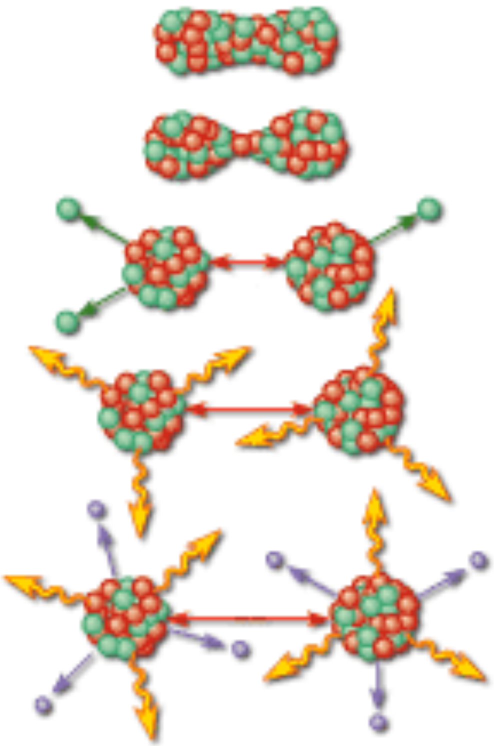
- Photon multiplicity: number of photons per fission event, N_γ
- Total photon energy: energy of photons emitted per fission

event, E_γ

- Statistical photons: continuous energy spectrum, no effect

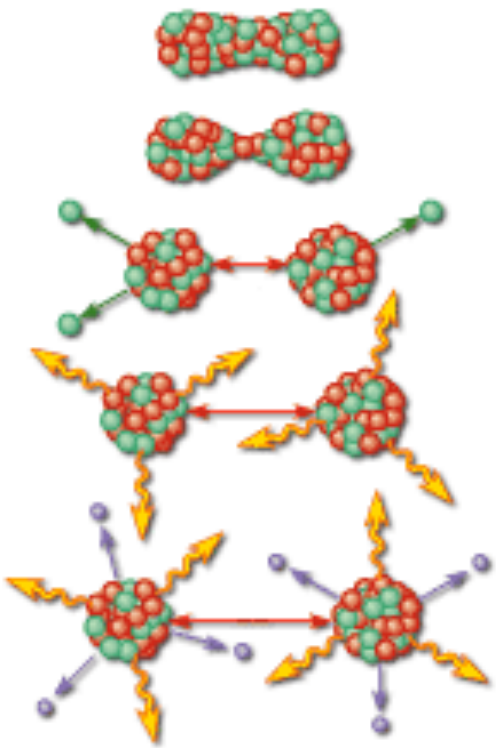
on rotational energy

- Yrast photons: quadrupole transitions, reduces nuclear spin

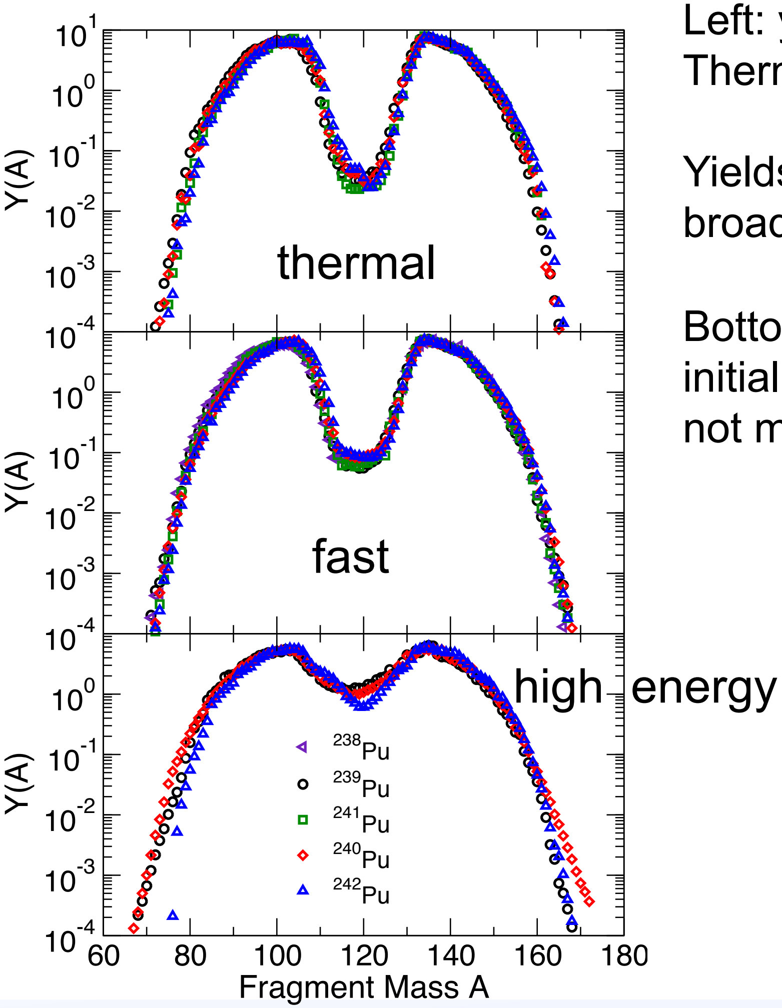


And Yet More Nomenclature

- Binary fission: split into 2 fragments
  - Symmetric fission: both fragments are near equal mass
  - Asymmetric fission: one fragment is heavy and the other is light
- Ternary fission: split into 3 fragments
- Spontaneous fission: internal excitation energy high enough for nucleus to fission without any external energy applied, $A_0 = A$, $E^* = 0$
- Neutron-induced fission: fission caused by incident neutron of sufficiently high energy to overcome fission barrier, $A_0 = A + 1$, $E^* = B_n + E_n$
- Photofission: fission induced by incident photon with high enough energy to overcome barrier, $A_0 = A$, $E^* = B_n + E_\gamma$
- Multichance fission: for sufficiently high incident energies (not for spontaneous fission), one or more neutrons could be emitted before fission – 0n, 1st chance; 1n, 2nd chance; 2n, 3rd chance; etc.
- Pre-equilibrium emission: incident neutron does not equilibrate and is emitted again, endpoint of neutron energy in this case is $E_{end} = E_n - B_n$



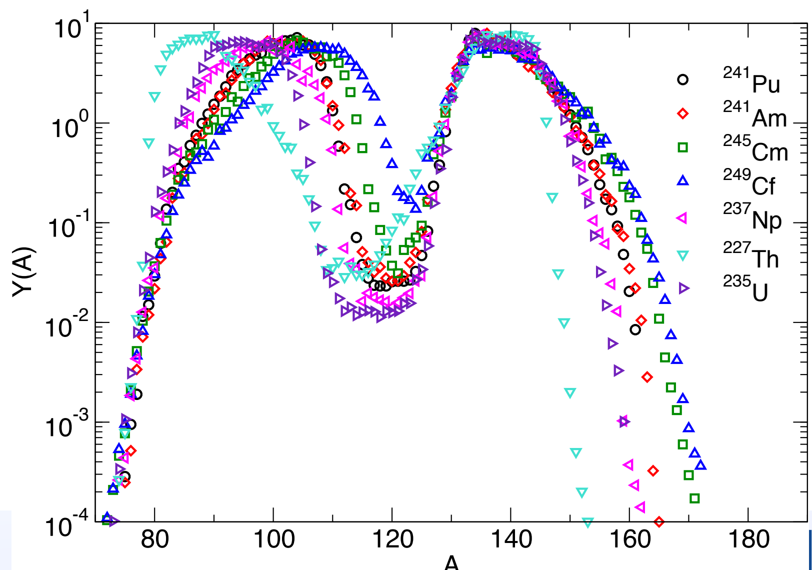
Fission Product Yields as a function of mass A



Left: yields for Pu isotopes at different energies – Thermal = 0.025 eV; Fast ~ 1 MeV; High energy ~ 14 MeV

Yields are asymmetric but become more symmetric and broader at higher energies, shapes similar for same Z (= 94)

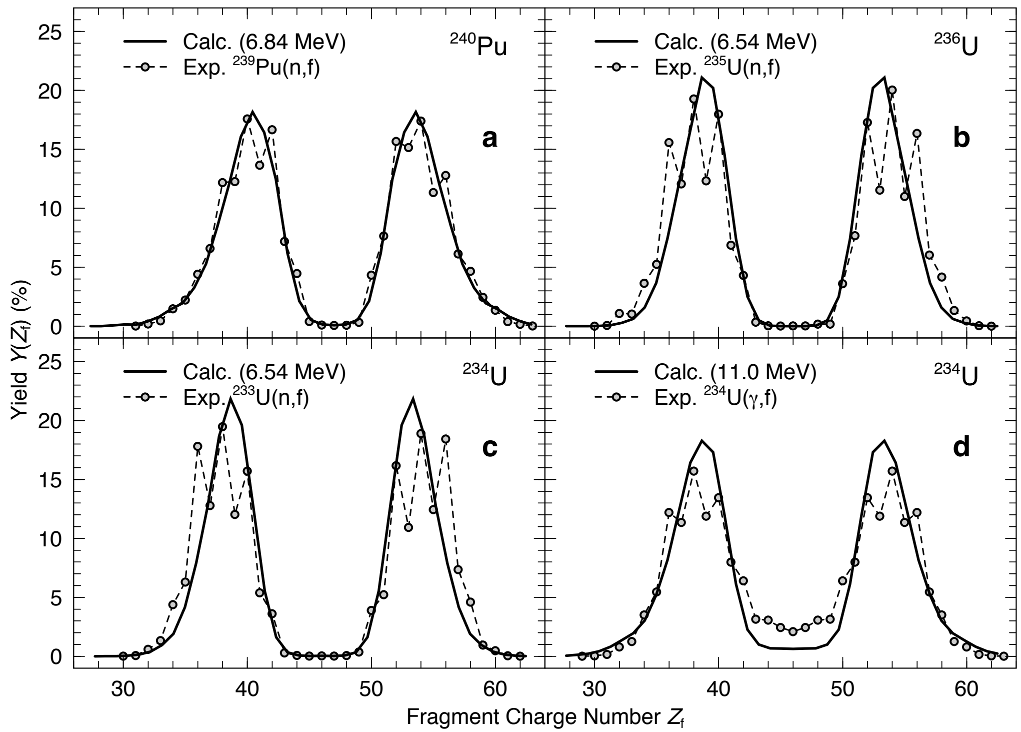
Bottom: illustrates the peak shift for the light fragment with initial A. Note that the heavy fragment mass yield peak does not move while that of the light fragment does



Fission Product Yields as a function of charge Z

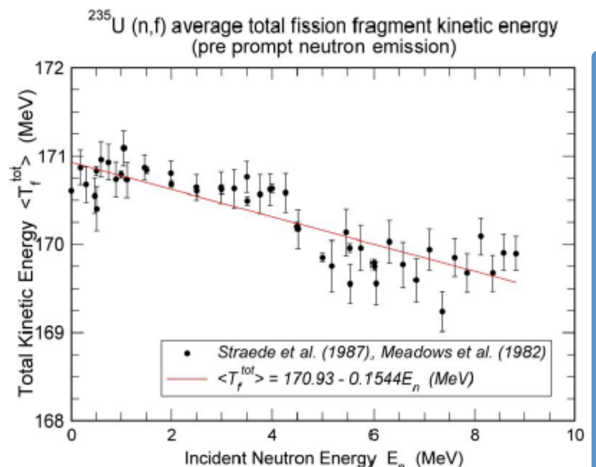
Points are a calculation based on shape evolution of a potential energy surface as it approaches fission

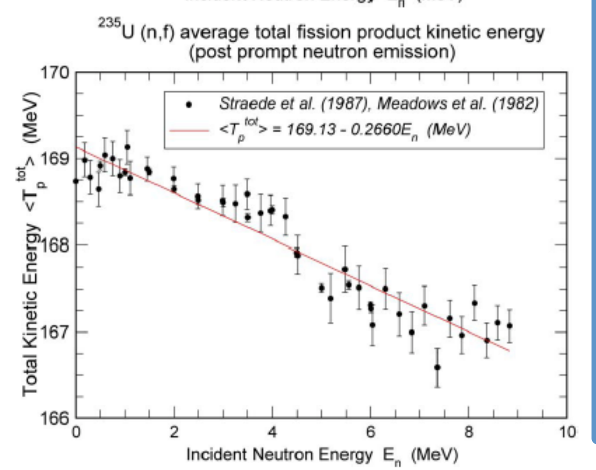
The model, by Randrup and Moller, has shown good agreement with a wide range of actinide data



Total Kinetic Energy of fragments

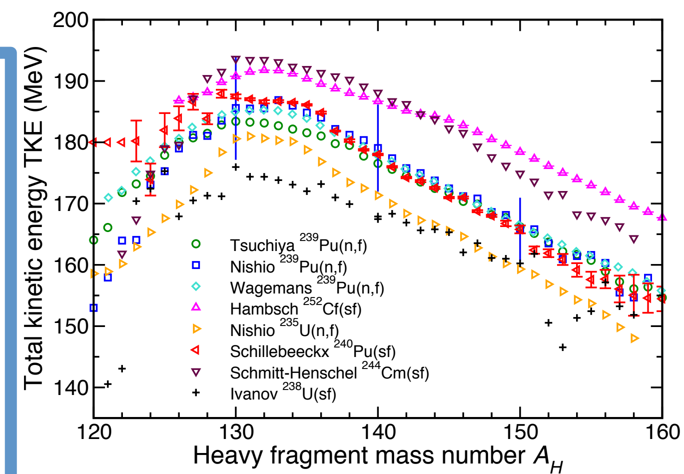
- Most energy of fission goes into motion of the fragments away from each other
- Average TKE tends to decrease slowly with incident neutron energy (left) but energy dependence of shape with heavy fragment mass TKE(A_H) is less well known

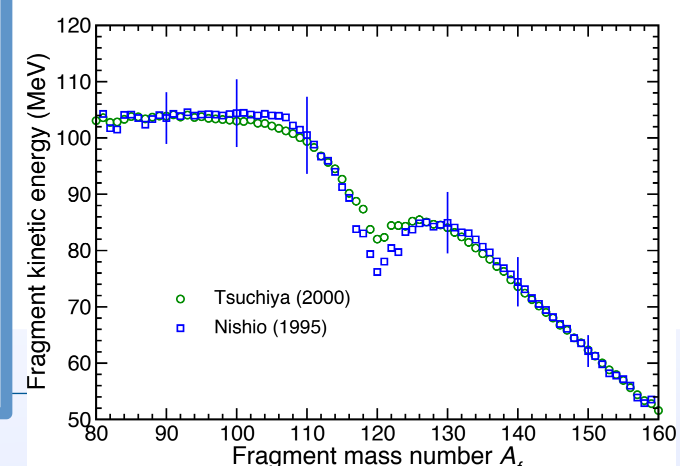




Left (top): fragment energy, integrated over A;
Left (bottom): product energy, integrated over A
Note the higher TKE for the fragments than for products and the steeper slope on the products
Both for ^{235}U(n,f)

Right (top): TKE vs A_H for several isotopes, highest TKE for most stable A_H, ~132
Right (bottom): Kinetic energy for single fragments from ^{239}Pu
Both at thermal energies

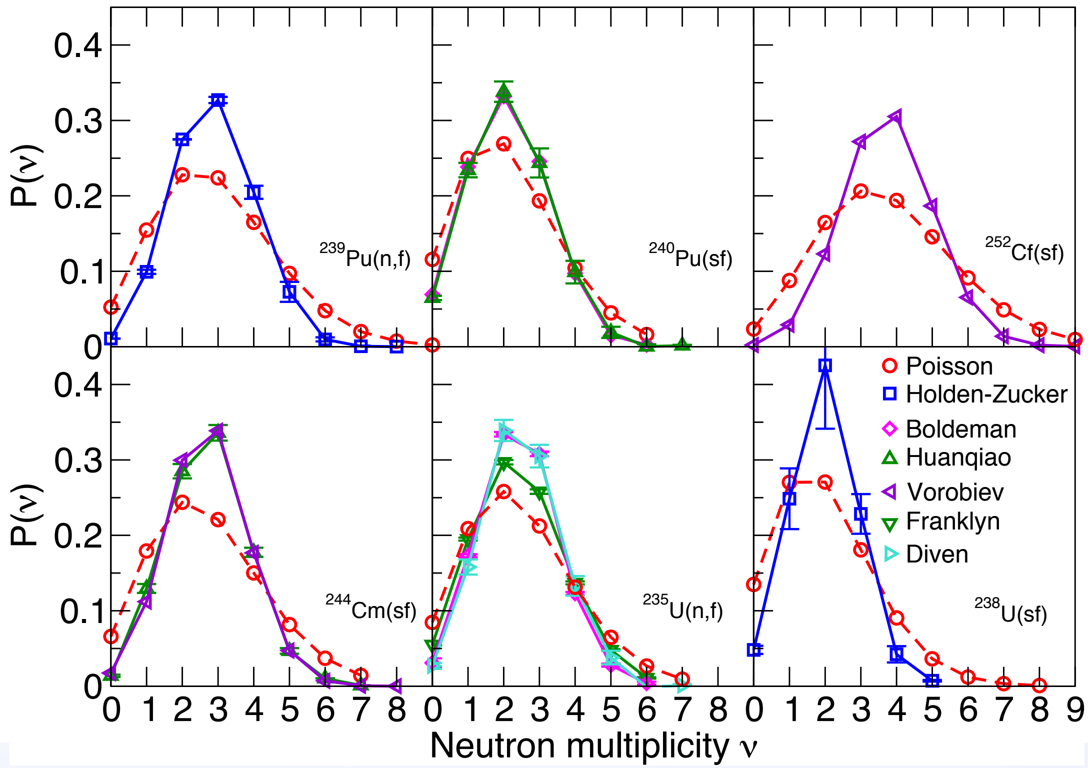




Neutron multiplicity distributions

Data on neutron multiplicity distributions are compared to a Poisson distribution

The data differ from a Poisson because not only is the neutron kinetic energy removed with each neutron but also its separation energy

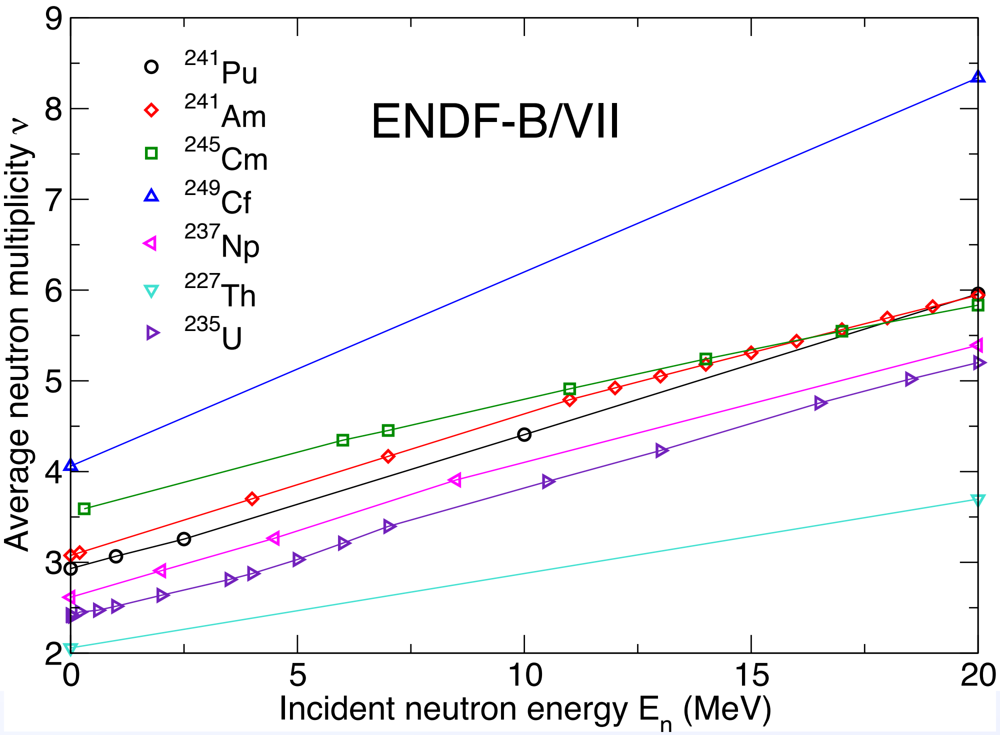


Energy dependence of neutron multiplicity

Evaluations of average neutron multiplicity as a function of incident neutron energy

‘Evaluations’ involve compiling data and deciding which are ‘better’; there is also
Some tweaking going on because the evaluations have to match certain criteria in applications

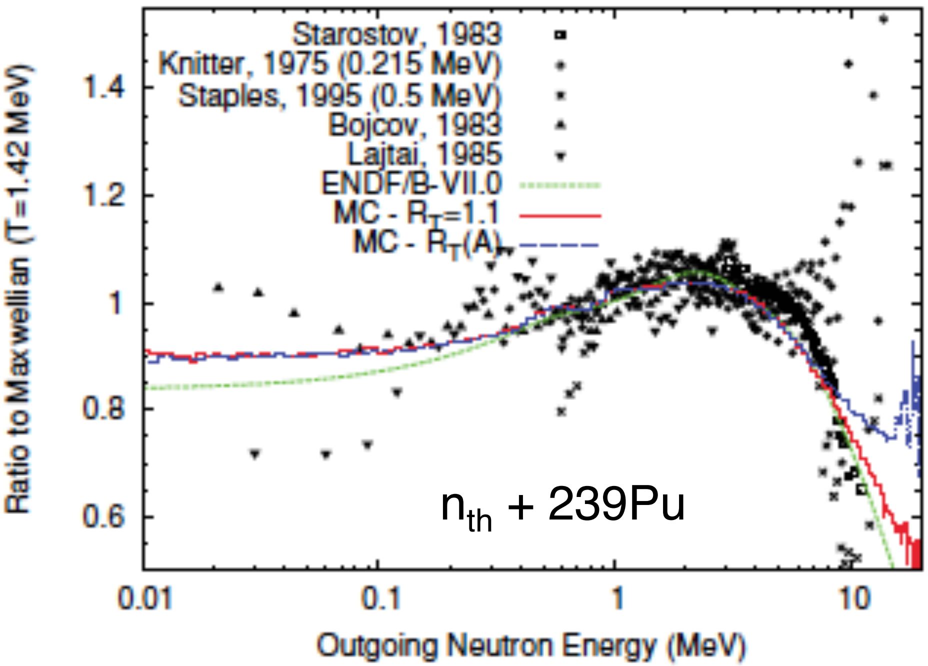
In some cases where there isn’t much data, the evaluations are mainly educated guesses

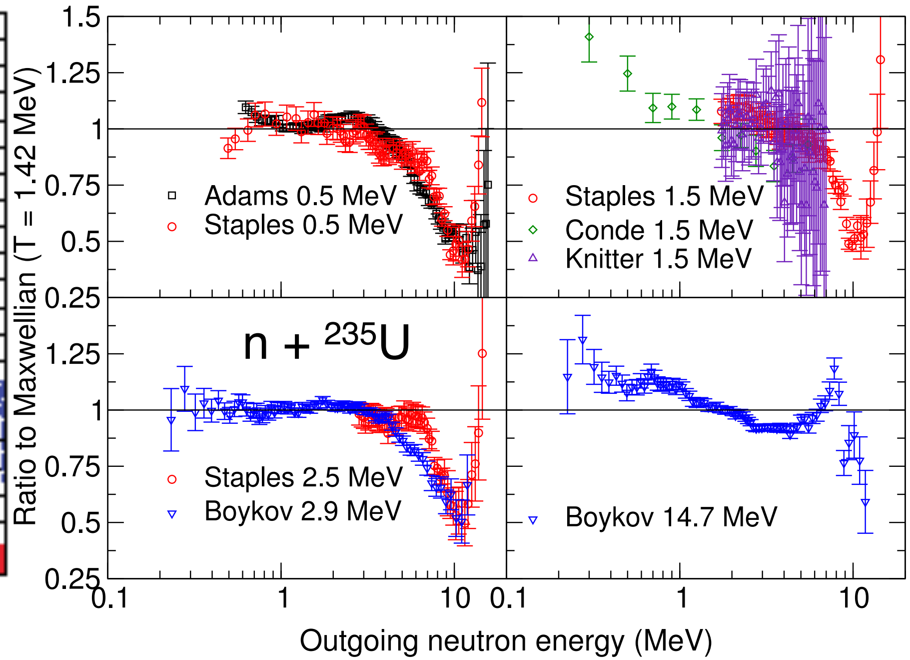


Neutron spectral shapes: comparison to a Maxwellian

A Maxwell distribution (Maxwellian), $dN/dE \approx \sqrt{E}\exp(-E/T)$, with constant temperature T, T = 1.42 MeV is often compared to the data, easier to see differences in a ratio on a linear Scale than individual distributions on a logarithmic scale

Note that the ‘kink’ in the Boykov 14.7 MeV data could be attributed to pre-equilibrium emission





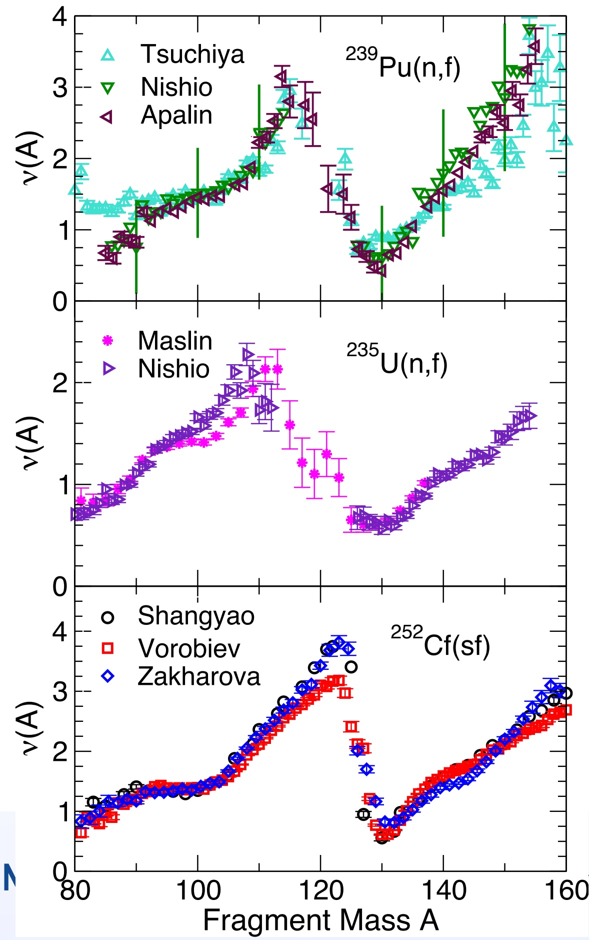
Trends in neutron and photon A dependence similar

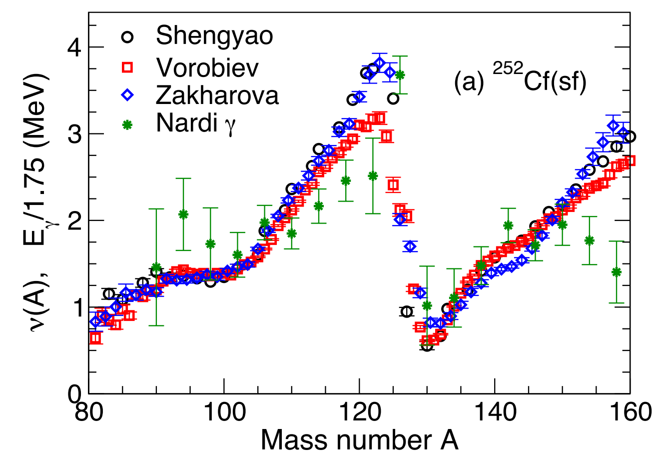
Both $\nu(A)$ and $E_\gamma(A)$ show a sawtooth shape but the slopes of the 'teeth' are not necessarily the same:
E_γ for ^{252}Cf(sf) seems to be flatter while N_γ seems to have a stronger A dependence than
E_γ for ^{235}U(n,f) while E_γ is more similar to $\nu(A)$, within large uncertainties

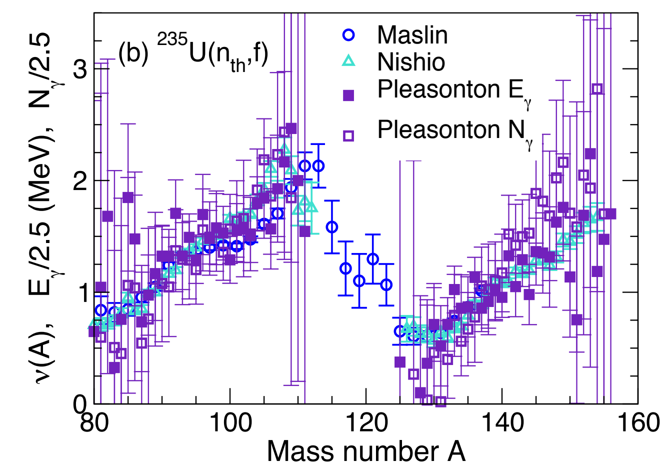
Sawtooth shape of $\nu(A)$ reflects shell structure: A = 132 is doubly-closed shell so hard to excite and thus few neutrons emitted in any case shown

Tooth is 'sharper' for larger A_0

Dependence of shape on neutron energy not well known

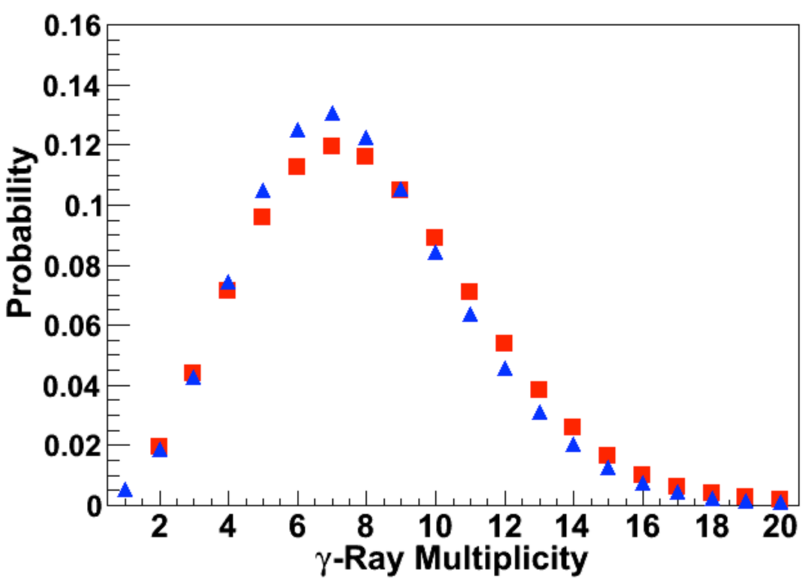


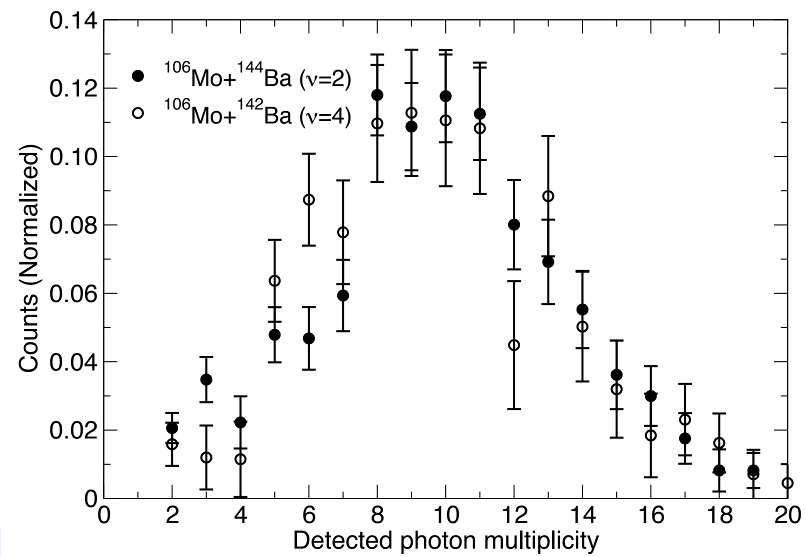




Photon multiplicity distributions

- Left: Photon multiplicity distribution measured in ^{252}Cf(sf) at LANSCE in Los Alamos
  - Photon distributions are more Poisson-like because there is no separation energy
- Right: Photon multiplicity distribution for 2 neutron emission (solid points) and 4 neutron emission (open points) measured at LBNL in ^{252}Cf(sf)
  - If fewer photons are emitted with higher neutron multiplicity, then there should be an anti-correlation in multiplicity and the $\nu = 4$ distribution should shift to the left of $\nu = 2$, if there is a correlation of more photons emitted at higher neutron multiplicity, shift should be to the right; not possible to distinguish





Data are often insufficient for comprehensive modeling of fission process

- Fission experiments have most often focused on measuring only a single type of observable, *e.g*. the fragment mass and/or charge or the number and/or energy of prompt neutrons or prompt photons
- Such inclusive data provides only limited guidance for fission modeling, in contrast to more exclusive data, *e.g*. prompt neutrons and/or prompt photons together with the fragment mass and/or charge
- Fission experiments largely focus on just a few cases, further limiting the experimental basis for modeling
- Some (n,f) data, such as $Y(A_f)$, $TKE(A_H)$ and $\nu(A_f)$, have been measured only at low incident energies
- Codes like **FREYA** can be used to study interdependencies and sensitivities, thus helping identify which further measurements might be most informative

Perils of comparing models to data

- Single particle observables such as average neutron multiplicity are sort of easy – they just require counting neutrons, sometimes within a given angle or energy bin but are basically counting experiments (these are good for many applications which require only average quantities
- Going beyond these measurements requires measuring e.g. neutrons *and* fragments
- Experiments measure products (the fission fragments reach the detectors after emitting neutrons and are thus ‘products’) but report measurement of fragments
- Thus any reported inclusive measurement such as $\nu(A)$, TKE(A) has already had some reverse analysis done on it to go back to fragments from products

Fission models

- There is no real ‘theory’ of fission: it’s difficult to do a fully many-body calculation, writing down the anti-symmetrized wavefunction of 230+ nucleons – some have tried but even going from some trial wavefunction to two distinct fragments is extremely difficult and more than marginal success with application to more than a single isotope is still years away
- Three things have been very important for application codes: the average neutron multiplicity, the prompt fission neutron spectrum (PFNS), and the fission cross section. The rest of the event is ignored, energy and momentum are not conserved and the same spectrum is sampled for all neutrons emitted in an event.
- The average multiplicity as a function of incident neutron energy is evaluated and tabulated in databases. For some isotopes it is very well known (claimed to be known better than 0.1%) and regarded as sacrosanct.
- The PFNS is also an evaluated quantity, based on the “Los Alamos” model. As we already saw, uncertainties in certain energy regions can still be large so a great deal of experimental effort has been aimed at reducing these uncertainties. (Hint: measuring neutron energies accurately is REALLY hard)

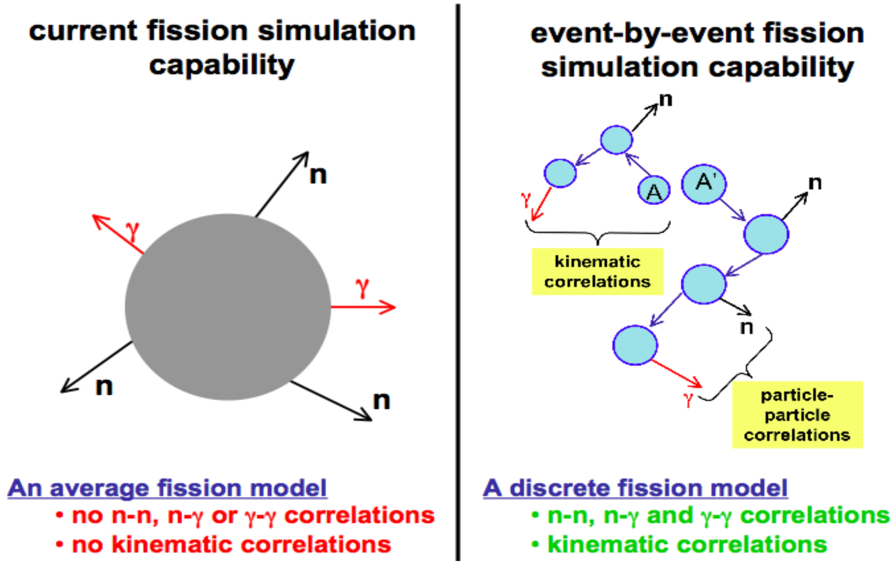
Los Alamos model (Madland & Nix, 1982)

- This approach has been the ‘gold standard’ in PFNS evaluations since it was first developed.
- It assumes that the light and heavy fragments are the ‘average’ ones, those that are the most probable. It also assumes an average value of the separation energy, Sn, based on the identities of the most probable fragments.
- They also make assumptions about the average fission Q value and the average total kinetic energy, TKE, to obtain the average total excitation energy. The average neutron multiplicity is then $\langle \nu \rangle = (\langle E^* \rangle - \langle E_\gamma \rangle)/(\langle S_n \rangle + \langle E \rangle)$ since the average energy emitted by photons is subtracted.
- The Weisskopf-Ewing spectral shape, $dN/dE \sim E \exp(-E/T_{max})$, is used with T_{max} the maximum temperature of the daughter nucleus, obtained for E = 0, giving an average neutron kinetic energy of $\langle E \rangle = 2T$
- The average neutron spectrum is obtained from this spectral shape folded with a triangular temperature distribution, $P(T) = 2T/(T_{max})^2$ for $T \leq T_{max}$; 0 for $T > T_{max}$; the average neutron spectrum is then $$\int_0^{T_{\max}} \frac{dN}{dE} P(T) dT = \frac{2E}{T_{\max}^2} \int_0^{T_{\max}} \exp(-E/T) \frac{dT}{T}$$ with an average energy of $\langle E \rangle = (4/3)T_{max}$
- Many variants of this model exist but all provide smooth PFNS for all incident energies

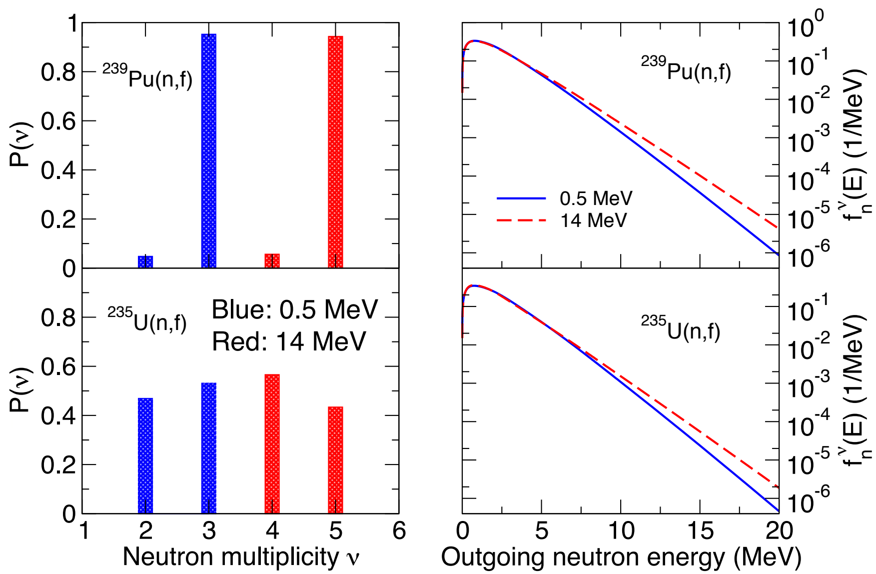
FREYA (Fission Reaction Event Yield Algorithm) developed at LLNL

- Model of complete fission events, just one example, there are others, as we'll see
- **FREYA** developed in collaboration with J. Randrup (LBNL)
- **FREYA** references: Phys. Rev. C **80** (2009) 024601, 044611; **84** (2011) 044621; **85** (2012) 024608; **87** (2013) 044602; **89** (2014) 044601; User Manual LLNL-TM-654899.
- General reference: R. Vogt and J. Randrup, "Nuclear Fission", Chapter 5 of 100 Years of Subatomic Physics, World Scientific, 2013.

How do complete event treatments differ from traditional fission models?



Fission model in frequently used simulation code **MCNP**:



- In 'average' models, fission is a black box, neutron and gamma energies sampled from same average distribution, regardless of multiplicity and energy carried away by each emitted particle; fluctuations and correlations cannot be addressed
- **Models like FREYA** generate complete fission events: energy & momentum of neutrons, photons, and products in each individual fission event; correlations are automatically included

- Traditionally, neutron multiplicity sampled between nearest values to get correct average value
- All neutrons sampled from same spectral shape, independent of multiplicity

Event-by-event modeling is efficient framework for incorporating fluctuations and correlations

Goal(s): *Fast* generation of (large) samples of complete fission events

Complete fission event: Full kinematic information on all final particles

Two product nuclei: $Z_H, A_H, \boldsymbol{P}_H$ and $Z_L, A_L, \boldsymbol{P}_L$

ν neutrons: $\{ \boldsymbol{p}_n \}, n = 1,\ldots,\nu$

N_γ photons: $\{ \boldsymbol{p}_m \}, m = 1,\ldots,N_\gamma$

Advantage of having *samples* of complete events:

Straightforward to extract *any* observable,
including fluctuations and correlations,
and to take account of cuts & acceptances

Advantage of *fast* event generation:

Can be incorporated into transport codes

Fragment mass and charge distribution

No quantitative models for $P(A_f)$ exists yet, so …

$P(A_f)$ is sampled *either* from the measured mass distribution *or* from five-gaussian fits to data: [W. Younes *et al*: PRC **64** (2001) 054613]

Mass number

$$P(A_f) = \sum_{m=-2}^{m=+2} \mathcal{N}_{|m|}\, \mathcal{G}_m(A_f) \qquad \sum_{m=-2}^{m=+2} \mathcal{N}_{|m|} = 1$$

$$\mathcal{G}_m(A_f) = (2\pi\sigma^2_{|m|})^{-\frac{1}{2}} \mathrm{e}^{-(A_f - \bar{A}_f - D_{|m|})/2\sigma^2_{|m|}}$$

Dependence on E_n: $$\mathcal{N}_{1,2}(E_n) = \frac{\mathcal{N}^0_{1,2}}{\mathrm{e}^{(E_n-\hat{E})/\tilde{E}} + 1} \qquad \hat{E} \approx 10\,\mathrm{MeV} \quad \tilde{E} \approx 1\,\mathrm{MeV}$$

Charge number

$$P_{A_f}(Z_f) \sim \mathrm{e}^{-(Z_f - \bar{Z}_f)/2\sigma_Z^2}$$

[W. Reisdorf *et al*: NPA **177** (1971) 337]

$$\bar{Z}_f = \frac{Z_0}{A_0} A_f \qquad \sigma_Z = 0.38 - 0.50$$

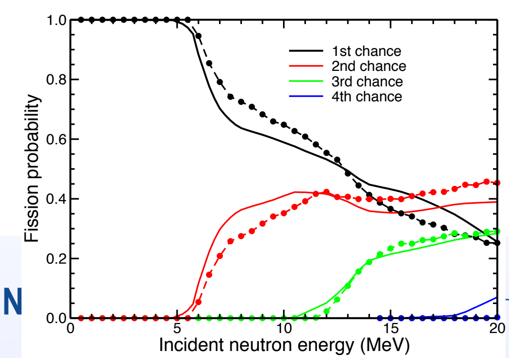
^{252}Cf ^{240}Pu

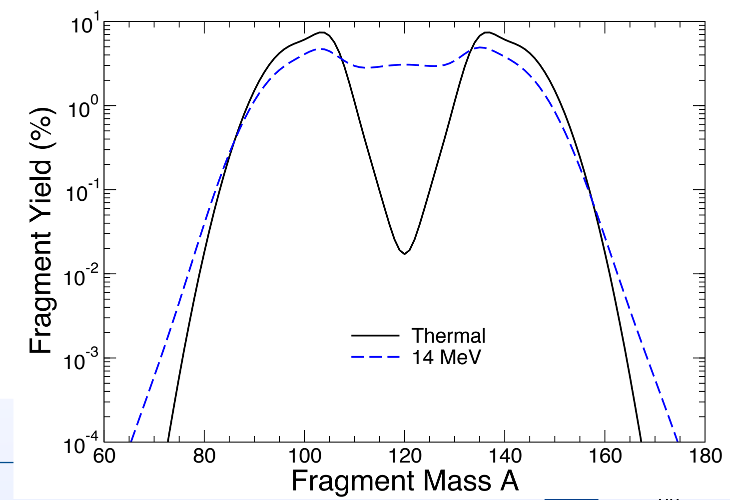
E_n = 14 MeV:

1st: 44%

2nd: 35%

3rd: 21%





Pre-equilibrium neutron emission

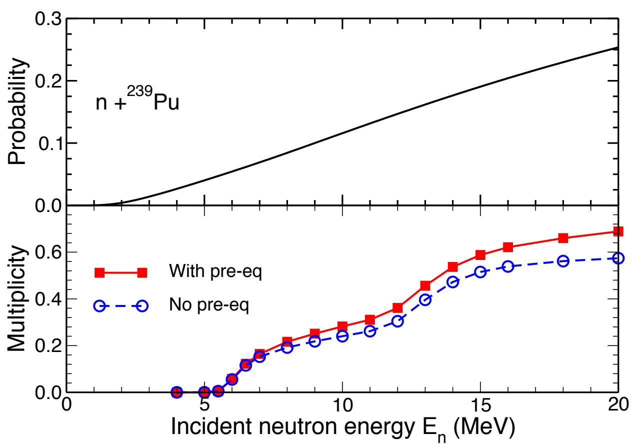
Based on the two-component exciton model by Koning & Duijvestin [NPA744]

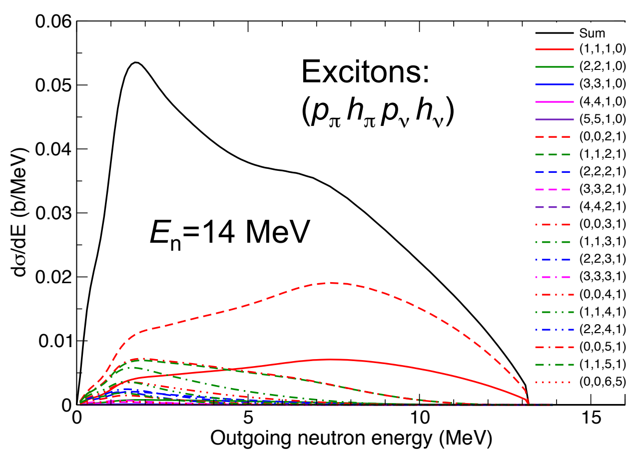
Master equation for $P(p_\pi\, h_\pi\, p_\nu\, h_\nu)$:

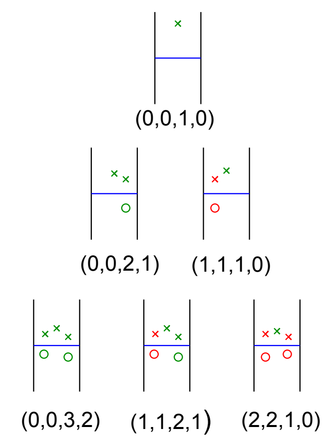
$$\frac{d\sigma_n}{dE} = \sigma_{\rm CN} \sum_{p_\pi=0}^{p_\pi^{\max}} \sum_{p_\nu=1}^{p_\nu^{\max}} W(p_\pi, h_\pi, p_\nu, h_\nu, E) \times \tau(p_\pi, h_\pi, p_\nu, h_\nu)\, P(p_\pi, h_\pi, p_\nu, h_\nu)$$

Emission rate:

$$W(p_\pi, h_\pi, p_\nu, h_\nu, E_k) = \frac{g_n}{\pi^2 \hbar^3} \mu_n E\, \sigma_{n,\rm inv} \frac{\omega(p_\pi, h_\pi, p_\nu - 1, h_\nu, E^* - E - S_n)}{\omega(p_\pi, h_\pi, p_\nu, h_\nu, E^*)}$$



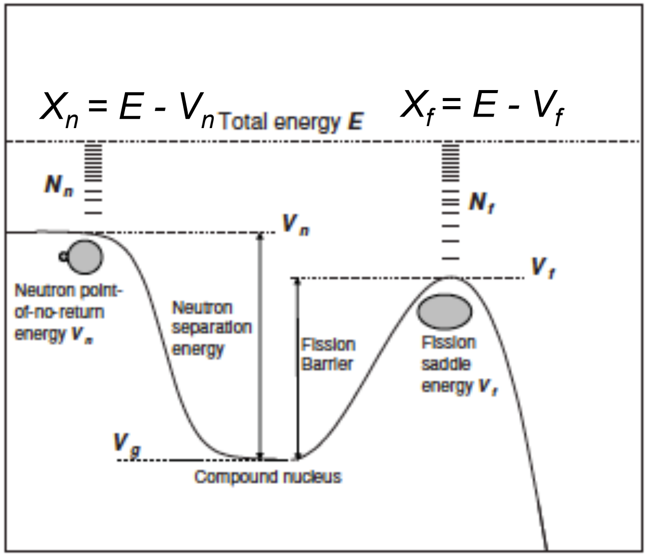




Calculations made by Erich Ormand

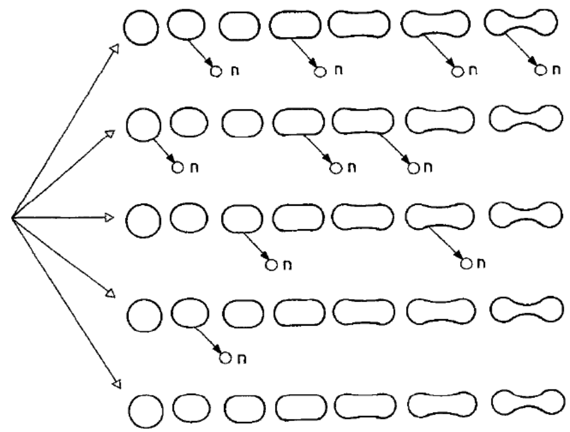
Vogt, Randrup, Brown, Descalle, Ormand: Physical Review C 80 (2009) 024601

Multichance fission based on fission-evaporation competition, transition state theory



$$\frac{\Gamma_n(E^*)}{\Gamma_f(E^*)} = \frac{2g_n\mu_n\sigma}{\pi\hbar^2}\frac{\int_0^{X_n}(X_n - x)\rho_n(x)dx}{\int_0^{X_f}\rho_f(x)dx}$$

Swiatecki et al:
PR C **78** (2008) 054604



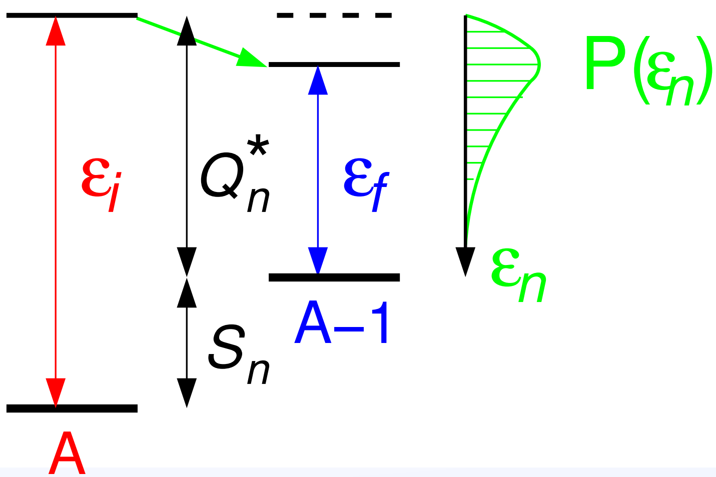
ν = 4; fifth chance fission

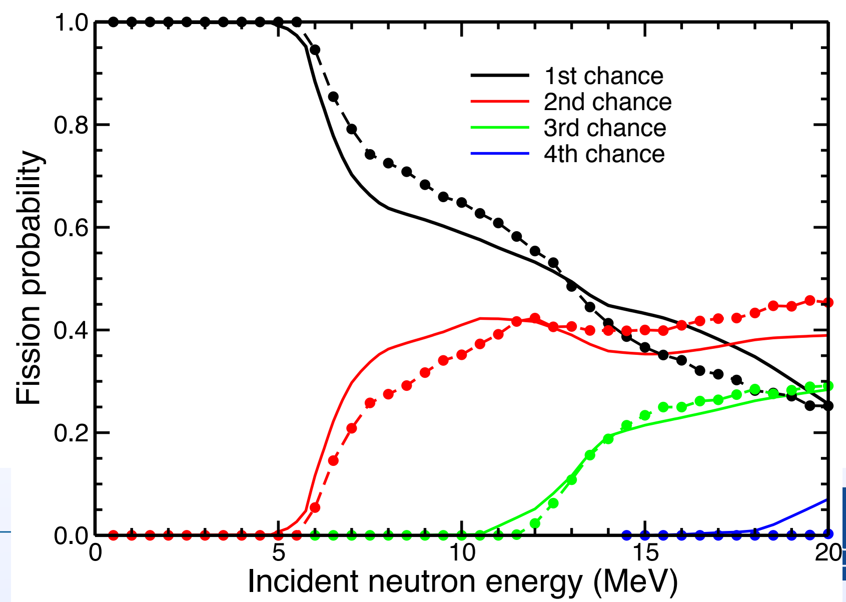
ν = 3; fourth chance fission

ν = 2; third chance fission

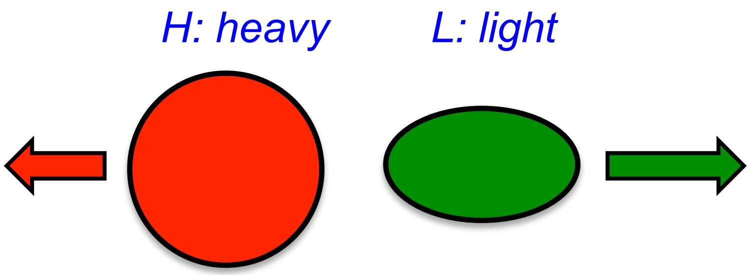
ν = 1; second chance fission

ν = 0; first chance fission





Fission fragment kinetic energies

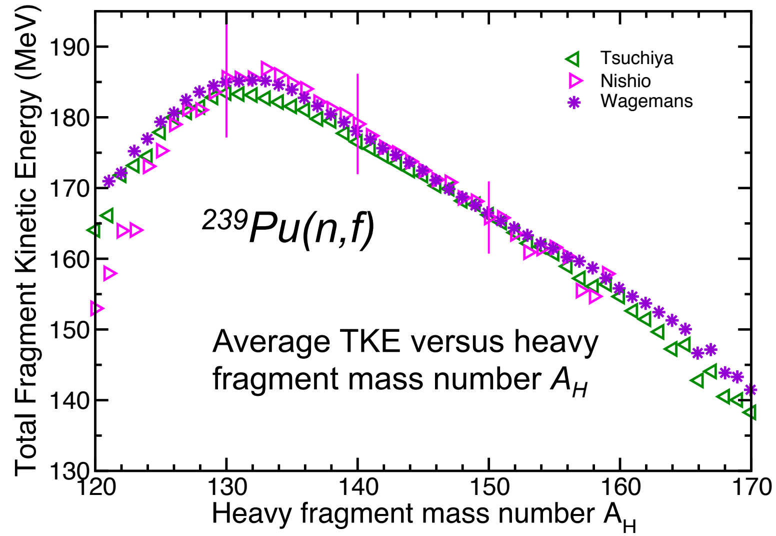


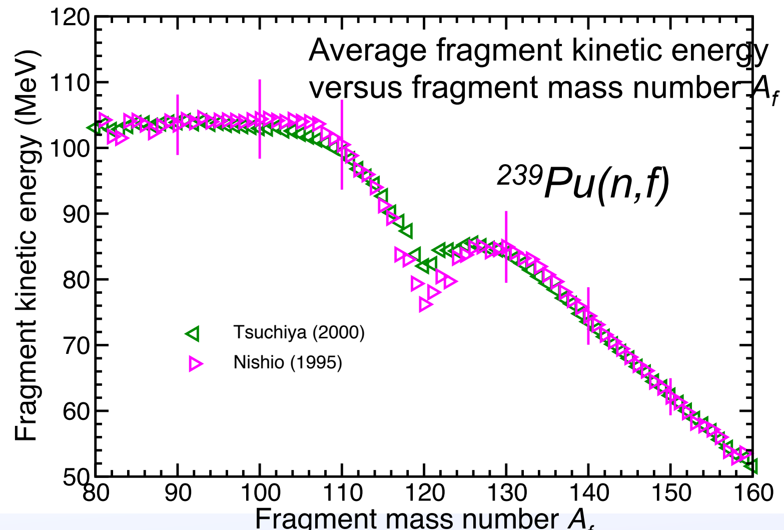
No models for $TKE(A_f)$ exists yet, so …

we adjust TKE to exp data:

$$\underline{\mathrm{TKE}} = \mathrm{TKE}_{\mathrm{data}} - \mathrm{dTKE}(E_n)$$

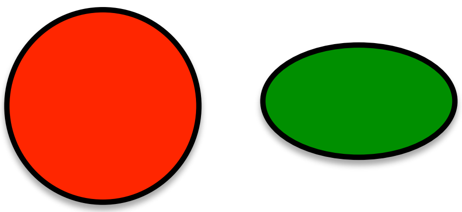
with an adjustable shift
to reproduce the mean
neutron multiplicity $<\nu>(E_n)$





Fragment excitation energies

H: heavy *L: light*



Q value: $Q_{LH} = M(^{240}Pu^*) - M_L - M_H$

Mean thermal excitation: $\underline{E}^* = Q_{LH} - \underline{TKE} = \underline{E}_L^* + \underline{E}_H^*$

Thermal equilibrium:

Common temperature: $T = [\underline{E}^*/(a_L + a_H)]^{1/2}$ *)

Excitation is shared: $\underline{E}_L^* : \underline{E}_H^* = a_L : a_H \Rightarrow \underline{E}_f^* = a_f T^2$

Thermal fluctuations: $\sigma^2(E_f^*) = 2\underline{E}_f^* T \Rightarrow \delta E_f^*$

Fragment excitation: $E_f^* = \underline{E}_f^* + \delta E_f^*$

Small adjustment: $\underline{E}_L^* \to x\, \underline{E}_L^*$ $(x>1)$ - dist?

Fragment momenta then follow from energy & momentum conservation:

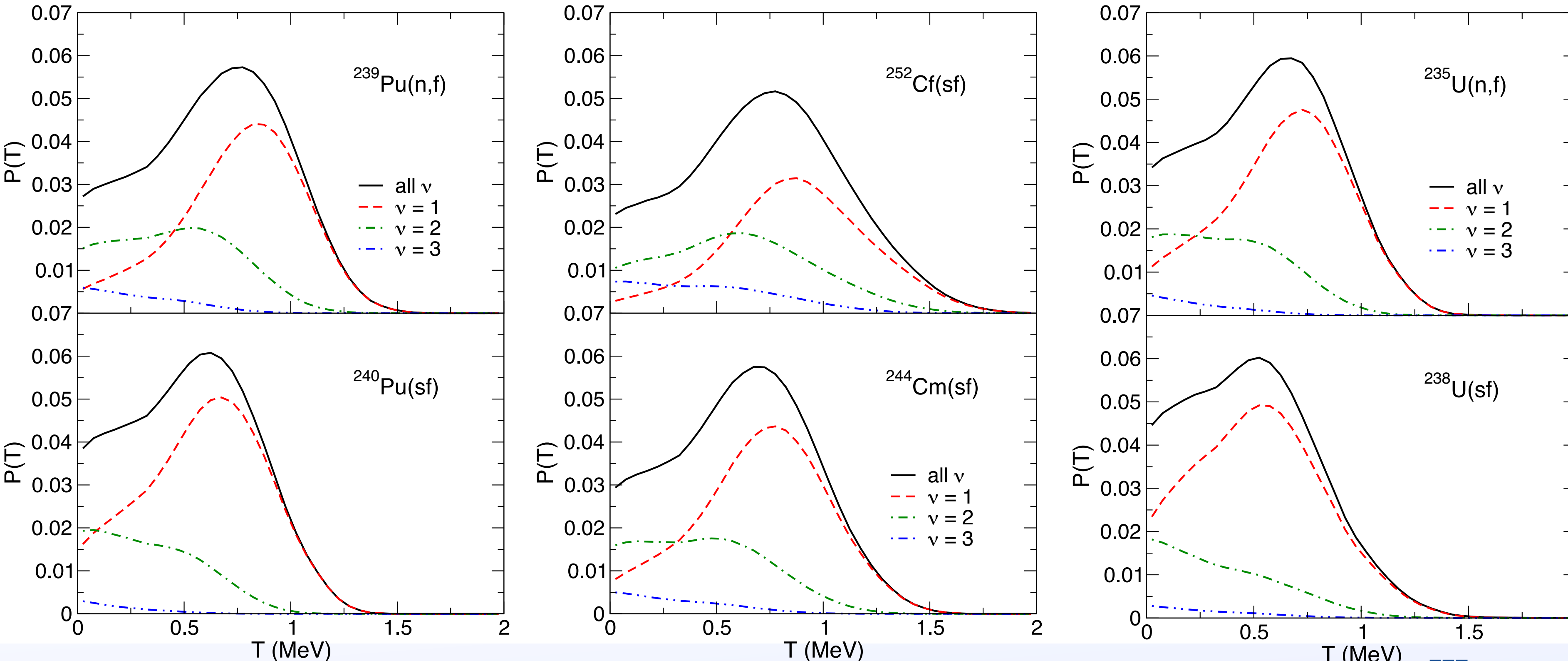
$$\begin{cases} TKE = \underline{TKE} - \delta E_L^* - \delta E_H^* \\ \mathbf{p}_L + \mathbf{p}_H = 0 \end{cases}$$

*) $a_A(E^*)$ from Kawano *et al*, J. Nucl. Sci. Tech. **43** (2006) 1

Temperature of daughter nuclei after neutron emission

Distribution of maximum temperature of fragment daughter nucleus after emission of one or more neutrons – cases that emit more neutrons on average are visibly hotter

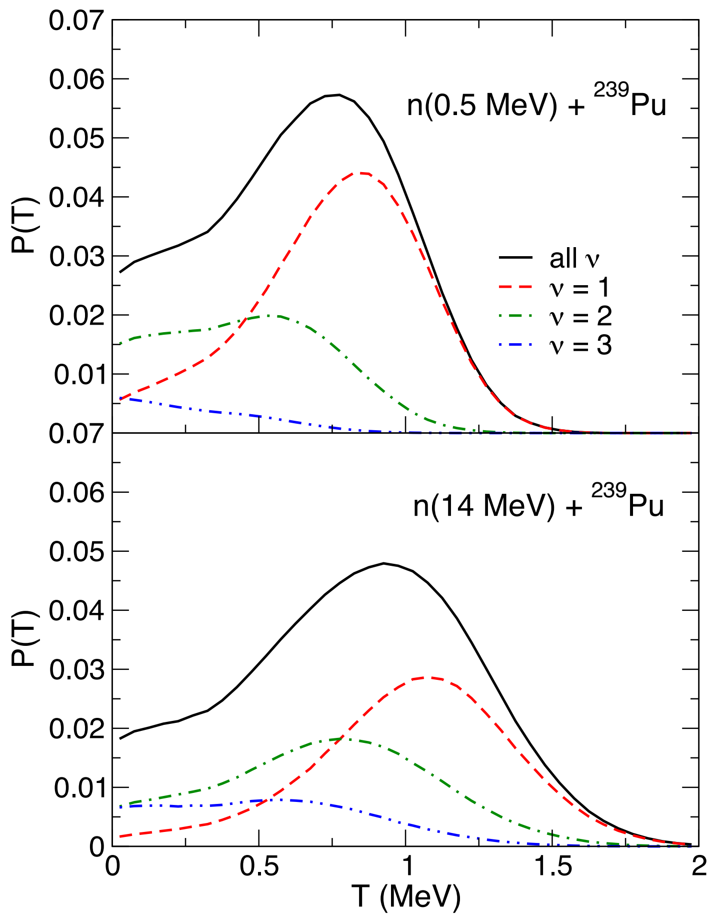
Shape is not triangular (as assumed by Madland and Nix)

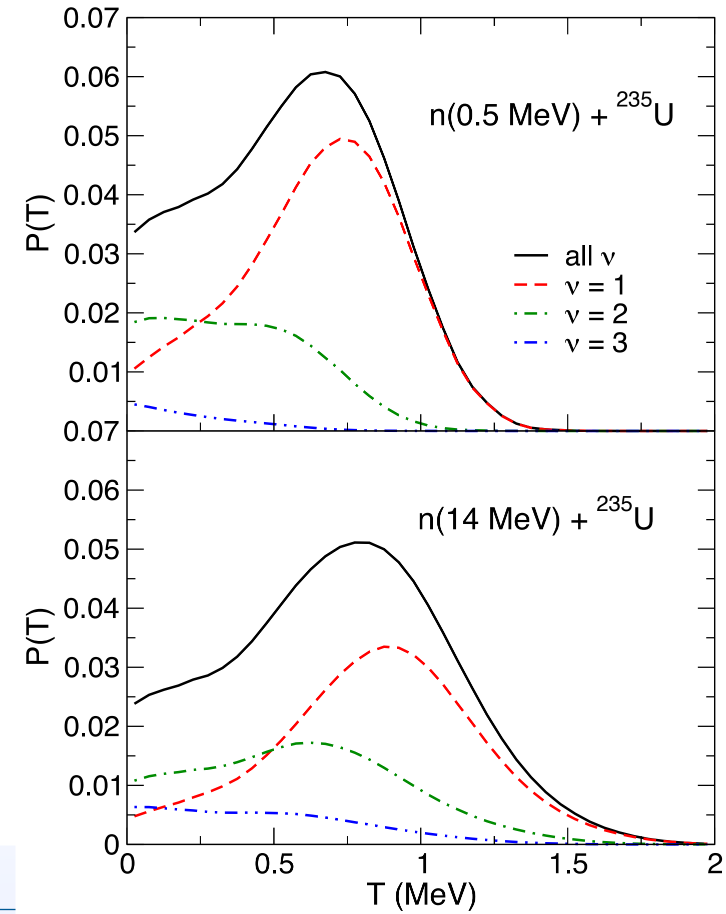


Energy dependence of daughter temperature distribution

Distribution of maximum temperature of fragment daughter nucleus after emission of one or more neutrons – higher energy, more neutron emission, is visibly hotter, even for 3 emitted neutrons

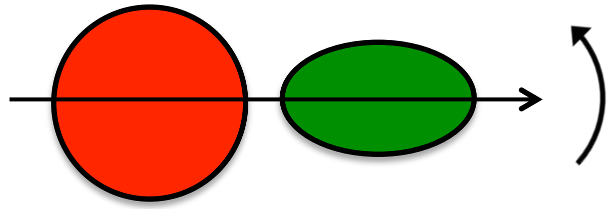
Shape is even less like a triangle





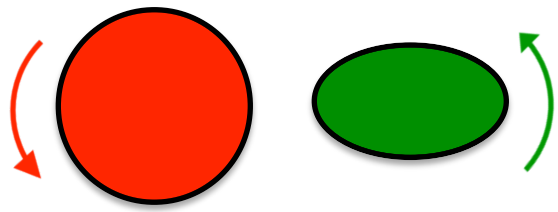
Angular momentum at scission: Rigid rotation plus fluctuations

Rigid rotation:



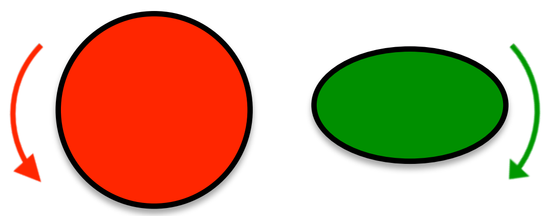
$\mathbf{S}_i = (\mathcal{I}_i/\mathcal{I})\mathbf{S}_0 + \delta\mathbf{S}_i$

Wriggling:



$\mathcal{I}_+ = (\mathcal{I}_{\mathrm{H}}+\mathcal{I}_{\mathrm{L}})\mathcal{I}/\mathcal{I}_{\mathrm{R}}$

Bending:

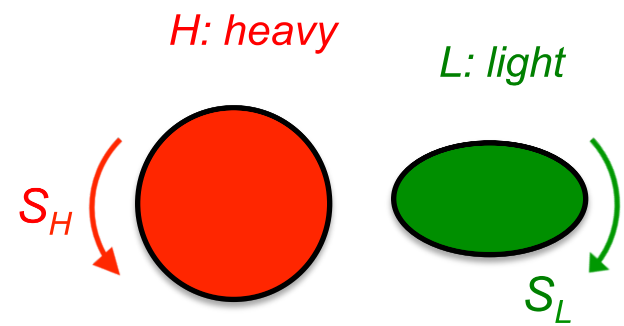


$\mathcal{I}_- = \mathcal{I}_{\mathrm{H}}\mathcal{I}_{\mathrm{L}}/(\mathcal{I}_{\mathrm{H}}+\mathcal{I}_{\mathrm{L}})$

$$\mathcal{I} = \mathcal{I}_{\mathrm{L}} + \mathcal{I}_{\mathrm{H}} + \mathcal{I}_{\mathrm{R}};\ \mathcal{I}_{\mathrm{R}} = \mu\mathbf{R}^2;\ \mathbf{R} = \mathbf{R}_{\mathrm{L}} - \mathbf{R}_{\mathrm{H}};\ \mu = m_N A_{\mathrm{L}} A_{\mathrm{H}}/(A_{\mathrm{L}} + A_{\mathrm{H}})$$

The dinuclear rotational modes (+ & -) have thermal fluctuations governed by an adjustable "spin temperature" $T_S = c_S\, T_{sc}$, where T_{sc} is the scission temperature

Fluctuations Contribute to Fragment Rotational Energy



Scission induces statistical agitation of dinuclear rotation modes – wriggling (s_+) and bending (s_-)
$s_\pm = (s_\pm^x, s_\pm^y, 0)$:

$P(s_\pm) \sim \exp(-s_\pm^2/2\mathcal{I}_\pm T_S)$

T_S: *related to scission temperature by* $T_S = c_S T_{sc}$
(used $c_S = 0, 0.1, 1$*)*

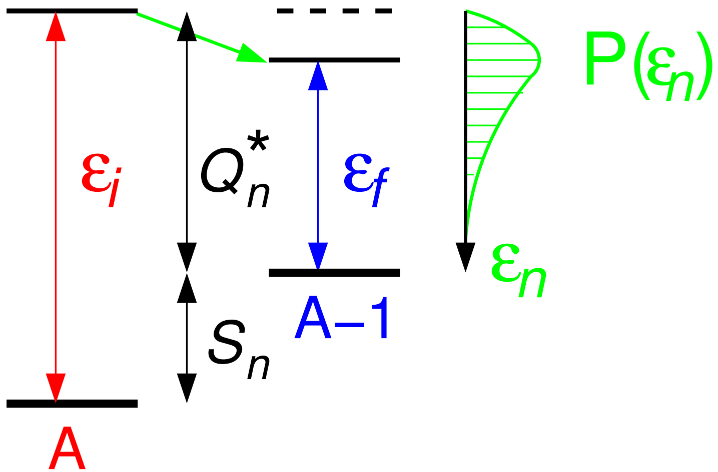
Fluctuating angular momentum components of fragments,
$\delta S_L^k = (\mathcal{I}_L/\mathcal{I}_+) s_+^k + s_-^k$; $\delta S_H^k = (\mathcal{I}_H/\mathcal{I}_+) s_+^k - s_-^k$;
Total angular momenta of fragment i are then $\mathbf{S}_i' = \mathbf{S}_i + \delta\mathbf{S}_i$
with orbital angular momentum $\mathbf{L}' = \mathbf{L} - \delta\mathbf{S}_L - \delta\mathbf{S}_H$; *contribution to dinuclear rotation modes* $\delta E_{rot} = S_+^2/2\mathcal{I}_+ + S_-^2/2\mathcal{I}_-$, *as well as rigid rotation part* E_{rot}, *is not available for statistical excitation*

Mean statistical excitation is reduced correspondingly and shared between fragments:

$$\underline{E^*} = Q_{LH} - \underline{TKE} - E_{rot} - \delta E_{rot} = \underline{E_L^*} + \underline{E_H^*}$$

Photon observables are very sensitive to fragment spin while neutrons are not

Neutron evaporation from fragments



$$M_i^* = M_i^{\mathrm{gs}} + \varepsilon_i$$

$$M_f^* = M_f^{\mathrm{gs}} + \varepsilon_f$$

$$M_i^* = M_f^* + m_{\mathrm{n}} + \epsilon$$

$$Q_{\mathrm{n}}^* = \varepsilon_i + Q_{\mathrm{n}} = \varepsilon_i - S_{\mathrm{n}}$$

$$Q_{\mathrm{n}} \equiv Q_{\mathrm{n}}^*(\varepsilon_i = 0) = M_i^{\mathrm{gs}} - M_f^{\mathrm{gs}} - m_{\mathrm{n}} = -S_{\mathrm{n}}$$

$$\epsilon + \varepsilon_f = M_i^* - M_f^{\mathrm{gs}} - m_{\mathrm{n}} = Q_{\mathrm{n}}^* = \left\{ \begin{array}{l} \varepsilon_f^{\max} \\ \epsilon^{\max} \end{array} \right.$$

$$T_f^{\max} = \sqrt{\varepsilon_f^{\max}/a_f} = \sqrt{Q_{\mathrm{n}}^*/a_f}$$

$$d^3\boldsymbol{p} \sim \sqrt{\epsilon}\, d\epsilon\, d\Omega$$

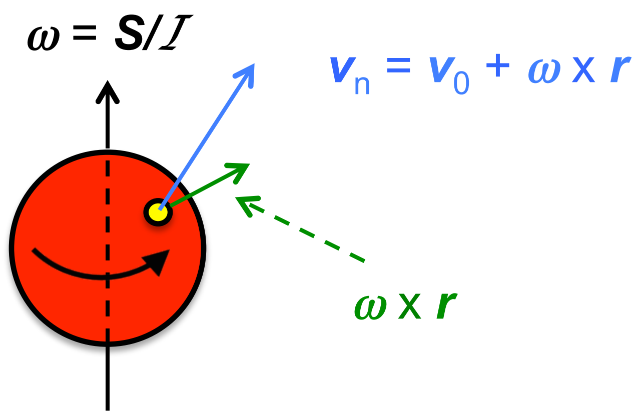
(non-relativistic)

Neutron energy spectrum:
$$\frac{d^3N}{d^3\boldsymbol{p}} d^3\boldsymbol{p} \sim \sqrt{\epsilon}\, \mathrm{e}^{-\epsilon/T_f^{\max}} \sqrt{\epsilon}\, d\epsilon\, d\Omega = \mathrm{e}^{-\epsilon/T_f^{\max}}\, \epsilon\, d\epsilon\, d\Omega$$

Lorentz boost both ejectile and daughter motion from emitter frame to laboratory frame

Neutron (and photon) emission in FREYA based on Weisskopf-Ewing theory which conserves only energy, charge, and mass number

Neutron evaporation from rotating fragments



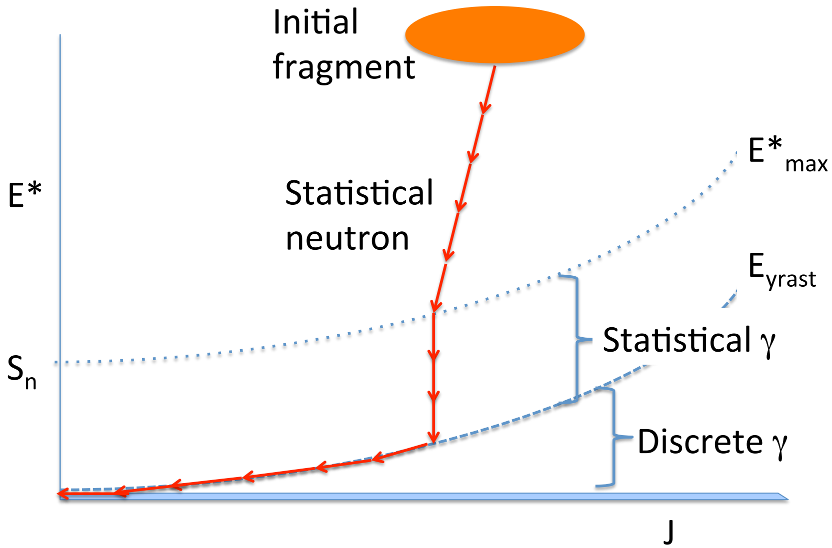
$$\boldsymbol{S}' = \boldsymbol{S} - \boldsymbol{r} \times \boldsymbol{p}_n$$

Usual thermal emission from the moving surface element, $\boldsymbol{v}_0$*, subsequently boosted with the local rotational velocity* $\omega \times \boldsymbol{r}$ *.*

Conserves energy as well as linear & angular momentum.

Photon emission follows neutron emission

After neutron evaporation has ceased, $E^* < S_n$, the remaining excitation energy is disposed of by sequential photon emission …



… first by statistical photon cascade down to the yrast line …

$$\frac{d^3N_\gamma}{d^3\boldsymbol{p}_\gamma} d^3\boldsymbol{p}_\gamma \sim c\,\mathrm{e}^{-\epsilon/T_i}\epsilon^2\,d\epsilon\,d\Omega$$ **<=** $$d^3\boldsymbol{p}_\gamma \sim \epsilon^2 d\epsilon\, d\Omega$$ *(ultra-relativistic)*

$$E_f^* = E_i^* - \epsilon_\gamma$$

… then by stretched E2 photons along the yrast line …

$$S_f = S_i - 2$$
$$\epsilon_\gamma = S_i^2/2\mathcal{I}_A - S_f^2/2\mathcal{I}_A$$
$$\mathcal{I}_A = 0.5 \times \tfrac{2}{5} A m_N R_A^2$$

Each photon is Lorentz boosted from the emitter to the laboratory frame

External parameters in FREYA which can be adjusted to data

- In addition to isotope-specific inputs such as Y(A) and TKE(A_H), there are also intrinsic parameters such as nuclear masses (Audi and Wapstra for experimentally-measured masses, supplemented by masses calculated by Moller, Nix, Myers and Swiatecki), barrier heights, pairing energies and shell corrections
- There are also external parameters that can be adjusted, either universally or per isotope
  - Shift in total kinetic energy, dTKE, adjusted to give the evaluated average neutron multiplicity
  - Asymptotic level density parameter, e_0, $a_i \sim (A/e_0)[1+ (\delta W_i/U_i)(1 - \exp(-\gamma U_i))]$ where $U_i = E^*_i - \Delta_i$, $\gamma = 0.05$, and the pairing energy, Δ_i, and shell correction, δW_i, are tabulated (if $\delta W_i \sim 0$ or U_i is large so that $1 - \exp(-\gamma U_i) \sim 0$, $a_i \sim A/e_0$)
  - Excitation energy balance between light and heavy fragment, x
  - Width of thermal fluctuation, $\sigma^2(E_f^*) = 2cE_f^*T$, c is adjustable (default = 1)
  - Multiplier of scission temperature, c_S, that determines level of nuclear spin
  - Energy where neutron emission ceases and photon emission takes over, $S_n + Q_{min}$
  - Default values: $e_0 \sim 10$/MeV, c = 1, $c_S = 1$, $Q_{min} = 0.01$ MeV
  - Specific to ^{252}Cf(sf): x = 1.3, dTKE = 0.5 MeV

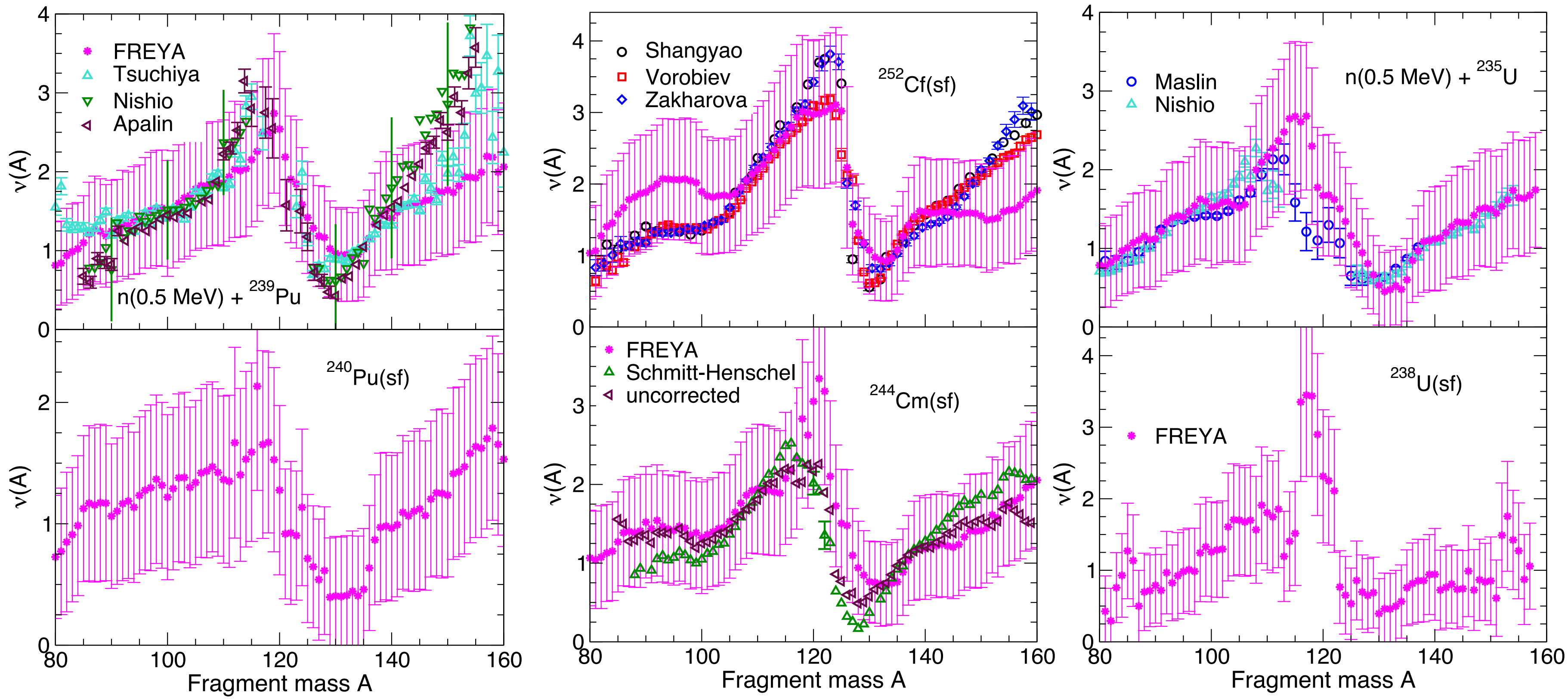
Other Monte Carlo fission codes

- CGMF (Talou et al), LANL
- FIFRELIN (Serot et al), France
- GEF (Schmidt and Jurado), Germany
- FREYA is based on Weisskopf-Ewing theory and thus emission is based only on charge, mass number and energy conservation, a fast procedure more useful for neutron transport codes
- CGMF and FIFRELIN are based on Hauser-Feshbach theory which includes angular momentum and parity as well so involves a sum over all outcomes that result in the same total angular momentum and parity: this is a very slow procedure and is so far limited to fewer nuclei than FREYA
- CGMF, FIFRELIN and FREYA use similar inputs of Y(A,Z) and TKE to ultimately extract the excitation energy
- Since CGMF and FIFRELIN have concentrated on fewer isotopes, they have tried to tune their results to some inclusive data such as $\nu(A)$; FREYA has focused more on using single global parameters to be somewhat more predictive
- GEF is a somewhat different beast, it models the potential energy surface of the fissioning (compound) nucleus to directly obtain the fragment yields and excitation energies, does not really address the TKE

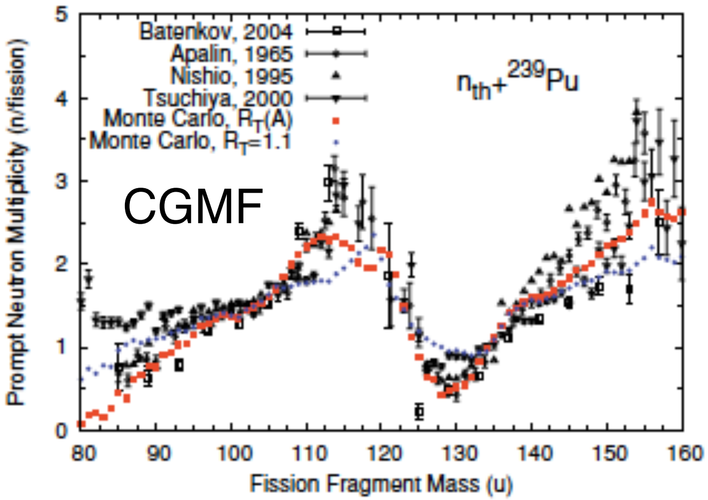
ν(A) for FREYA spontaneous and thermal fission

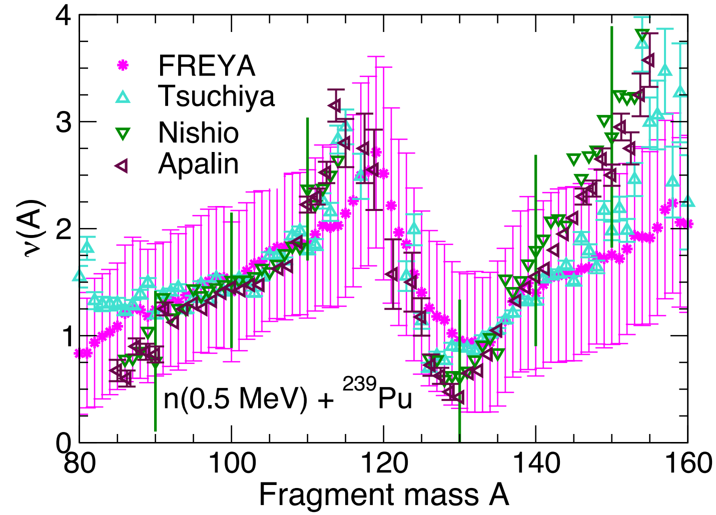
Mean neutron multiplicity as a function of fragment mass; agrees with sawtooth shape of data

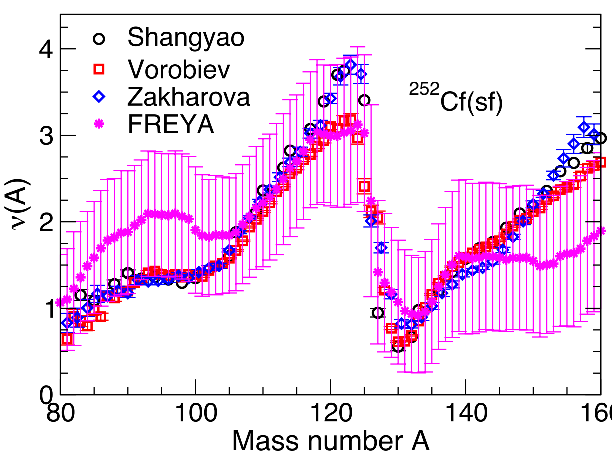
Not all cases have data to compare to **FREYA**, smoothness of sawtooth dependent on quality of yield and TKE data

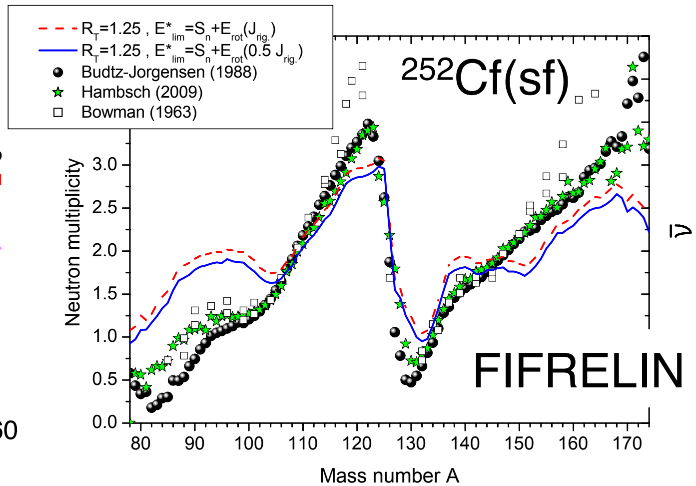


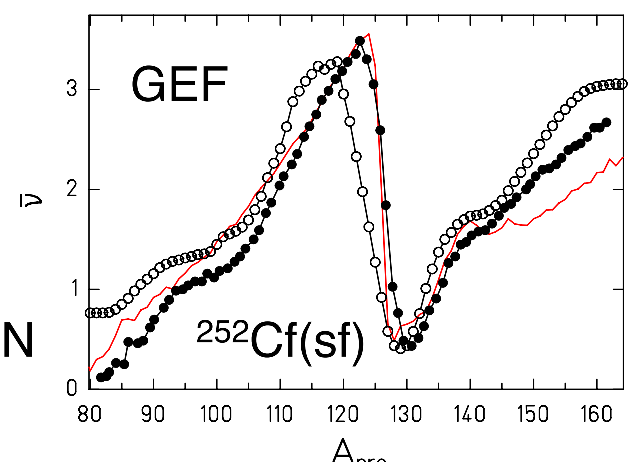
Model comparison: ν(A)









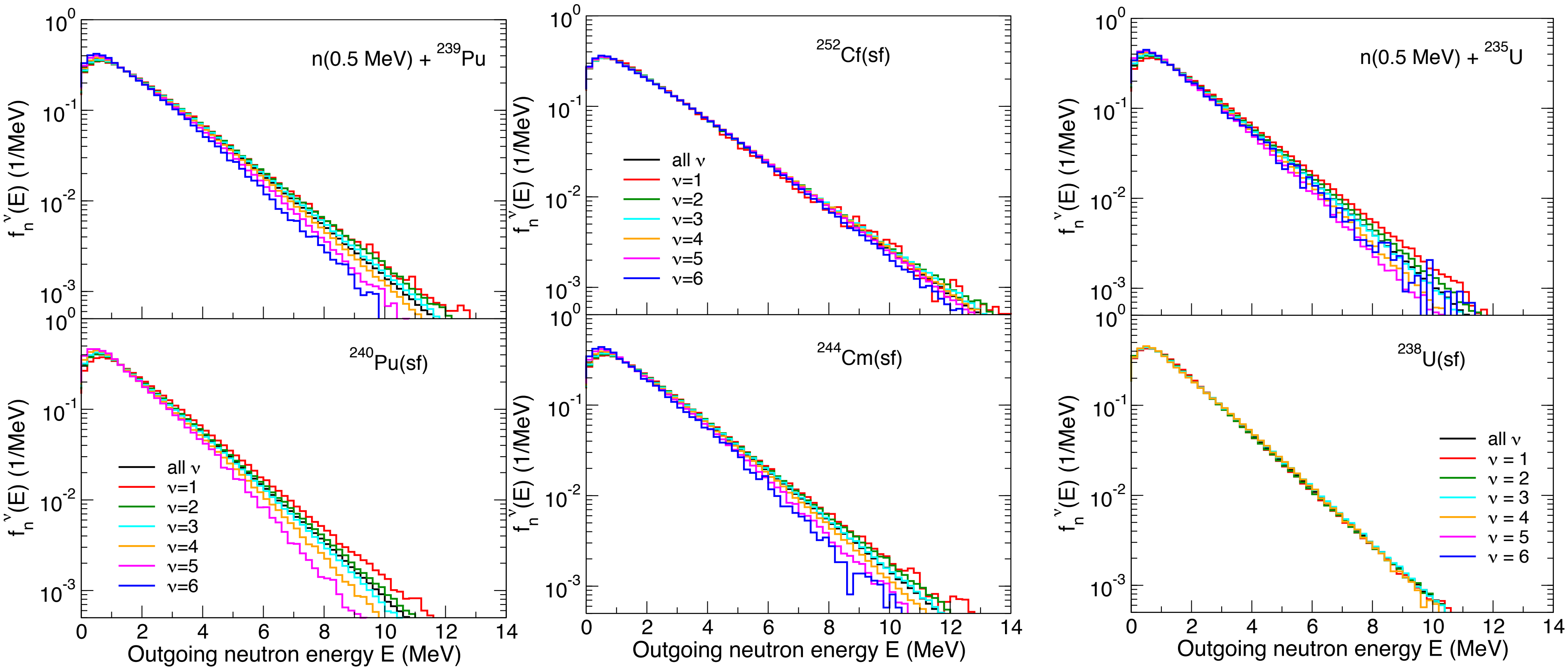


Correlations between neutron number and energy

Spectral shapes shown, all normalized to unity for better comparison

Most cases show considerable softening of the spectrum for increased neutron multiplicity

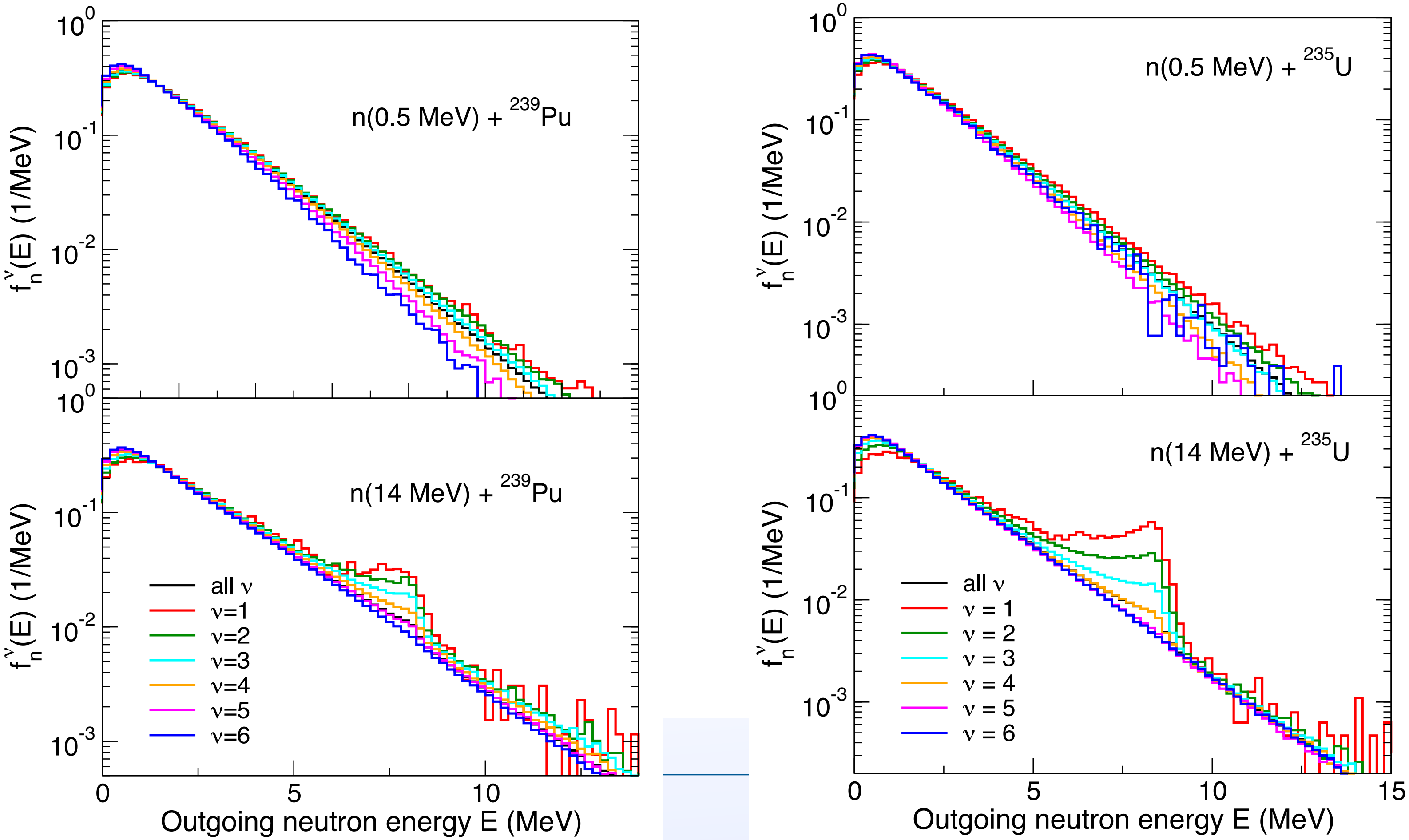
^{252}Cf(sf) and ^{238}U(sf) more tightly correlated



Energy dependence of prompt fission neutron spectra

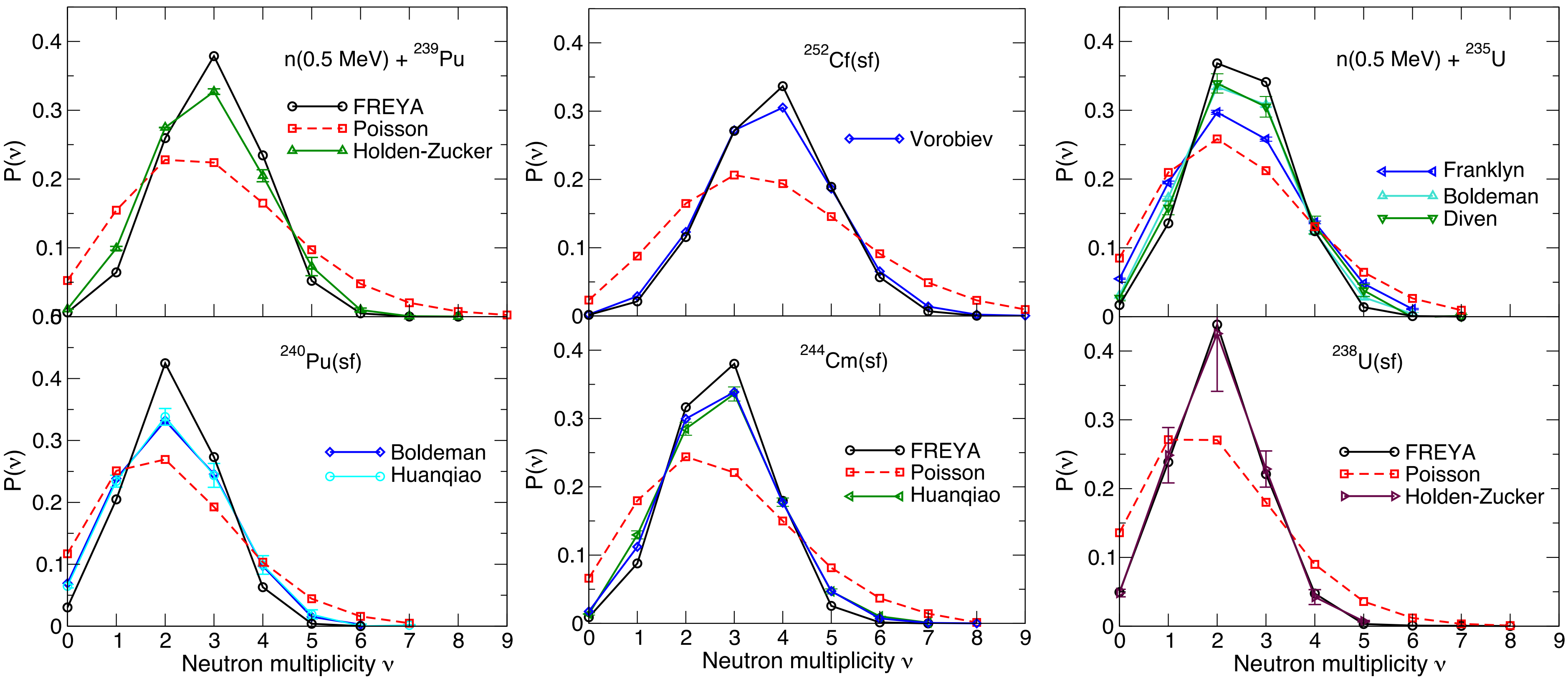
‘Pile-up’ in 14 MeV spectra at E_n-B_f due to energy conservation: there can be no pre-fission neutrons with energy greater than E_n-B_f, otherwise fission would not occur

Bump shows single pre-fission neutron emission, strongest for ν=1, reduced when evaporated neutrons are also present, high energy tail is from first chance fission



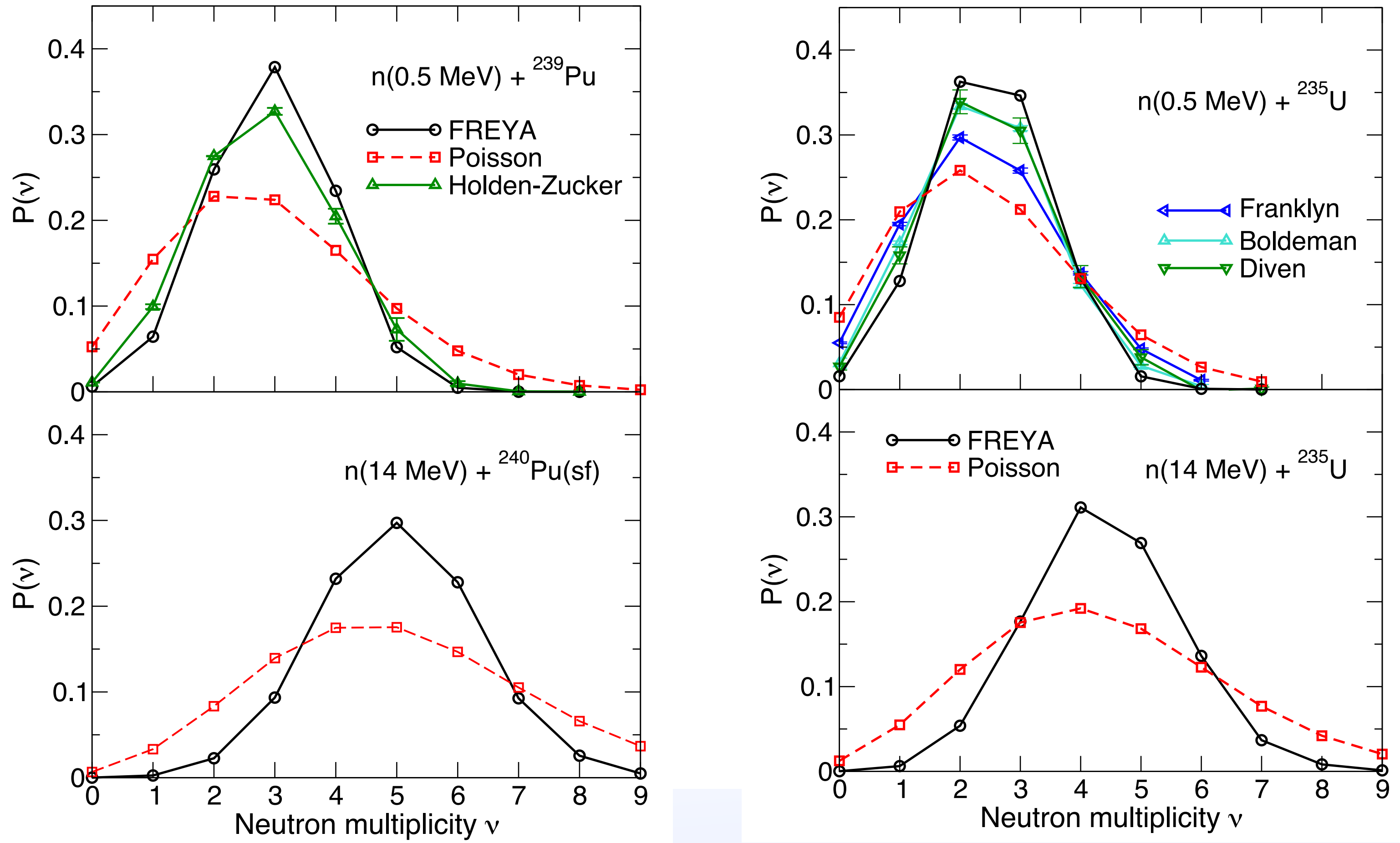
Probability for prompt neutron emission

Since each neutron emitted reduces the excitation energy not only by its kinetic energy ε_n ($\langle\varepsilon_n\rangle = 2T_f^{max}$) but also by the (larger) separation energy $S_{n,}$ the neutron multiplicity distribution is narrower than a Poisson



Energy dependence of neutron multiplicity distribution

As incident neutron energy increases, P(ν) is peaked at higher multiplicity and distribution broadens, reflecting higher probabilities of fluctuations with large multiplicities

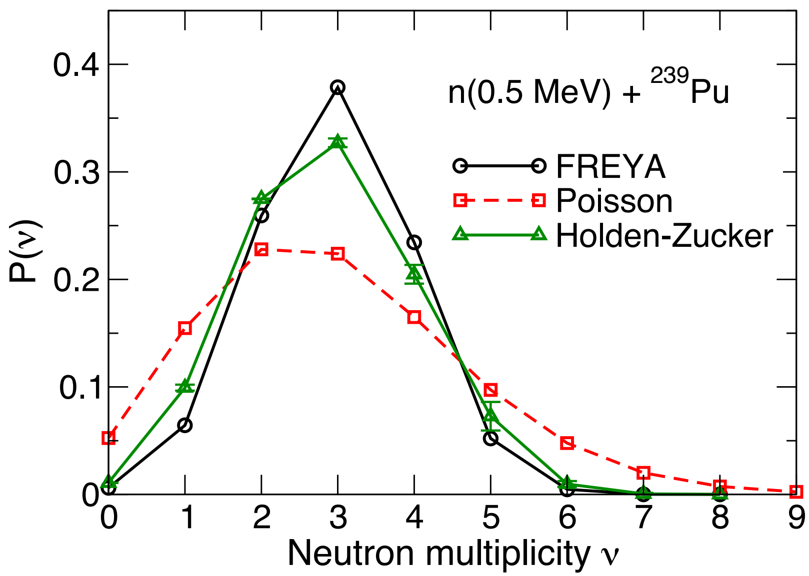


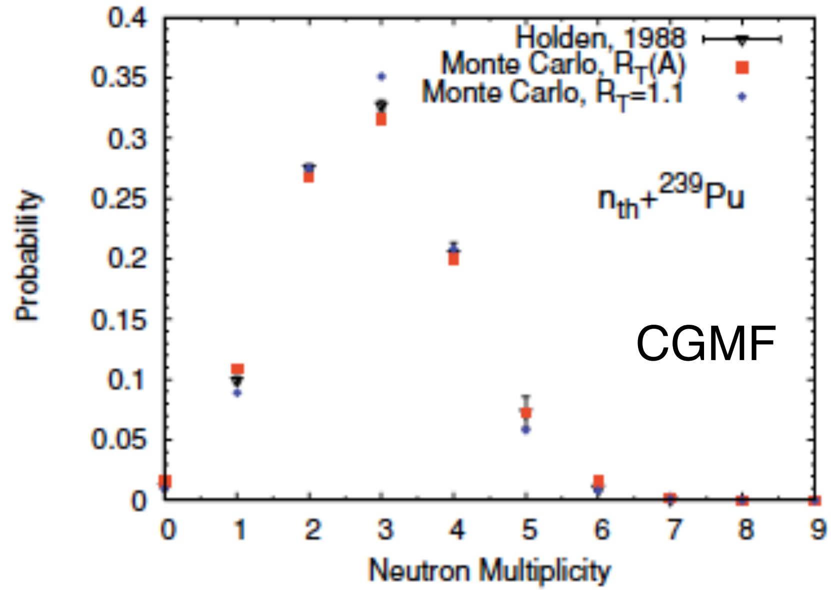
Model comparison: neutron multiplicity distribution

Neutron-induced fission of ^{239}Pu is calculated in FREYA (left) and CGMF (right)

FREYA result is similar to R_T = 1.1 in CGMF, not surprising because $R_T(A)$ is tuned to $\nu(A)$ data

Holden-Zucker (Holden) is compilation of data on a number of isotopes, e.g. for ^{239}Pu it represents an average over several data sets





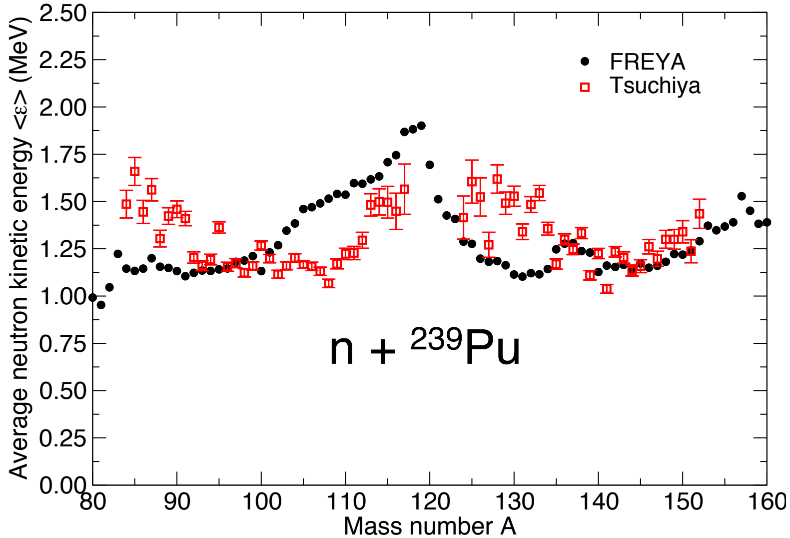
Model comparison: neutron kinetic energy vs mass

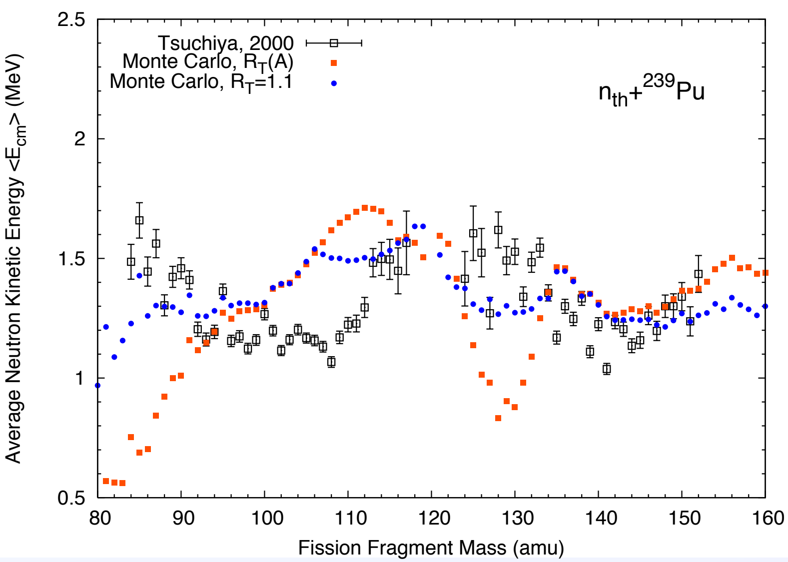
Neutron kinetic energy was measured by Tsuchiya et al as a function of fragment mass

FREYA (left) and CGMF (right) compared to data, note different scales on the y-axes

FREYA and RT = 1.1 in CGMF are very similar except near symmetry

Note that tuning RT(A) to n(A) generally decreases agreement with data, especially at A < 90 and 120 < A < 135 – latter region is because fewer neutrons are emitted at closed Shell and, in CGMF, these neutrons are less energetic

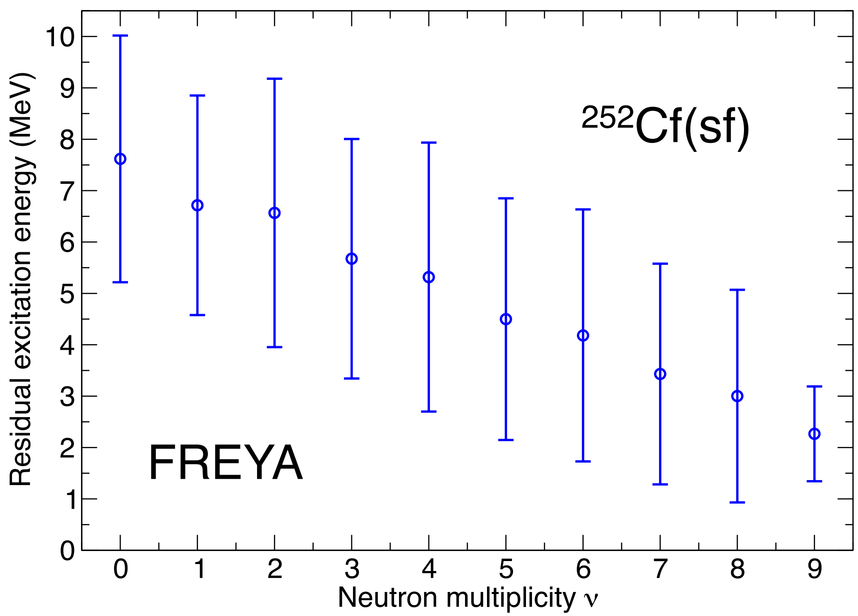


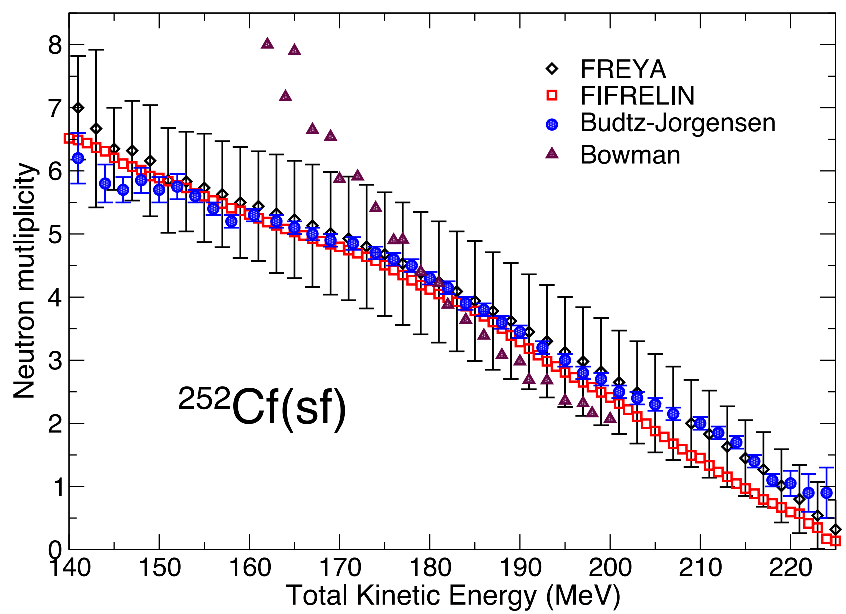


Other inclusive ‘observables’

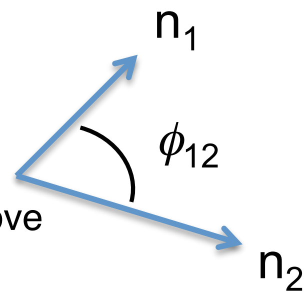
(Left) Residual excitation energy is how much is left after neutron emission stops, depends on Q_{min}, the more neutrons emitted, the more energy they take away; increasing Q_{min} would increase residual excitation energy – essentially what is left over for photons, equivalent to E_{γ}

(Right) Neutron multiplicity vs TKE: Budtz-Jorgensen data and model calculations are averaged Over Y(A,Z) while Bowman data are for yields of specific fragment pairs; models are consistent





Two-neutron angular correlations reflect emitter source

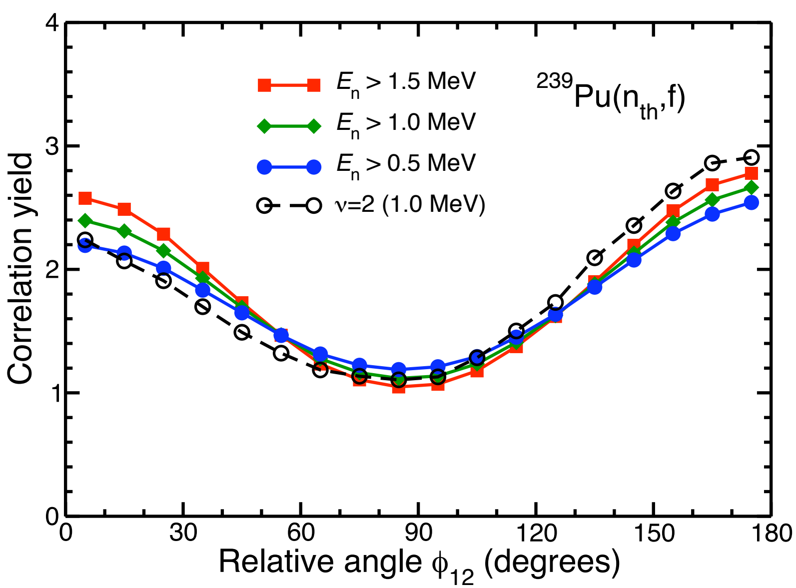


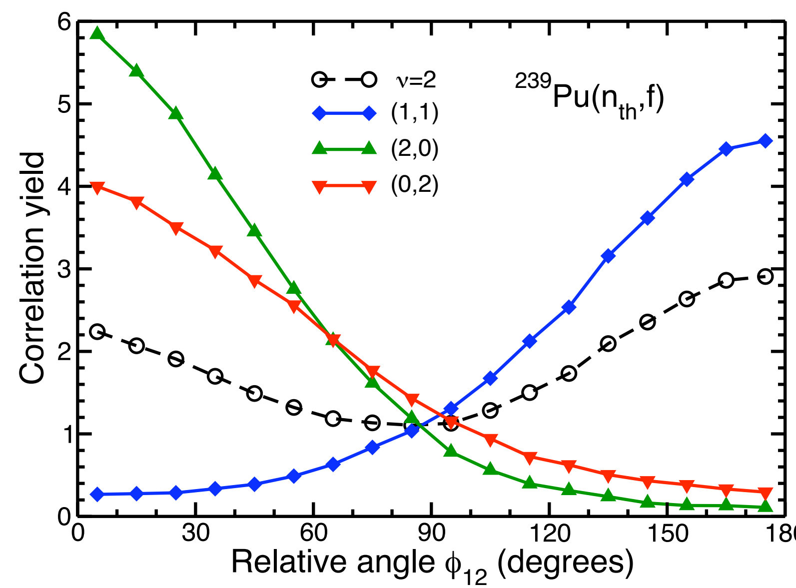
Correlations between neutrons when exactly 2 neutrons with $E_n > 1$ MeV are emitted:

One from each fragment (blue) back to back; both from single fragment emitted in same direction, tighter correlation when both from light fragment (green) than from heavy (red); open circles show sum of all possibilities

Correlations of neutrons with energies above a specified threshold energy

Yield forward and backward is more symmetric for higher-energy neutrons

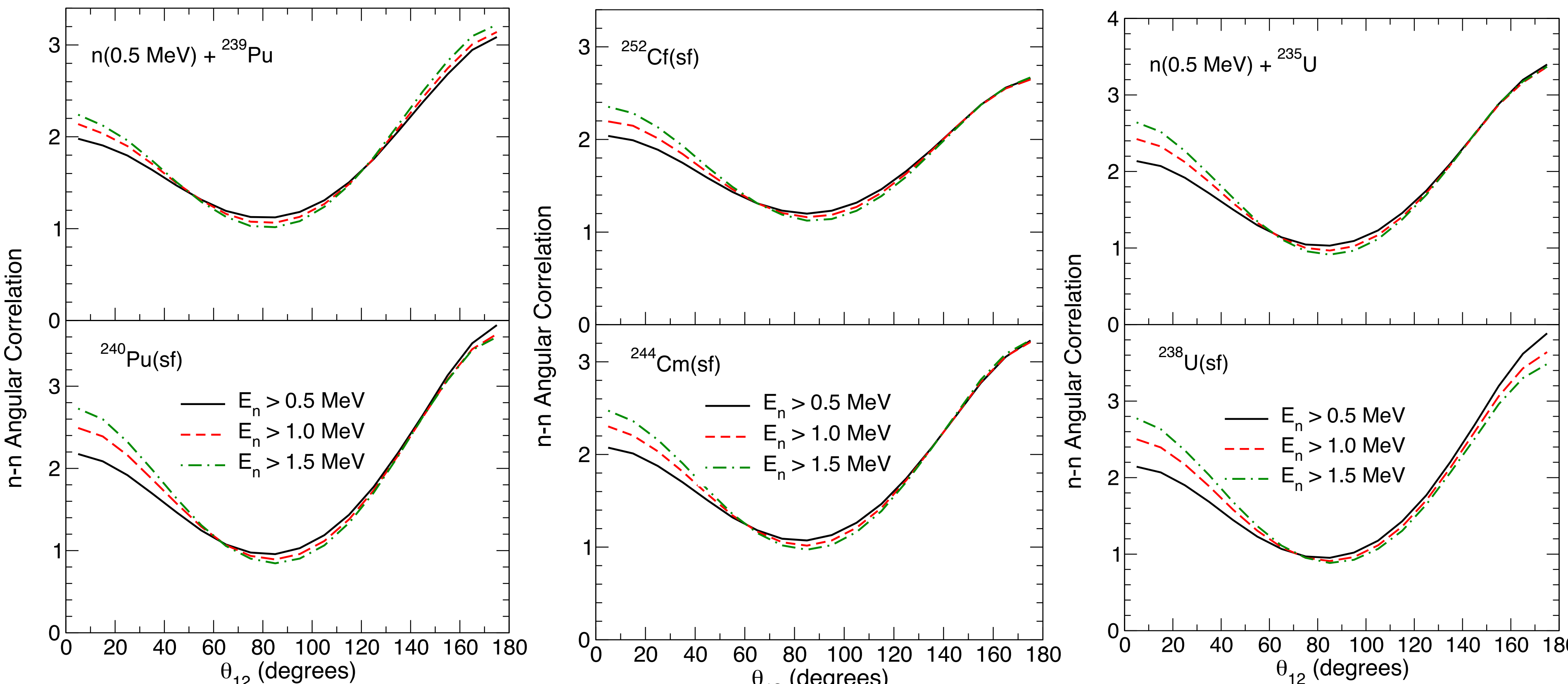




Examples of two-neutron correlations in FREYA

Back-to-back correlation is stronger for ^{240}Pu(sf) and ^{238}U(sf) since both emit about 2 neutrons on average

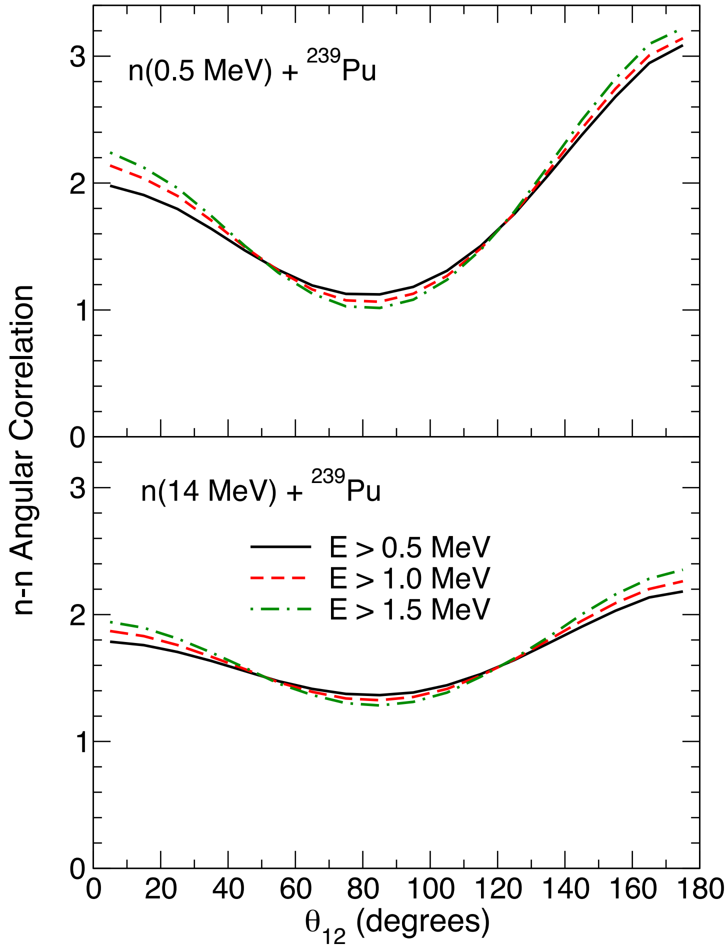
Cases with larger multiplicities, like ^{252}Cf(sf), show weaker two-neutron correlations

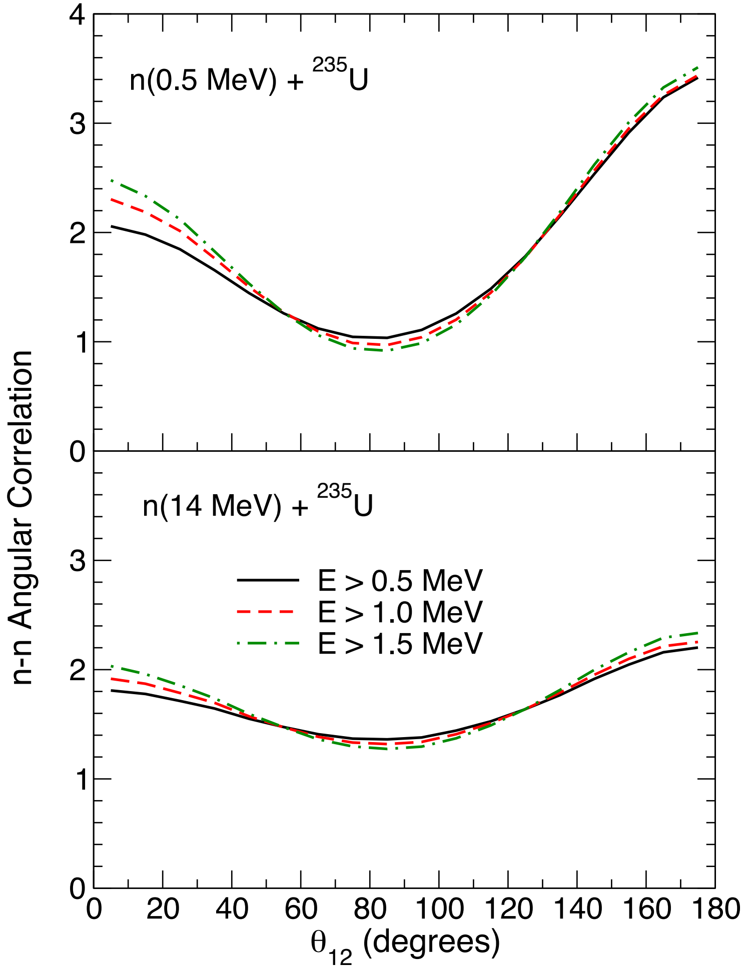


Energy dependence of two-neutron angular correlations

Back-to-back direction of emission is reduced at higher energies since two energetic neutrons can come from same fragment as often as one from each fragment

Correlations get washed out because more neutrons are emitted



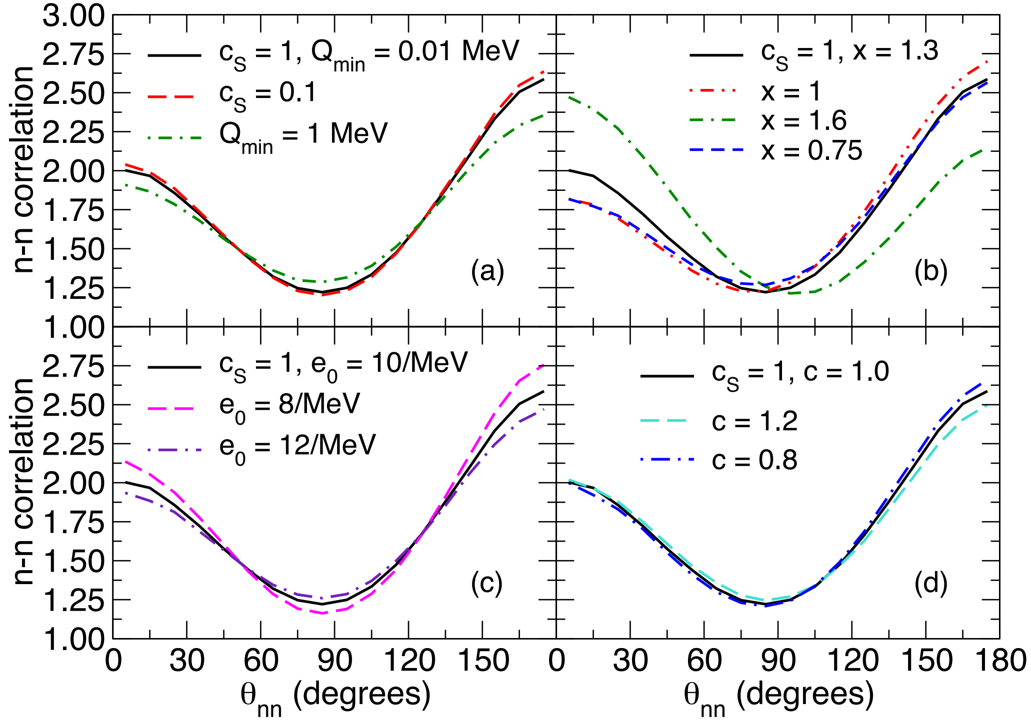


Sensitivity of correlations to input parameters

Changing Q_{min}, c_S, e_0 and c does not have a strong effect on the shape of the n-n correlations

Only changing x strongly modifies the correlation shape: x < 1.3 default reduces the correlation at $\theta_{nn} = 0°$ while leaving that at 180° unchanged; x > 1.3 (giving more excitation to light fragment) produces a significantly stronger correlation at $\theta_{nn} = 0°$

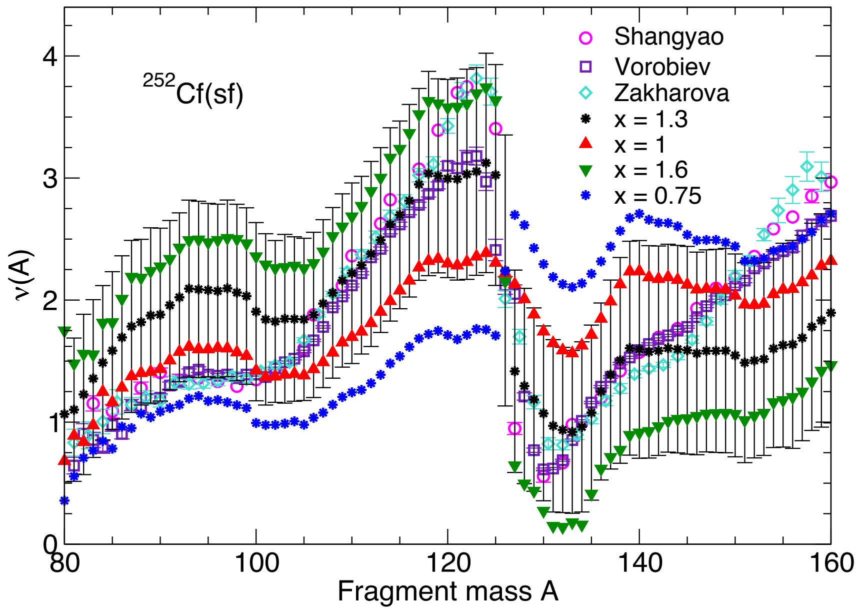
Correlation shape is relatively robust with respect to model parameters

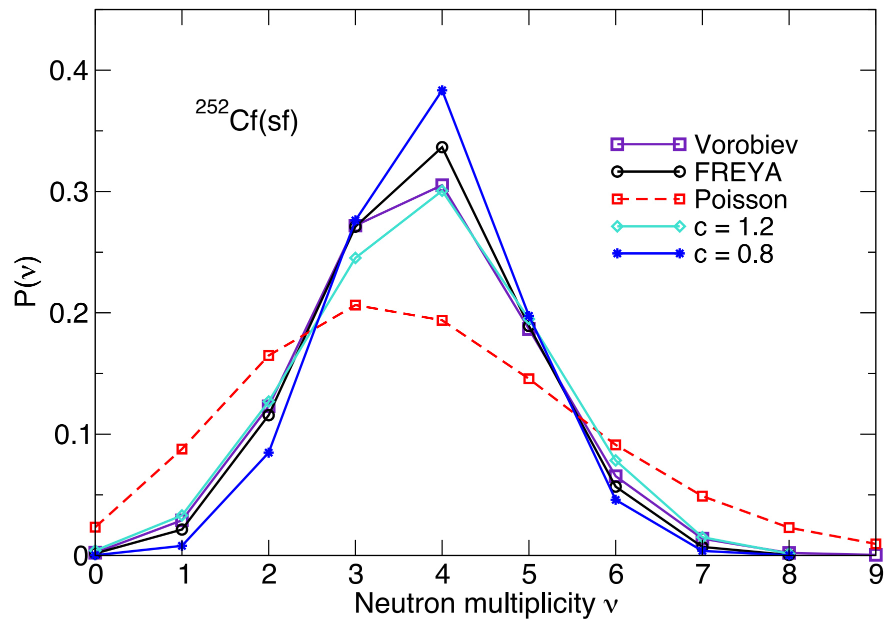


Effect of changing input parameters on other observables

(Left) changing x reduces agreement with ν(A) in the range of highest yield, $100 < A < 140$; x = 1.3 gives best agreement in this range, x = 0.75 gives too much energy to the heavy fragment, x = 1 does somewhat better for $A < 100$ but is bad everywhere else, x = 1.6 is far off

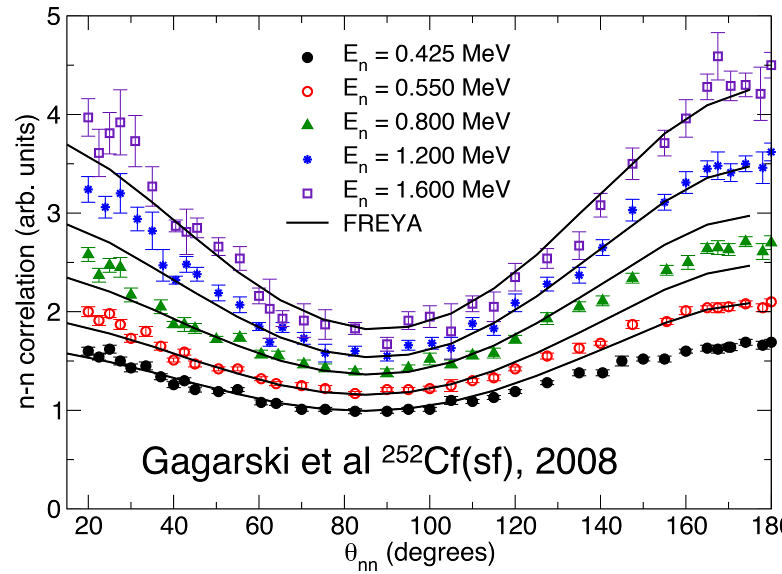
(Right) changing the width of the thermal distributions reduces the agreement of **FREYA** with the Vorobiev P(ν) data, increasing c makes P(ν) too broad, decreasing c makes it too narrow

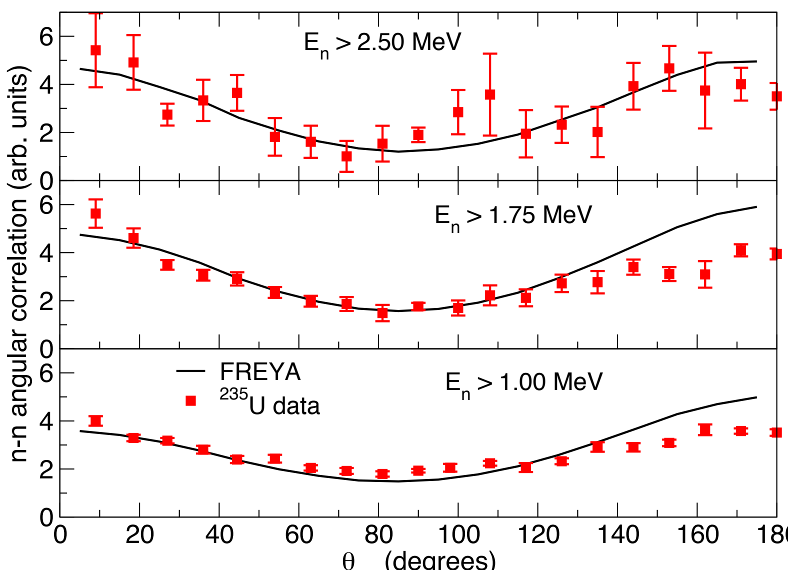




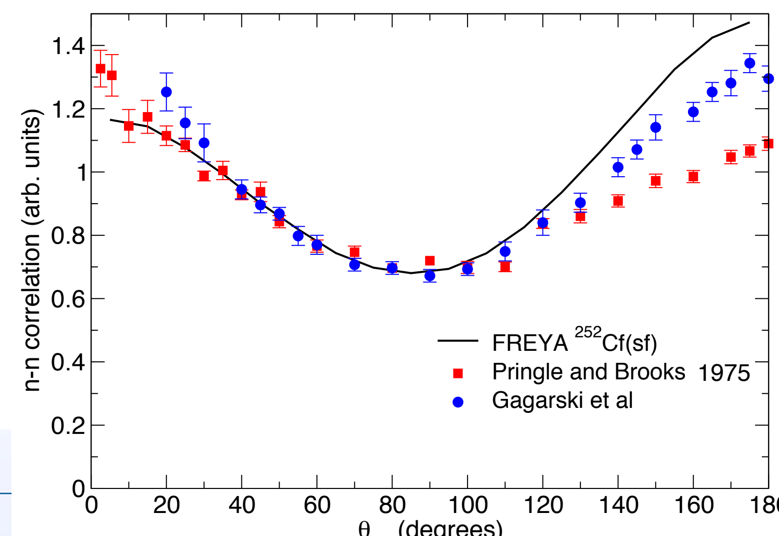
Default version of FREYA gives rather good agreement with angular correlation data

- All experiments took measurements at different angles, discriminating between photons and neutrons by timing, Gagarski et al used time of flight, others used pulse shape discrimination
- Newer data seems to show higher back-to-back correlation, more consistent with **FREYA**, than older data
- Higher Q_{min} might bring data and calculations closer together at lower energies and $\theta_{nn} > 120°$ where calculation and data are most discrepant





Franklyn et al, 1978

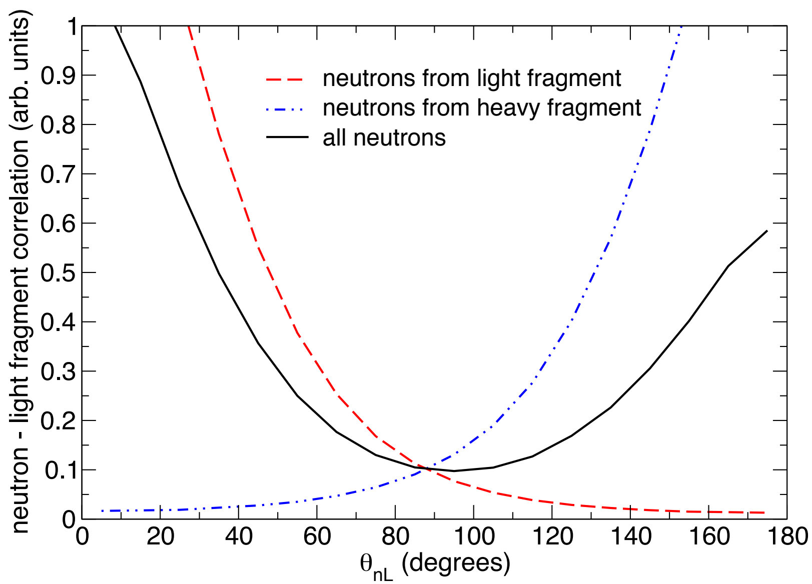


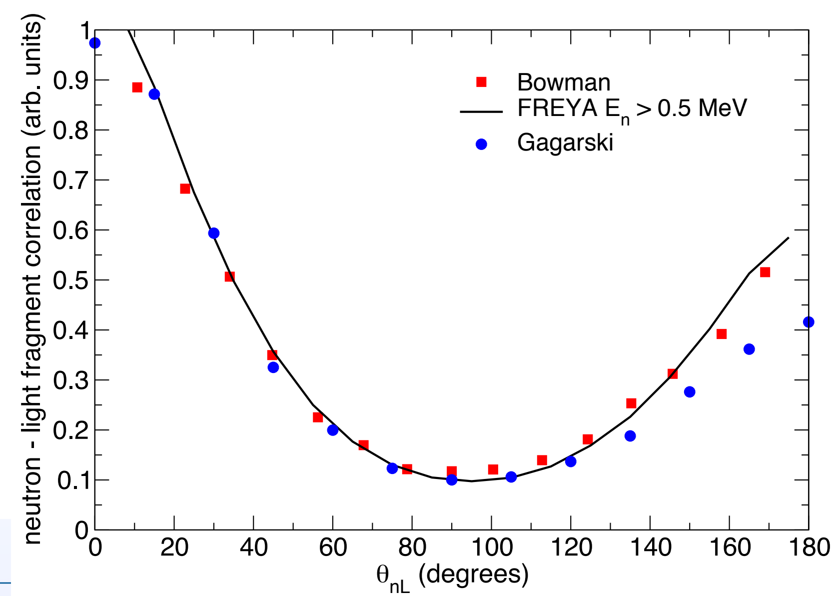
Correlation between neutron and light fragment

Neutron emission can also be correlated with individual fragments

(Left) Angle of neutrons emitted by either the light or heavy fragment or both fragments with respect to the direction of the light fragment: neutrons from light fragment emitted preferentially toward $\theta_{nL} = 0°$; neutrons from heavy fragment are typically moving opposite the light fragment in the lab frame, $\theta_{nL} = 180°$; correlation becomes more tightly peaked for higher neutron kinetic energies, here $E_n > 0.5$ MeV

(Right) **FREYA** result is compared to data, light fragment is determined and correlation is made with all measured neutrons, as in black curve at left; good agreement is seen





Other possible neutron correlation observables

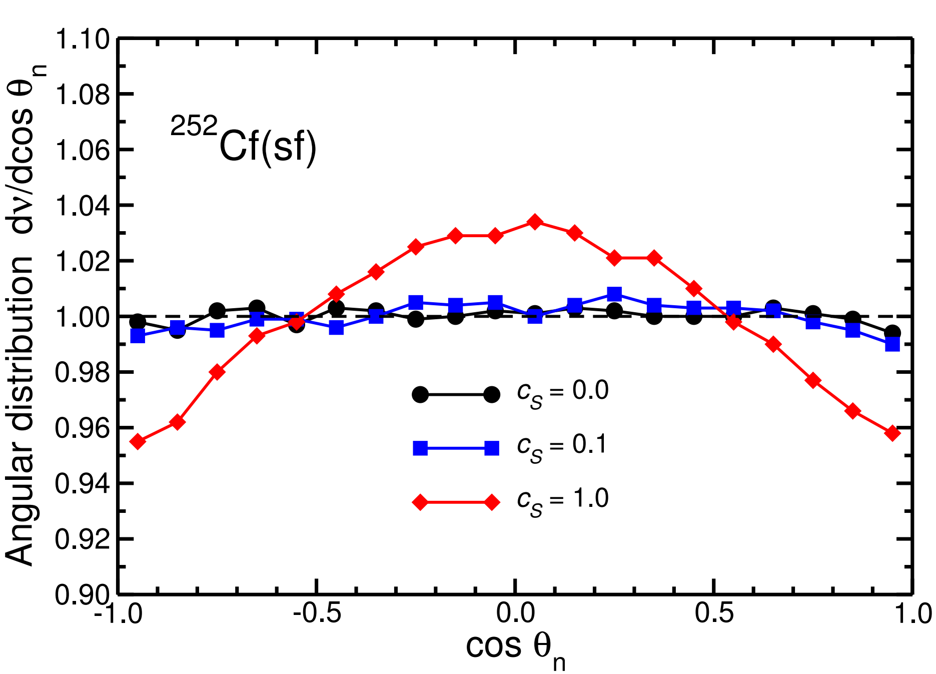
Angular distribution of neutrons evaporated from rotating nucleus acquires oblate shape – rotational boost enhances emission in plane perpendicular to angular momentum of emitter centrifugal effect quantified by 2nd Legendre moment

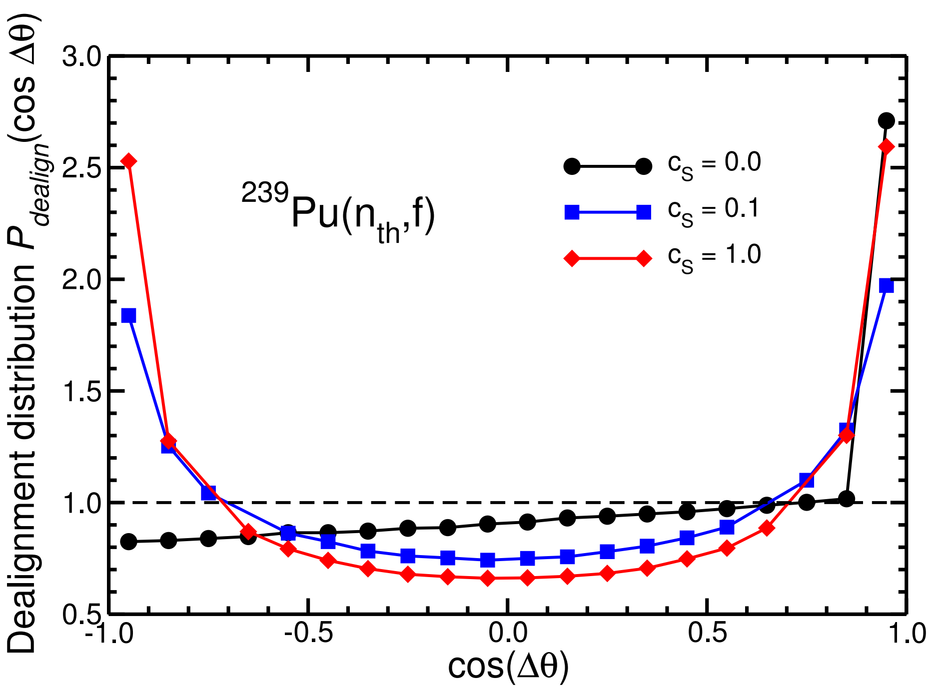
$$\langle P_2(\cos\theta)\rangle = \langle P_2(\boldsymbol{p}\cdot\boldsymbol{S}/|\boldsymbol{p}||\boldsymbol{S}|)\rangle$$

0 for isotropic emission; + for prolate (polar);
- for oblate (equatorial) – small effect overall

Neutron-induced fission endows compound nucleus with small initial angular momentum $\boldsymbol{S}_0$, giving the fragments non-vanishing angular momentum along $\boldsymbol{S}_0$ in addition to that acquired from fluctuations; fragment angular momentum modified by each neutron emission

angle between initial angular momentum of compound nucleus and fragment after evaporation is the dealignment angle $\Delta\theta$ ($\boldsymbol{S}_i'\cdot\boldsymbol{S}_0 = S_i' S_0 \cos\Delta\theta$)





Summary

- Event-by-event treatment shows significant correlations between neutrons that are dependent on the fissioning nucleus
- **FREYA** agrees rather well with most neutron observables for several spontaneously fissioning isotopes and for neutron-induced fission
- Comparison with n-n correlation data very promising
- Photon data do not present a very clear picture – clearly more experiments with modern detectors needed to verify older data
- Refined modeling of photon emission in **FREYA** is planned
- Incorporation of **FREYA** into **MCNP6**, **FREYA1.0** with neutrons, released as open source in July 2013, is in progress
- **FREYA1.0** is available from http://nuclear.llnl.gov//simulation/main2.html
- User manual also available online

Homework

- Prove that $\langle E \rangle = 2T$ for the Weisskopf-Ewing spectrum and the average energy of the PFNS in the Los Alamos model is $\langle E \rangle = (4/3)T_{max}$
- Download **FREYA** and run example problems.