Lawrence Livermore National Laboratory

Applications of Event-by-Event Fission Modeling with FREYA

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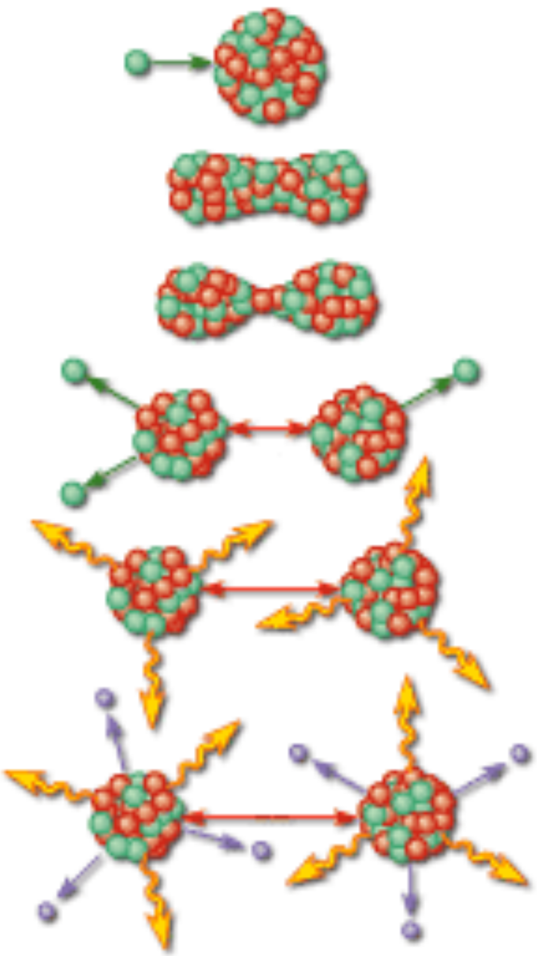
We are developing FREYA (Fission Reaction Event Yield Algorithm) for correlation studies and spectral evaluations

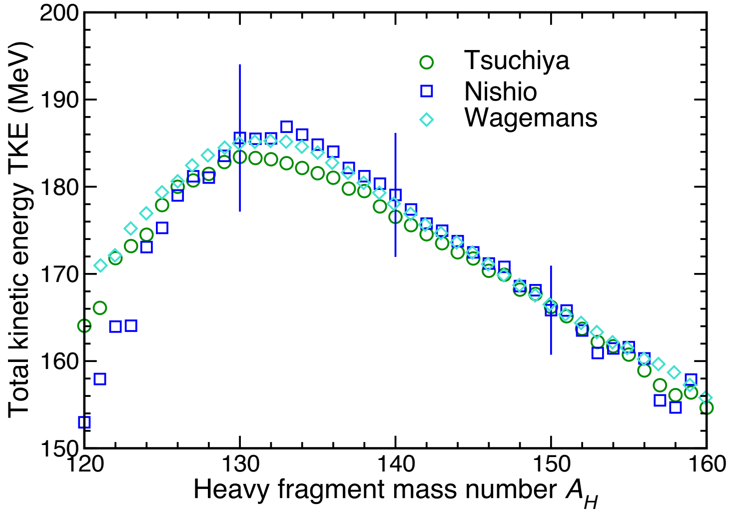
- J. Randrup (LBNL) is collaborator on **FREYA** development
- Other past and present LLNL collaborators: D. A. Brown (BNL), M. A. Descalle, C. Hagmann, W. E. Ormand, J. Pruet (NNSA), W. Younes
- Papers: Phys. Rev. C **80** (2009) 024601, 044611 **84** (2011) 044621; another submitted

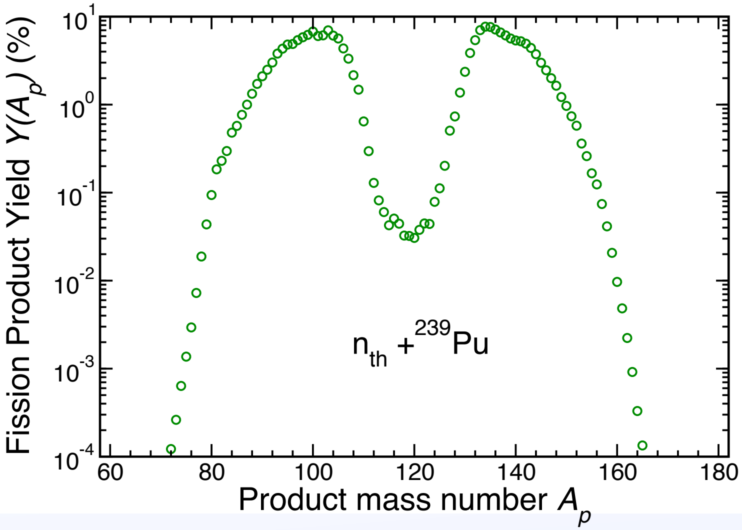
How FREYA works

- Assume binary fission of compound nucleus with mass A_c and charge Z_c formed by incident neutrons with energy E_n on actinide with mass $A_c - 1$
- Sample mass and charge of light, L, and heavy, H, fragments from fission fragment distributions, conserving mass and charge
- Determine fission Q from fragments, divide Q value between fragment kinetic and excitation energies
- Fix total kinetic energy, TKE, by sampling kinetic energy due to mutual Coulomb repulsion, obtain total excitation energy by conservation, TEE = Q – TKE
- Divide TEE between light and heavy fragments
- Allow for temperature fluctuations in small systems; adjust TKE accordingly to retain total energy conservation
- Evaporate neutrons from each fragment until excitation energy is too low for further neutron emission
- Prompt gamma emission follows after prompt neutron emission ceases



FREYA requires information about fragment yields, TKE, and average neutron multiplicity

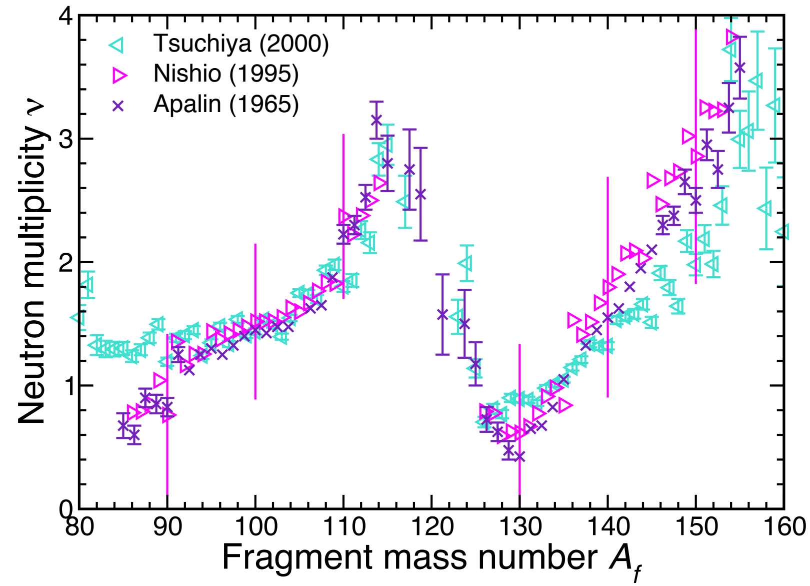




Extract shape of TKE(A_H) from thermal data and assume energy independence, moves TKE up and down

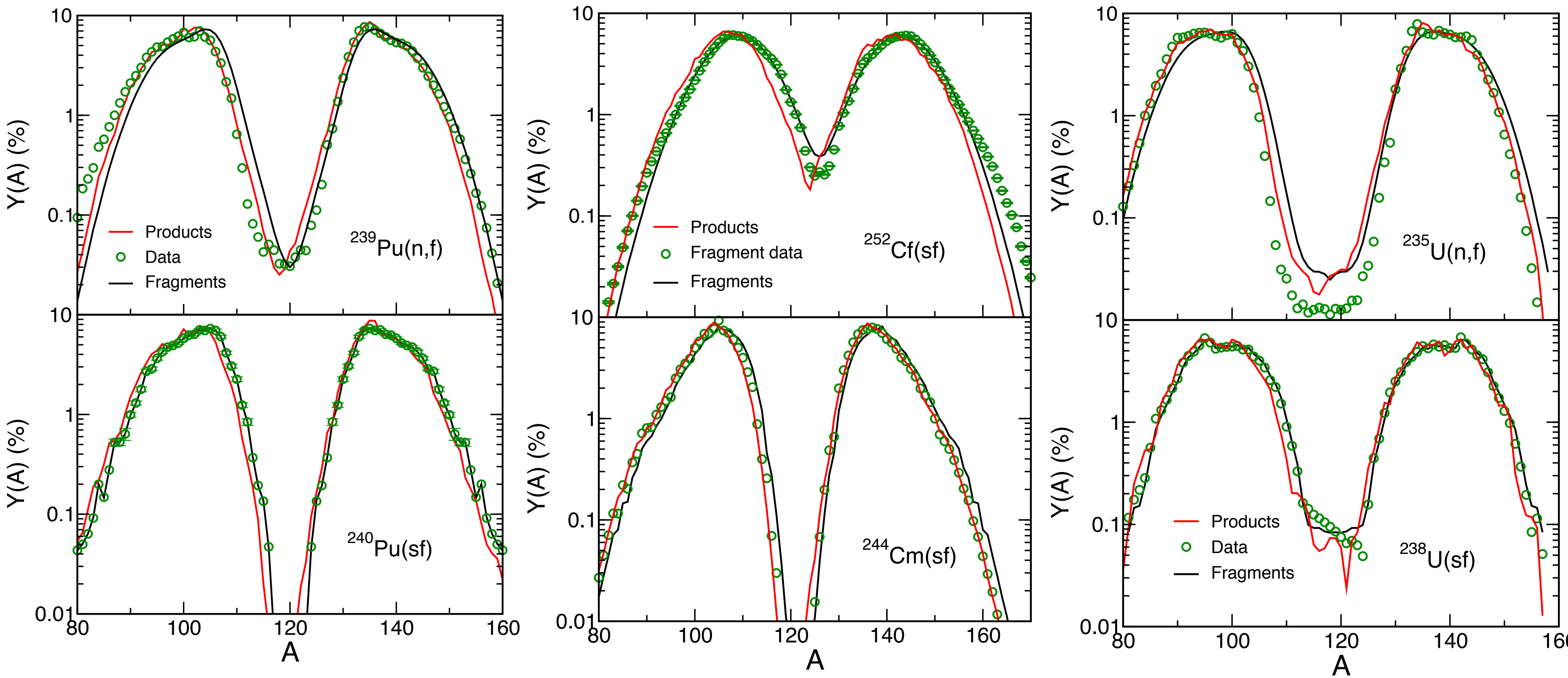
Level density parameter needed but assume it is independent of fissioning isotope

Sawtooth shape of ν(A) falls out from TKE shape and energy balance



Reported yields are either of fragments or products

Data are for fragment yields (spontaneous fission) and product yields (n,f), curves are from **FREYA** before and after neutron evaporation

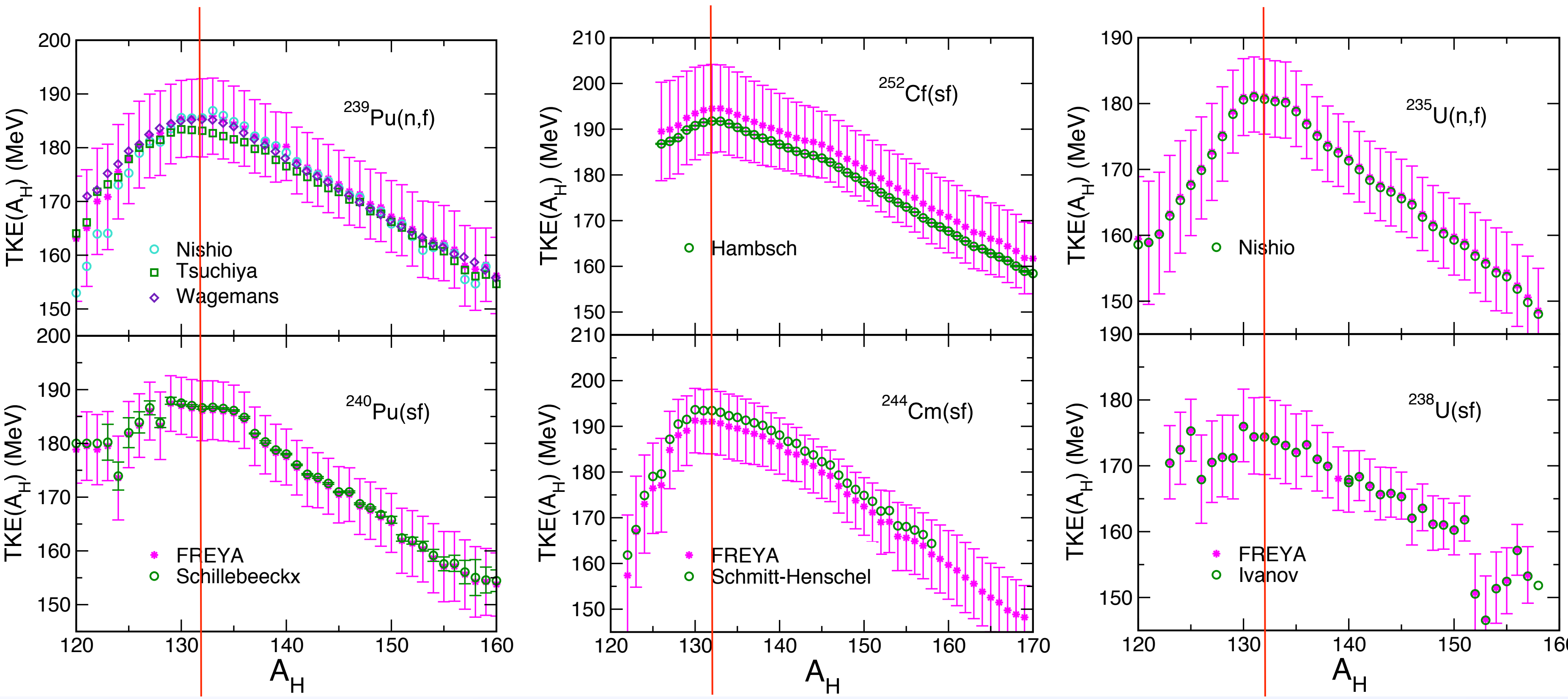


Shape of TKE(A_H) reflects shell structure of fragments

Peak of TKE(A_H) is near doubly-closed shell, $Z_H = 50$ and $N_H = 82$ (red line at $A_H = 132$)

dTKE (centroid of **FREYA** points, bars are variance in Z_H for given A_H) generally small

^{238}U(sf) and ^{240}Pu(sf) suffer from limited statistics (2800 events for ^{238}U)



Prompt neutron evaporation from excited fragments

Q value for neutron emission (maximum possible excitation of daughter nucleus)

$$Q_\mathrm{n} = M_i^\mathrm{gs} + E_i^* - M_f^\mathrm{gs} - m_\mathrm{n}$$

where M_f^gs is ground state mass of daughter nucleus

Assume kinetic energy of evaporated neutron, $\epsilon_\mathrm{n} = p_\mathrm{n}^2/2m_\mathrm{n}$, is isotropic in rest frame of emitting nucleus with $v_\mathrm{n} \propto \sqrt{\epsilon_\mathrm{n}}$ ($d^3\mathbf{p}_\mathrm{n} \propto \sqrt{\epsilon_\mathrm{n}} d\epsilon_\mathrm{n}$) so that

$$\begin{aligned} \frac{d^3\nu}{d^3\mathbf{p}_\mathrm{n}} d^3\mathbf{p}_\mathrm{n} &\propto \sqrt{\epsilon_\mathrm{n}}\, \mathrm{e}^{-\epsilon_\mathrm{n}/T_f^\mathrm{max}} \sqrt{\epsilon_\mathrm{n}} d\epsilon_\mathrm{n}\, d\Omega \\ &= \epsilon_\mathrm{n}\, \mathrm{e}^{-\epsilon_\mathrm{n}/T_f^\mathrm{max}} d\epsilon_\mathrm{n}\, d\Omega \ , \end{aligned}$$

Resulting excitation energy and mass of daughter nucleus

$$E_f^* = Q_\mathrm{n} - \epsilon_\mathrm{n} \quad M_f^* = M_f^\mathrm{gs} + E_f^*$$

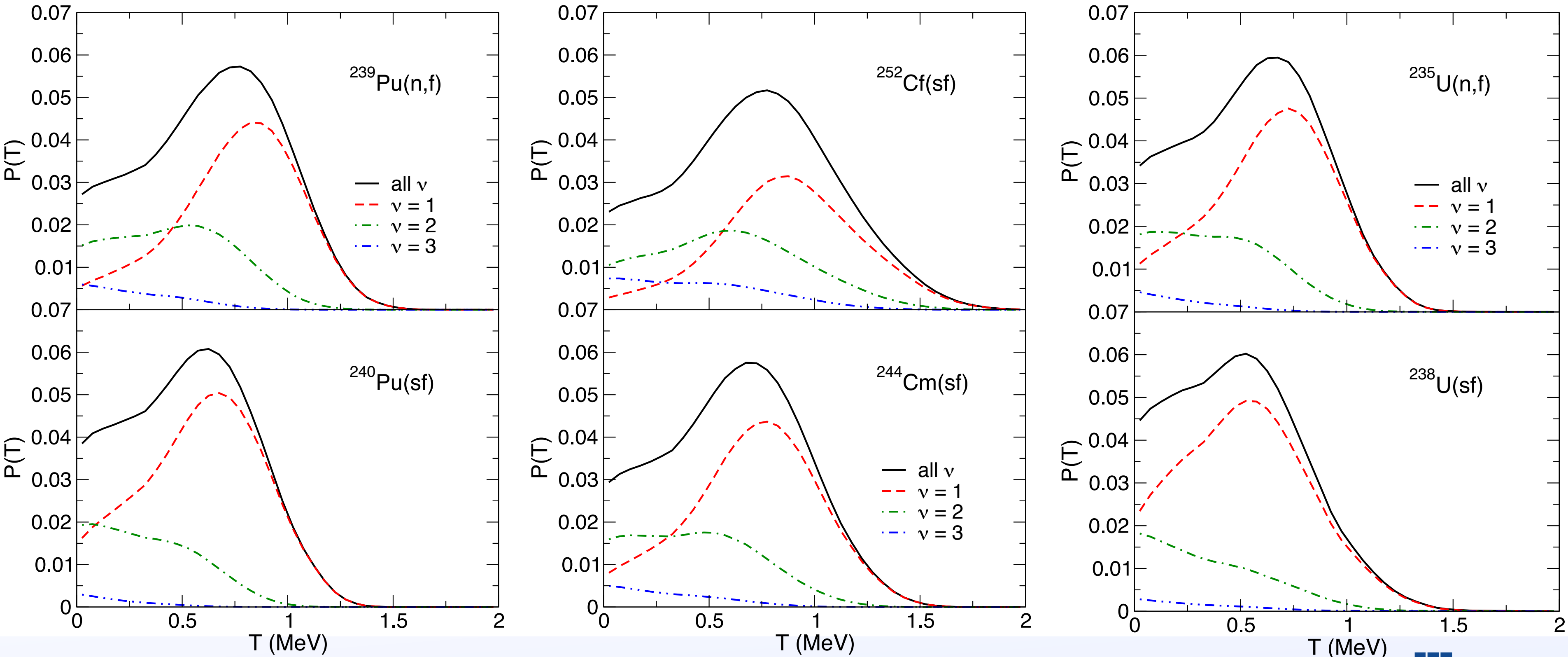
Emission continues until no further emsion energetically possible, $E_f^* < S_\mathrm{n}$ where S_n is neutron separation energy of daughter,

$$S_\mathrm{n} = M(^AZ) - M(^{A-1}Z) - m_\mathrm{n}$$

Residual temperature of daughters after neutron emission

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

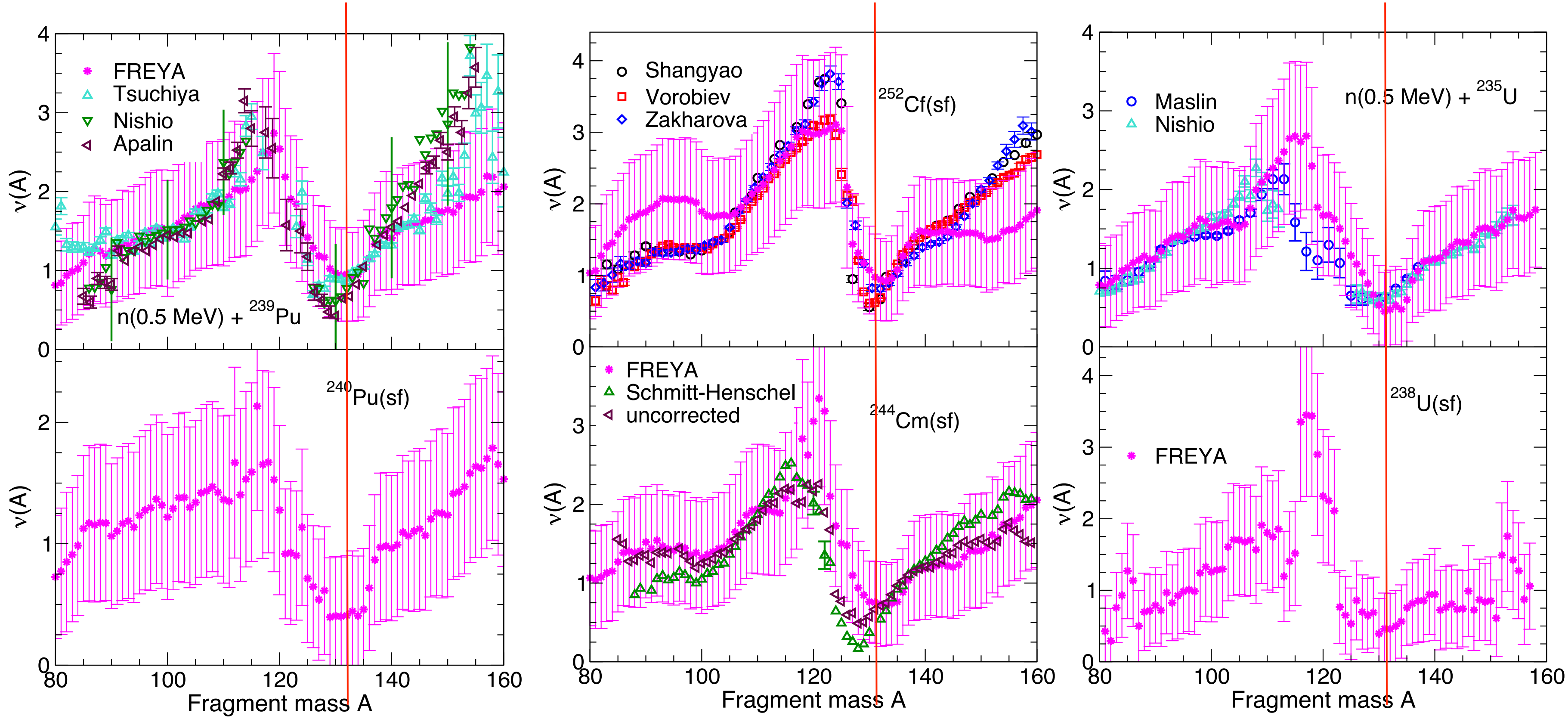
Shape is not triangular



Neutron multiplicity as a function of fragment mass

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

Note that not all isotopes have data to compare to FREYA, smoothness of sawtooth dependent on quality of Y(A) and TKE data – dip in $\nu(A)$ coincides with the peak of TKE(A_H), red line at A = 132

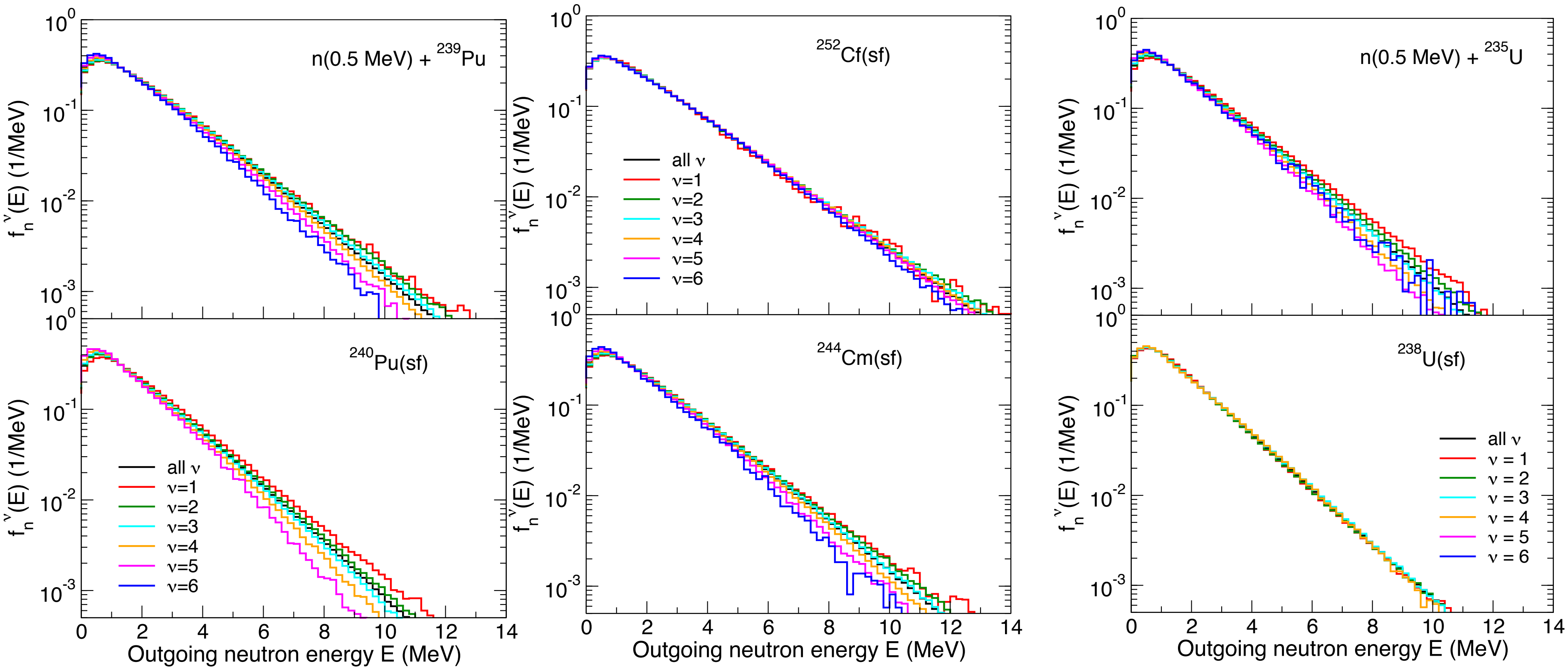


Neutron number-energy correlations

Spectral shapes shown, all normalized to unity for better comparison

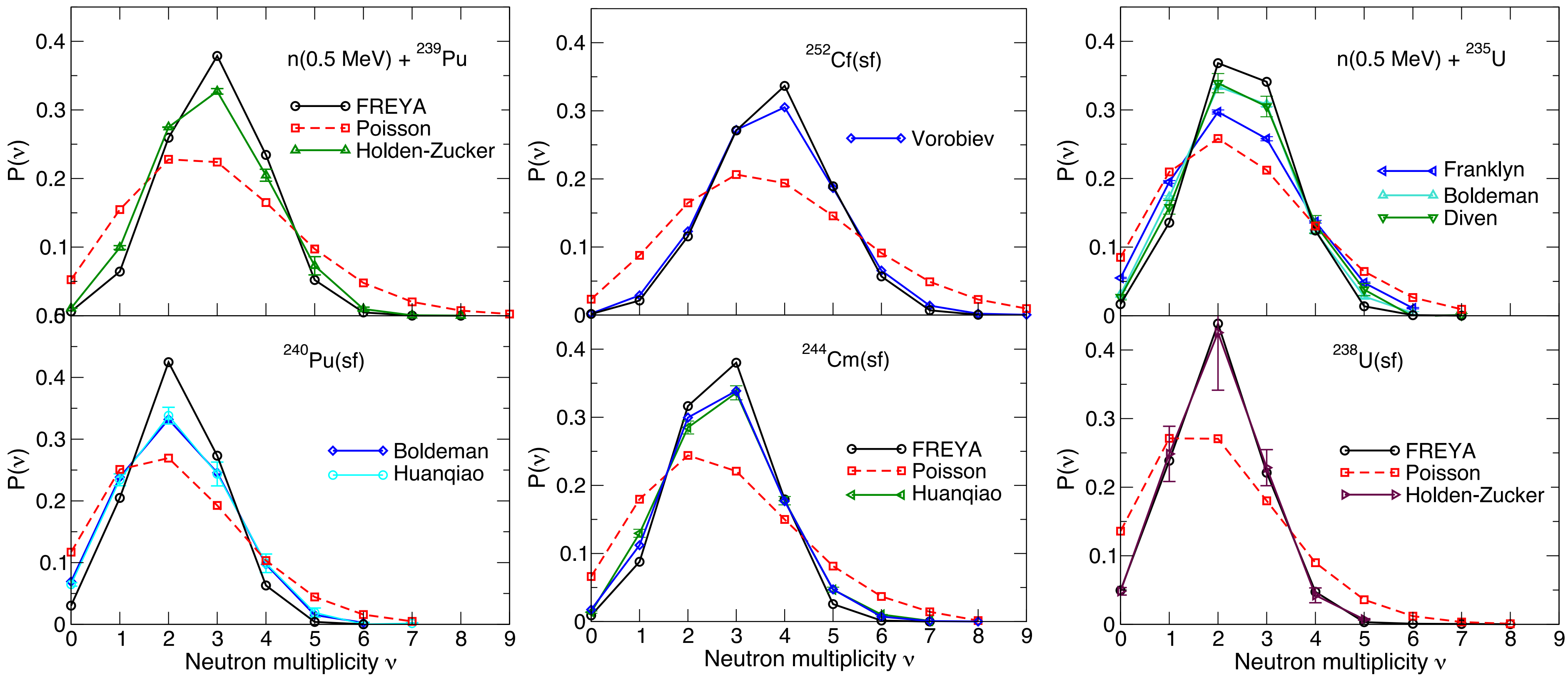
Most isotopes show considerable softening of the spectrum for increased neutron multiplicity

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



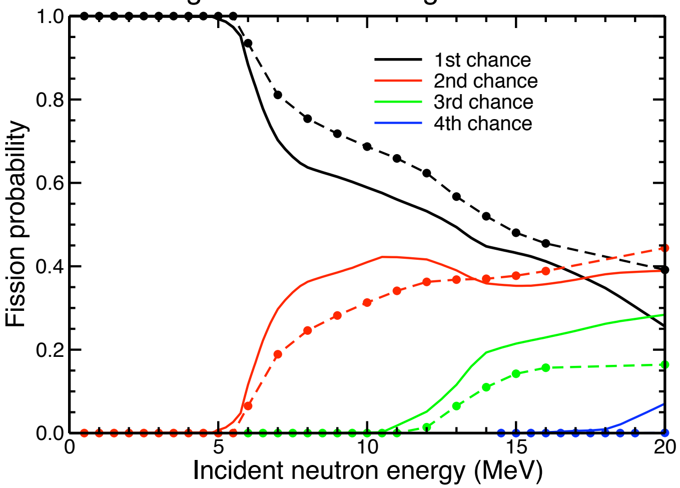
Probability for prompt neutron emission

Since each neutron emitted reduces excitation energy both by its kinetic energy (proportional to the temperature of the daughter nucleus) and the (larger) separation energy $S_{n,}$ the neutron multiplicity distribution is narrower than a Poisson

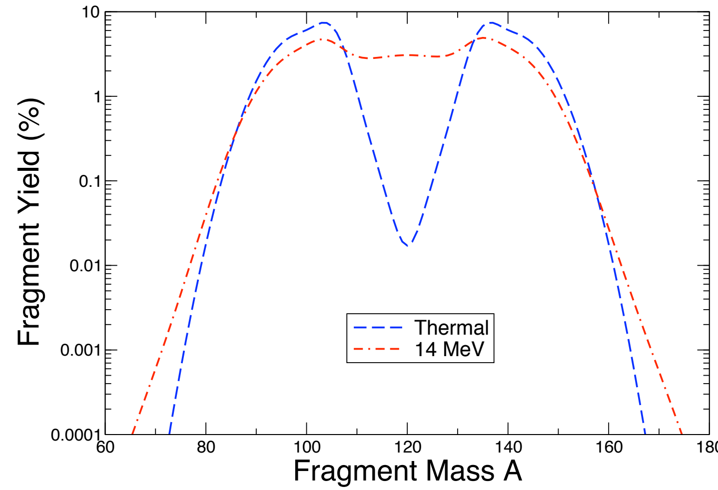


Spectral evaluations require additional inputs at high incident neutron energy

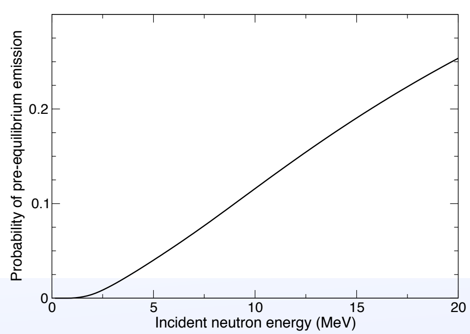
- **Multi-chance fission**, emission of one or more neutrons from excited compound nucleus pre-fission, turns on when incident neutron energy is above neutron separation energy for compound nucleus (^{240}Pu, 1[st] chance; ^{239}Pu, 2[nd] chance; ^{238}Pu, 3[rd] chance)
- Comparison to ENDF ^{239}Pu evaluation (**GNASH** calculation, not measured) with **FREYA** using same barrier heights but fitted level density parameter

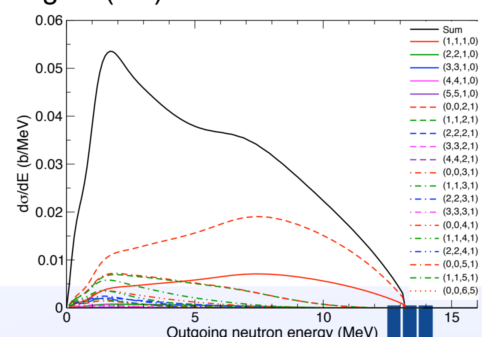


- **Transition from asymmetric to symmetric fission:** more symmetric with increasing incident neutron energy



- **Pre-equilibrium emission:** captured neutron fails to equilibrate and is re-emitted; biggest effect for smallest number of intermediate excited states (right) and high incident neutron energies (left)



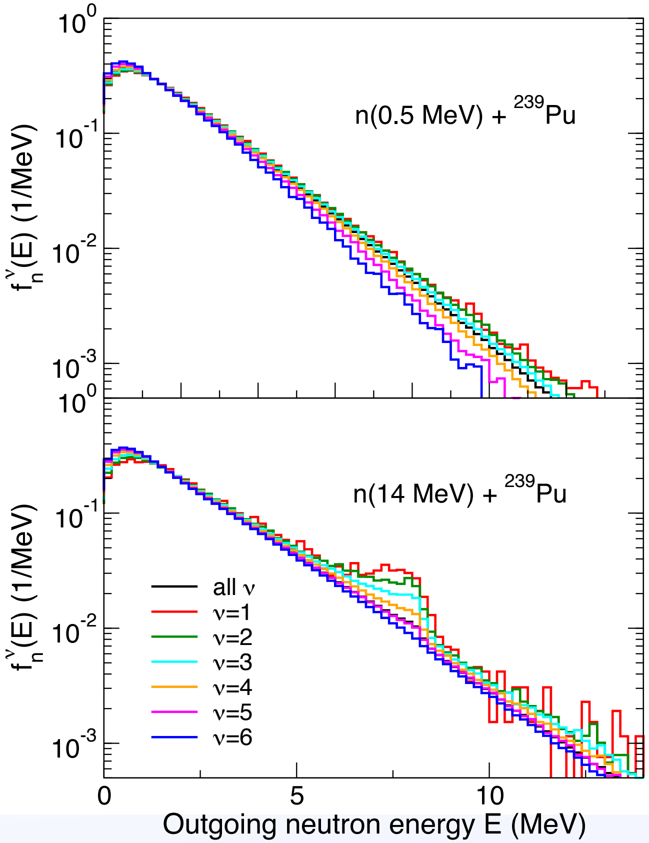


- **Missing ingredients to improve analysis at all incident neutron energies:**
  - **more comparison data e.g. Y(A,TKE)**
  - **more differential data like n(A_f)**
  - **better modeling of yields, kinetic energies with 'hot' fission (dynamics: Schunk, Younes)**

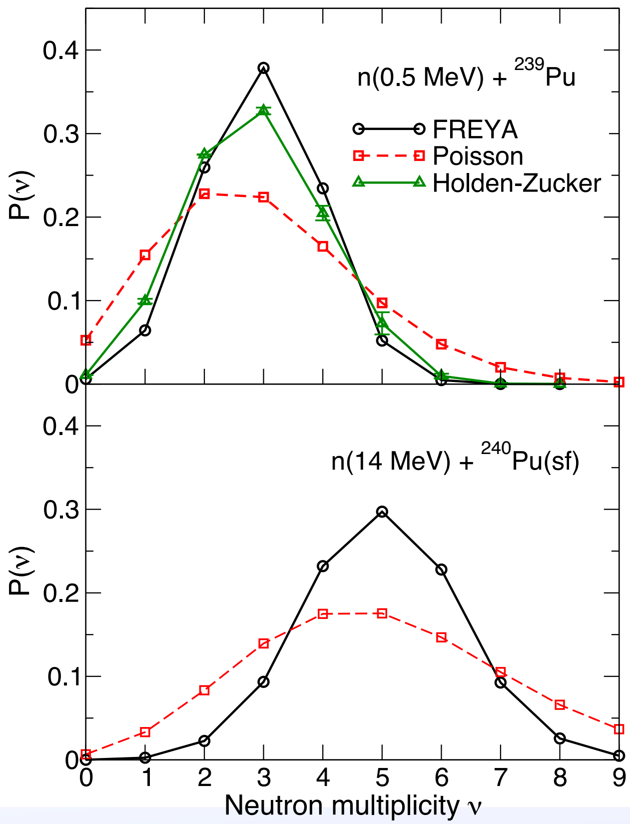
Energy dependent differences from average fission model (1)

FREYA accounts for softening of the PFNS after neutron evaporation

'kink' in spectrum due to pre-fission emission, small for all ν, enhanced for ν=1,2,3

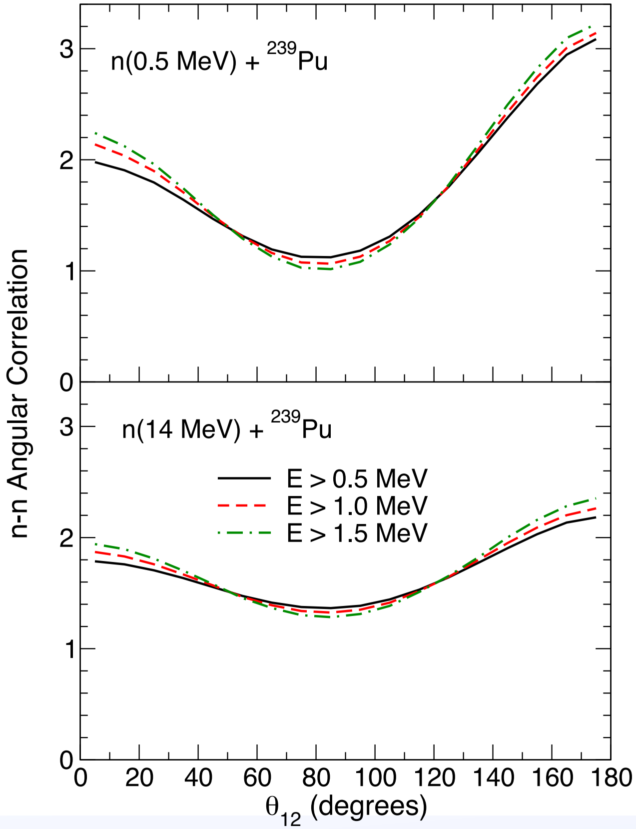


Since each neutron emitted reduces excitation energy both by its kinetic energy (proportional to the temperature of the daughter nucleus) and the (larger) separation energy S_n, the neutron multiplicity distribution is narrower than a Poisson



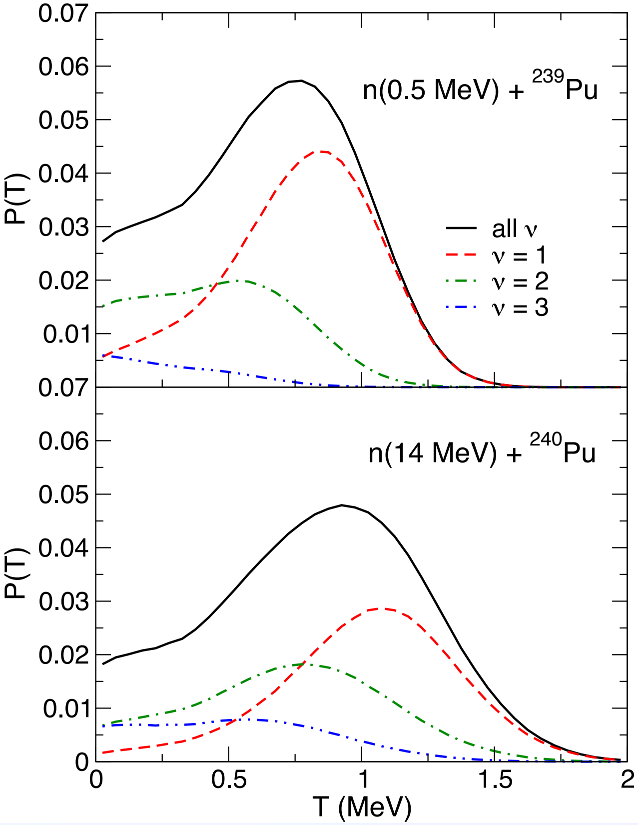
Energy dependent differences from average fission model (2)

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



Probability of maximum temperature of fragment daughter nucleus after emission of one or more neutrons – higher energy, more neutron emission, is visibly hotter

Shape is not triangular



Choosing FREYA input parameters

We tune three parameters to average neutron multiplicity, $\overline{\nu}$ at a given incident energy

- Shift of TKE(A_H), dTKE, from average over measured TKE values at thermal energies. The shape is assumed to be independent of energy, shell effects do not kick in to change this until incident energies well above 20 MeV.

- The level density parameter, a, sets fragment temperature for neutron evaporation. The asymptotic form, $a = A/e_0$, was used by Madland & Nix, more correct should be back-shifted Fermi gas approach

$$a_i(E_i^*) = \frac{A_i}{e_0}\left[1 + \frac{\delta W_i}{U_i}[1 - e^{-\gamma U_i}]\right]$$

  where $U_i = E_i^* - \Delta_i$, Δ_i is the fragment pairing energy, δW_i is the shell correction, and $\gamma = 0.05$. If shell corrections are negligible, $\delta W \approx 0$ and $a_i \sim A_i/e_0$. We take e_0 as a second parameter.

- Relative excitation of light and heavy fragments. Observations suggest that light fragments are more excited, leading to higher multiplicities than from statistical (even) partition of the excitation energies. We take

$$\begin{aligned} \overline{E}_L^* &= x E_L^* \\ \overline{E}_H^* &= \overline{\mathrm{TEE}} - \overline{E}_L^* \end{aligned}$$

Evaluation method

Use Monte Carlo approach to Bayesian inference (a la inverse problem theory) to obtain fit parameters

- We assume e_0 and x are independent of incident neutron energy
- We vary dTKE linearly between fixed points at incident energies of 10^{-11}, 0.25, 1, 5, 14 and 20 MeV; points chosen to map contours of $\overline{\nu}(E)$ and reasonably cover multichance fission thresholds
- Fit only to $\overline{\nu}$ at each energy (10^{-11}, 0.25, 0.5, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 20) MeV
- For each energy, we generate a set of model parameters, $d\text{TKE}, e_0, x$ uniformly distributed in parameter space
- For each parameter set, we generate 1M FREYA events at each energy and compare the calculated $\overline{\nu}$ – with energy-energy covariance – to the evaluation
- Best estimate is obtained from likelihood-weighted average of all parameter sets at all energies; best fit is that with largest likelihood
- Make evaluation using best fit; test; repeat if necessary

Summary

- Event-by-event models show significant correlations between neutrons that are dependent on the fissioning nucleus
- Such correlations may be exploited in fast neutron detection systems
- Version of **FREYA** is being added inline to Monte Carlo tools used by experimentalists
- Useful interplay between models and data but better, more up-to-date measurements, such as from fission TPC and ChiNu would be valuable