FREYA Update

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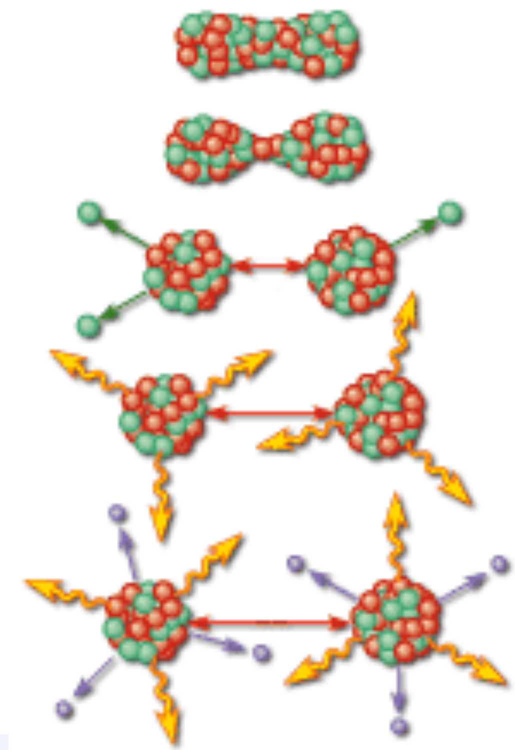
Outline

- A flexible modeling tool is needed for fast simulation of fission events for applications
- Our code **FREYA** has been developed to address this need
- We have studied a small number of fissioning systems so far
  - Spontaneous fission of ^{252}Cf, ^{244}Cm, ^{240}Pu, and ^{238}U
  - Neutron induced fission of ^{239}Pu and ^{235}U for $E_n \leq 20$ MeV
- Neutron observables and correlations have been studied in detail for all isotopes
- Photon observables are studied for ^{252}Cf(sf) and ^{235}U(n,f) up to now
- In this talk we
  - Introduce **FREYA**
  - Present neutron results for ^{239}Pu(n,f) and ^{252}Cf(sf), compare to data
  - Present photon results for ^{235}U(n,f) and ^{252}Cf(sf)
  - Discuss future work

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

- **FREYA** developed in collaboration with J. Randrup (LBNL)
- Phys. Rev. C **80** (2009) 024601, 044611; **84** (2011) 044621; **85** (2012) 024608; **87** (2013) 044602
- Collaborators: D. A. Brown (BNL), M. A. Descalle (LLNL), W. E. Ormand (LLNL), J. Pruet (NNSA) and W. Younes (LLNL)



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

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

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

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

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]

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

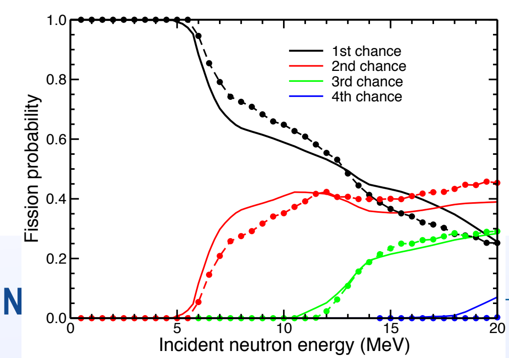
^{252}Cf ^{240}Pu

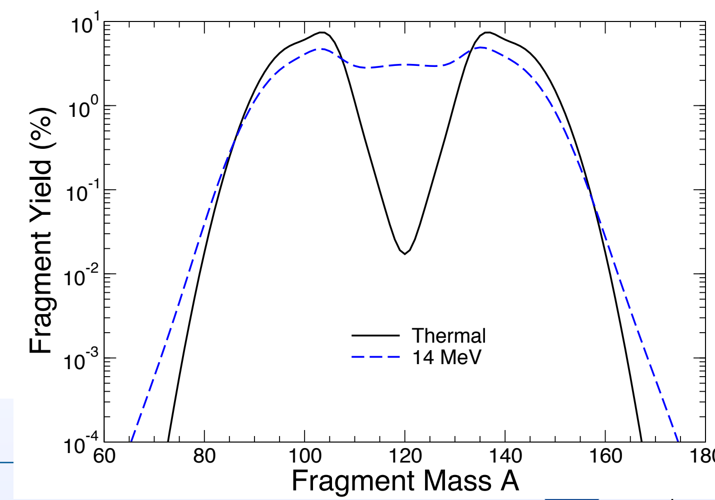
E_n = 14 MeV:

1st: 44%

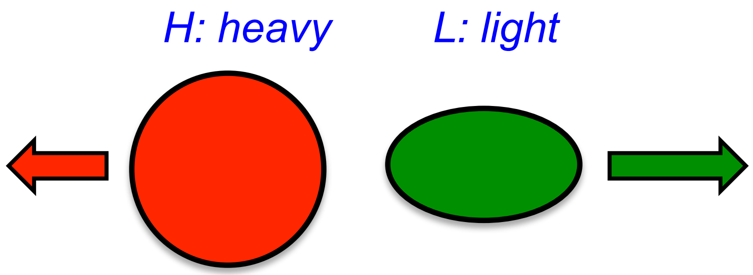
2nd: 35%

3rd: 21%





Fission fragment kinetic energies

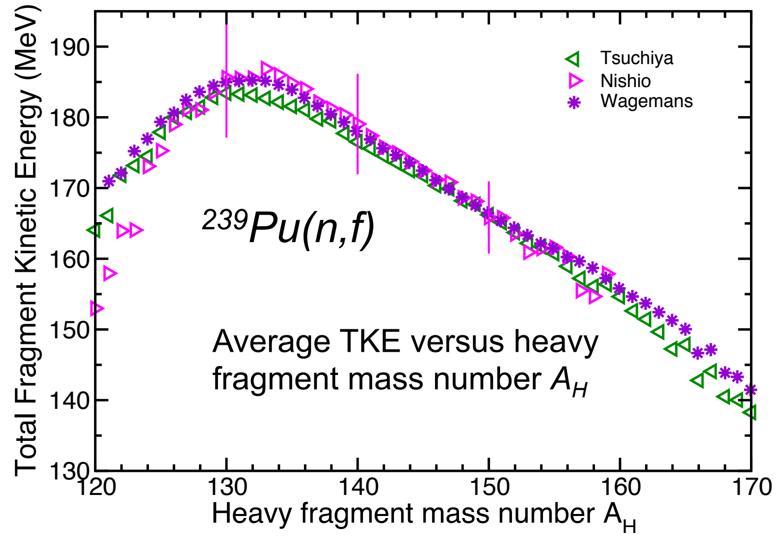


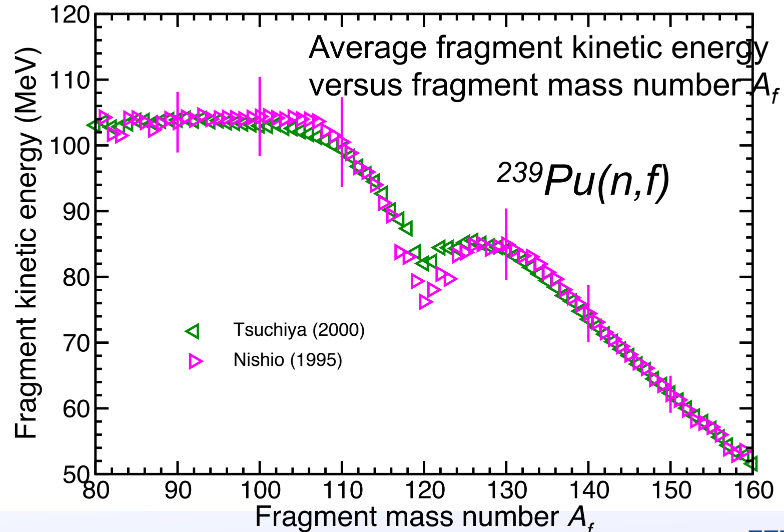
No models for $TKE(A_f)$ exists yet, so …

we adjust TKE to exp data:

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

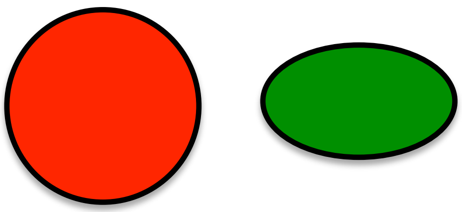
with an adjustable shift
to reproduce the mean
neutron multiplicity $<\nu>(E_n)$





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

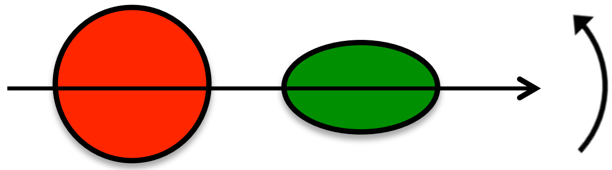
Fragment momenta then follow from energy & momentum conservation:

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

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

Angular momentum at scission: Rigid rotation plus fluctuations

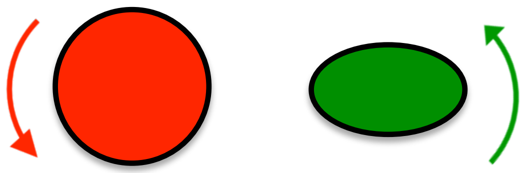
Rigid rotation:



$\boldsymbol{S}_f = (\mathcal{I}_f/\mathcal{I}_{\rm tot})\boldsymbol{S}_0 + \delta\boldsymbol{S}_f$

The dinuclear rotational modes have thermal fluctuations that are governed by an adjustable "spin temperature" T_S:

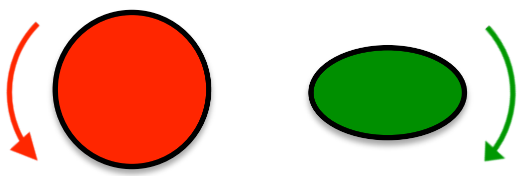
Wriggling:
(2 modes)



$\mathcal{I}_{\rm wrig} = (\mathcal{I}_{\rm H}+\mathcal{I}_{\rm L})\ \mathcal{I}_{\rm tot}/\mathcal{I}_{\rm rel}$

Sample $\boldsymbol{S}_{wrig}$ *from* $P(\boldsymbol{S}_{wrig}) \sim \exp(-S_{wrig}^2/2\mathcal{I}_{wrig}T_S)$

Bending:
(2 modes)



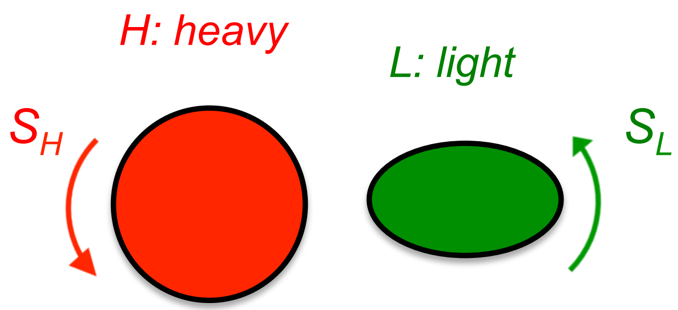
$\mathcal{I}_{\rm bend} = \mathcal{I}_{\rm H}\mathcal{I}_{\rm L}/(\mathcal{I}_{\rm H}+\mathcal{I}_{\rm L})$

Sample $\boldsymbol{S}_{bend}$ *from* $P(\boldsymbol{S}_{bend}) \sim \exp(-S_{bend}^2/2\mathcal{I}_{bend}T_S)$

Fragment spins

$$\boldsymbol{S}_\mathrm{H} = (\mathcal{I}_\mathrm{H}/\mathcal{I}_\mathrm{tot})\boldsymbol{S}_0 + (\mathcal{I}_\mathrm{H}/\mathcal{I}_\mathrm{wrig})\boldsymbol{S}_\mathrm{wrig} + \boldsymbol{S}_\mathrm{bend}$$

$$\boldsymbol{S}_\mathrm{L} = (\mathcal{I}_\mathrm{L}/\mathcal{I}_\mathrm{tot})\boldsymbol{S}_0 + (\mathcal{I}_\mathrm{L}/\mathcal{I}_\mathrm{wrig})\boldsymbol{S}_\mathrm{wrig} - \boldsymbol{S}_\mathrm{bend}$$



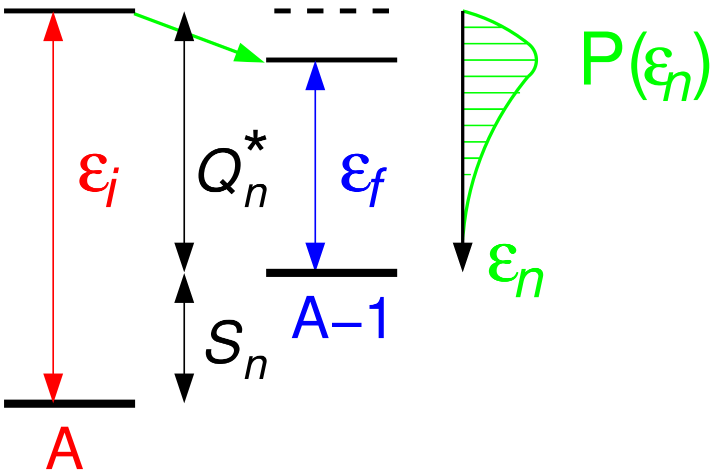
The rotational energy $E_{rot} = S_L^2/2\mathcal{I}_L + S_H^2/2\mathcal{I}_H$
is not available for internal excitation

The mean internal excitation is reduced correspondingly: $\underline{E}^* = Q_{LH} - \underline{TKE} - E_{rot} = \underline{E_L}^* + \underline{E_H}^*$

$\underline{E}^*$ *is shared between the two fragments*

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

Neutron evaporation from fragments



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

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

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

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

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

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

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

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

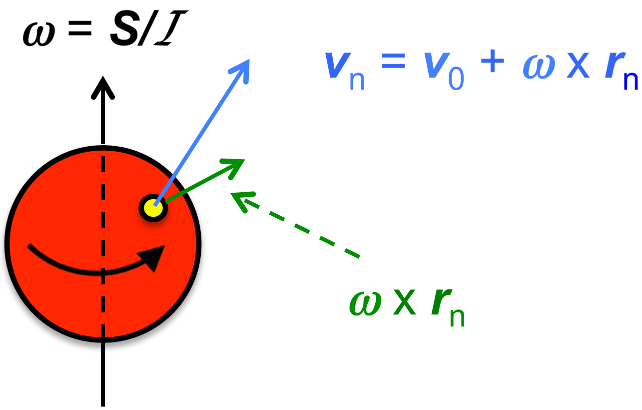
(non-relativistic)

Neutron energy spectrum:

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

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

Neutron evaporation from rotating fragments



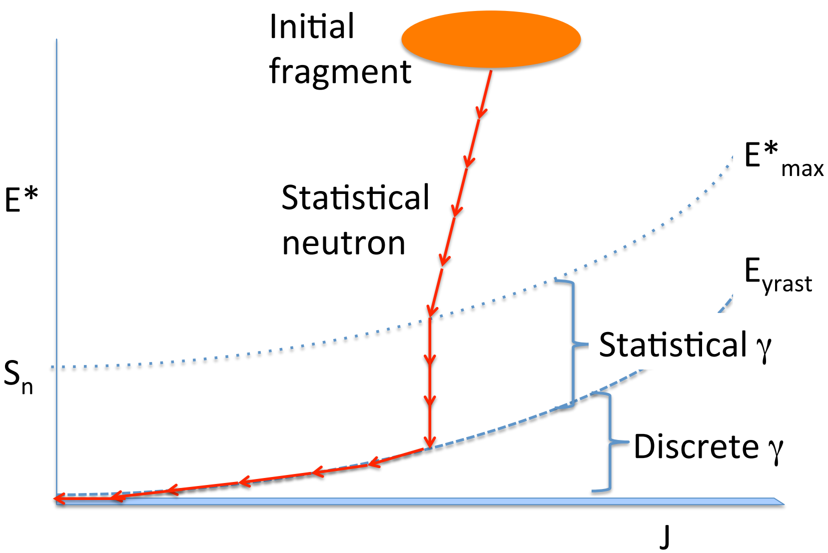
$$\boldsymbol{S}' = \boldsymbol{S} - \boldsymbol{r}_{\mathrm{n}} \times \boldsymbol{p}_{\mathrm{n}}$$

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

Conserves energy as well as linear & angular momentum.

Photon 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 …

$$\frac{d^3N_\gamma}{d^3\boldsymbol{p}_\gamma} d^3\boldsymbol{p}_\gamma \sim c\,\mathrm{e}^{-\epsilon/T_i}\epsilon^2\, d\epsilon\, d\Omega \quad \Leftarrow \quad d^3\boldsymbol{p}_\gamma \sim \epsilon^2 d\epsilon\, d\Omega$$

(ultra-relativistic)

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

… then by stretched E2 photons along the yrast line …

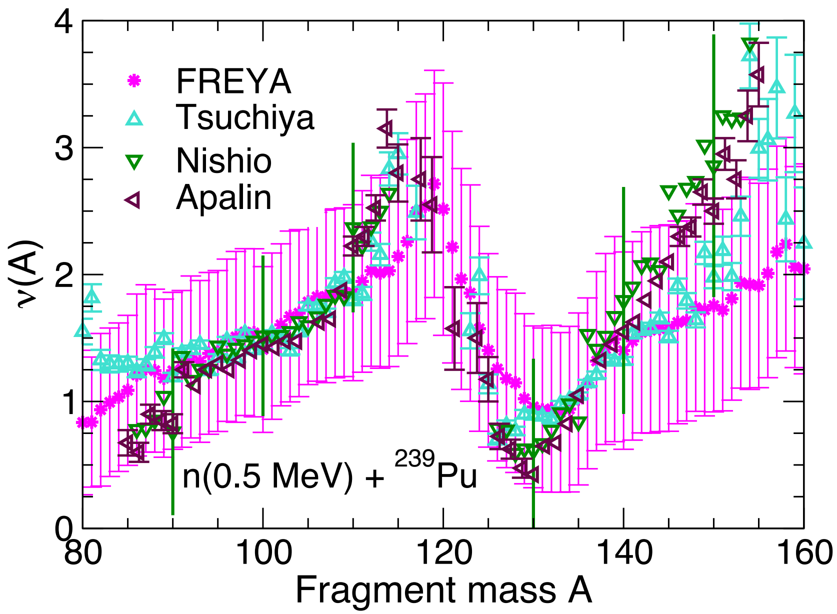
$$S_f = S_i - 2$$
$$\epsilon_\gamma = S_i^2/2\mathcal{I}_A - S_f^2/2\mathcal{I}_A$$
$$\mathcal{I}_A = 0.5 \times \tfrac{2}{5} A m_N R_A^2$$

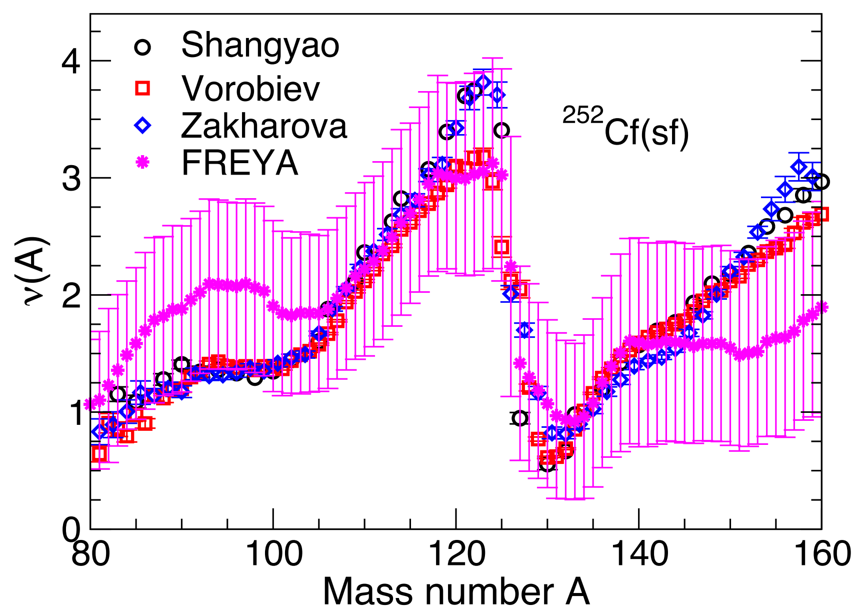
Each photon is Lorentz boosted from the emitter to the laboratory frame

Neutron observables: sawtooth ν(A)

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

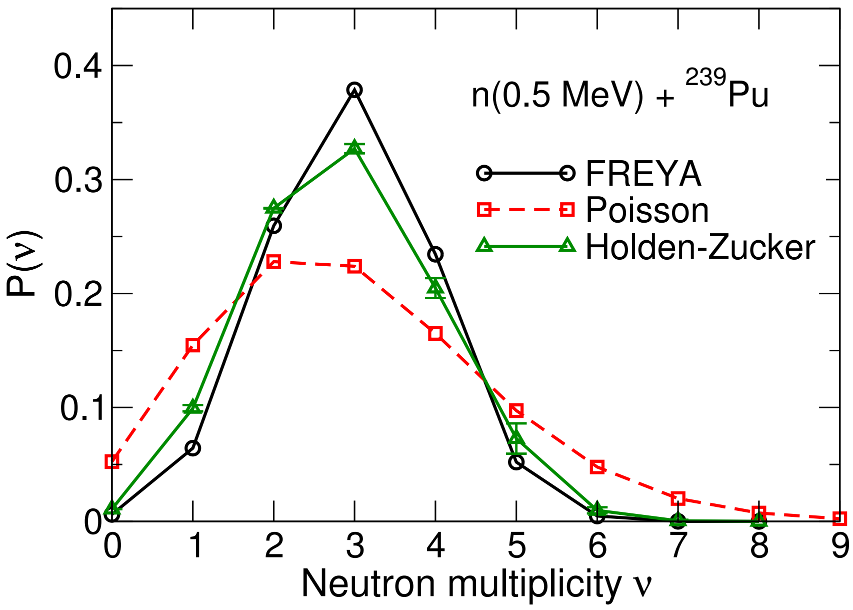
ν(A) calculation shows dispersion in Z for a given mass (**FREYA** ‘error bars’)

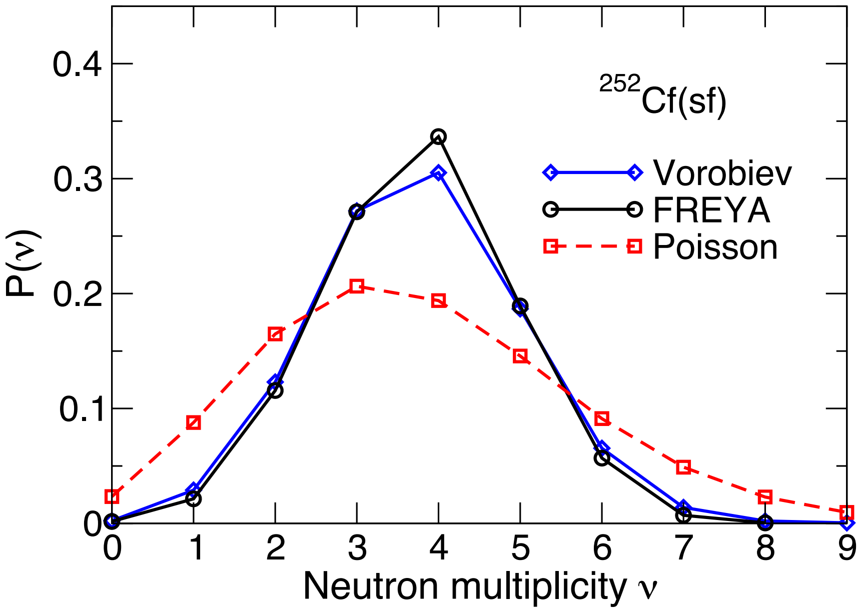




Neutron observables: multiplicity distribution P(ν)

Neutron multiplicity distribution, different from Poisson due to removal of neutron separation energy, S_n, as well as neutron kinetic energy, ε_n

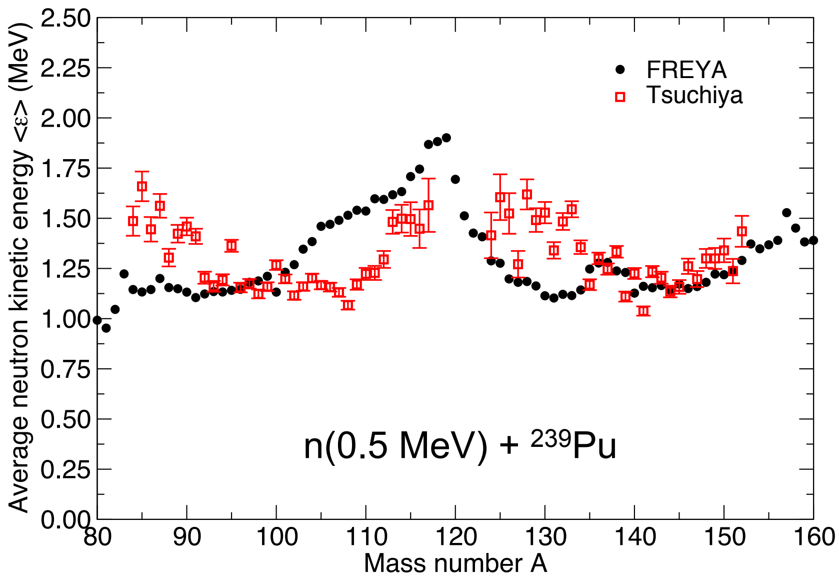


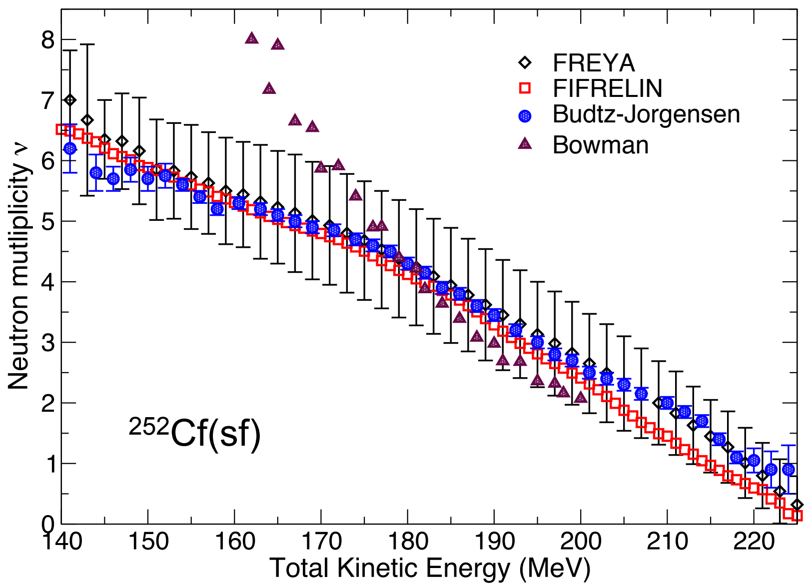


Other neutron observables

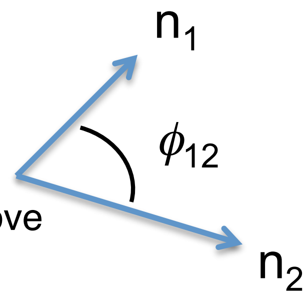
Average neutron kinetic energy as a function of fragment mass, dispersion not shown

Neutron multiplicity as a function of TKE in **FREYA** follows Budtz-Jorgensen data, Averaged over yields as a function of A and TKE very well; Bowman data, for fragment pairs only, has a different slope





Two-neutron angular correlations reflect emitter source

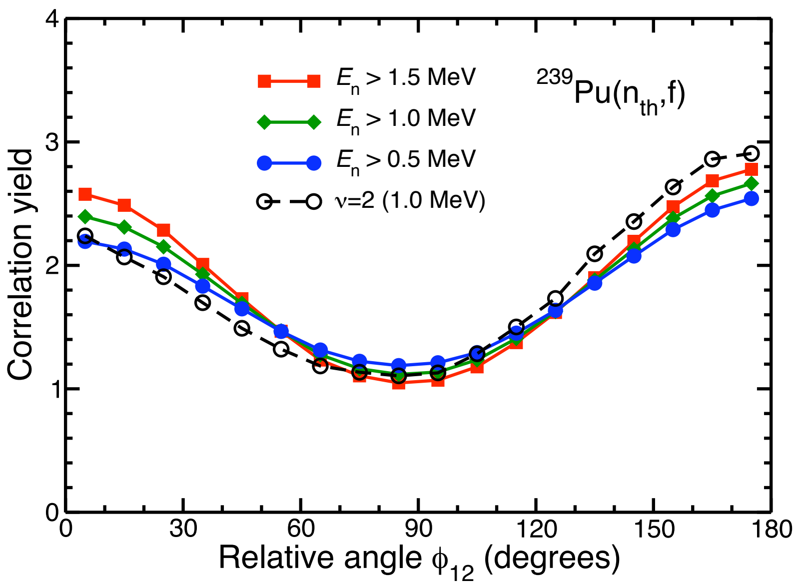


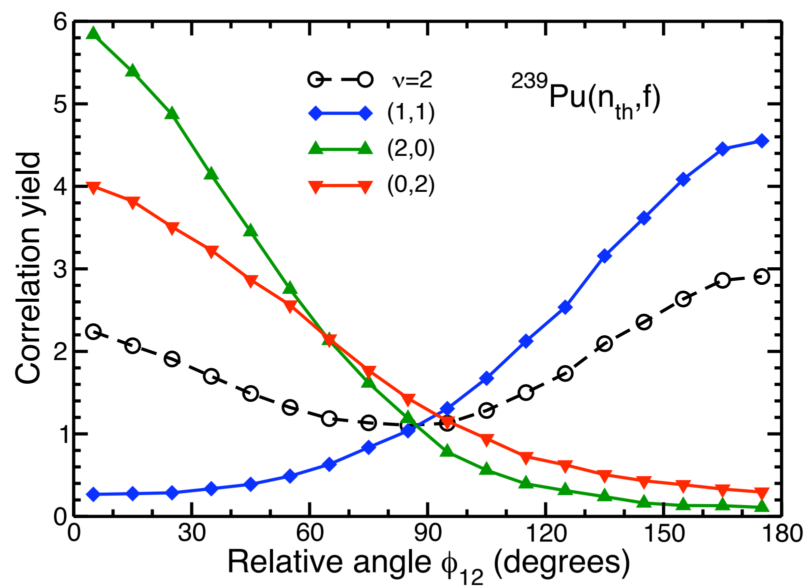
Correlations of neutrons with energies above a specified threshold energy

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

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

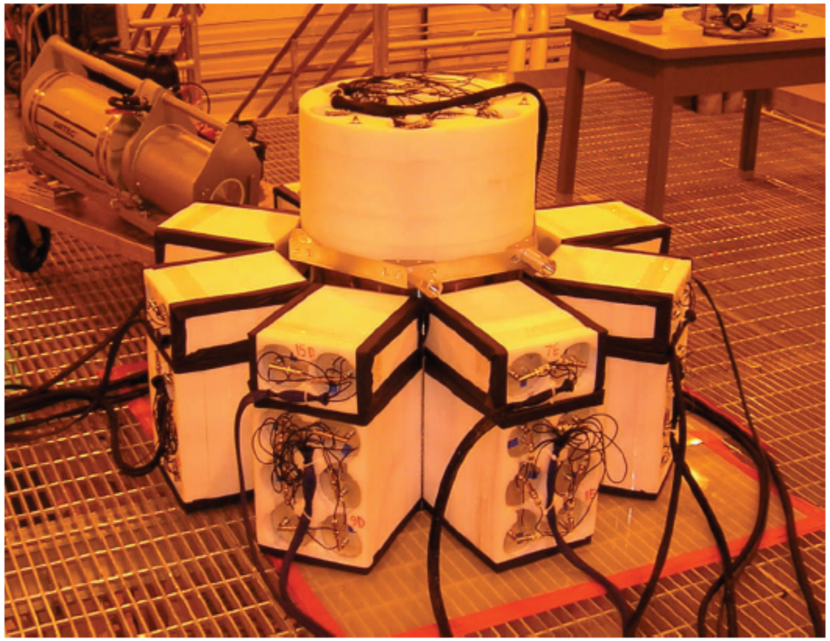
One from each fragment (blue) back to back; both from single fragment emitted in same direction, tighter correlation when both from light fragment (green) than from heavy (red); open circles show sum of all possibilities



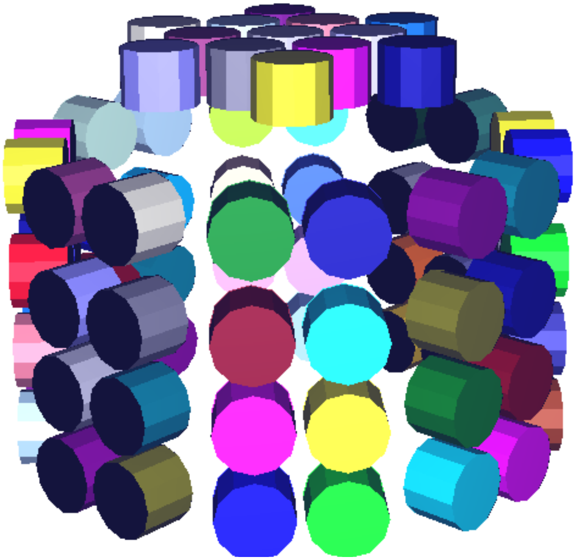


Angular Correlations Testable in a Real Detector: 77 Cell Detector (Birthday Cake) Array

- Liquid Scintillator
  - Xylene cells: 3” long, 4” diameter
  - neutron-gamma differentiation via pulse shape discrimination



Detector (left) simulated as cells (right) in **MCNP** code



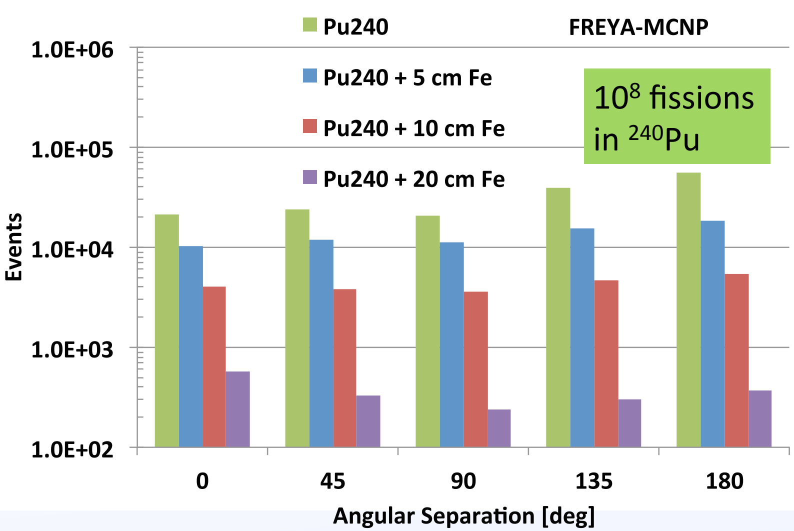
8-cell octants + 13 cells on top

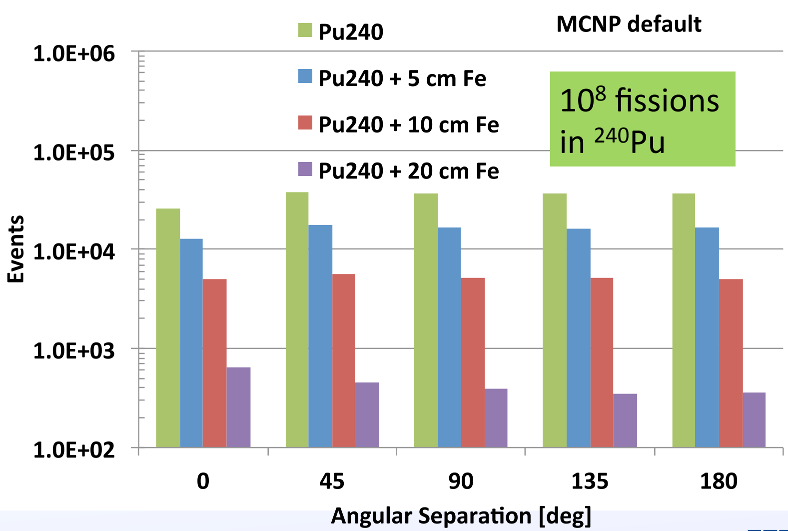
Angular Correlations in the Birthday Cake Array

- Simulated detector setup
  - 64 scintillators (top not included)
  - Tally coincidences between octants
  - Each cell only hit once
  - Source placed in center of array
  - Angular correlations studied for 2 neutrons hitting same octant (*e.g*. 1-1, 0°) through 2 neutrons in opposite octants (*e.g*. 1-5, 180°)
  - Studied differences between general purpose simulation code **MCNP** with and without **FREYA** included

Simulation Results: Angular Correlations (C. Hagmann)

- **MCNP5 + FREYA**
  - –Distinct angular correlations predicted, strongest at 180° relative neutron separation
  - –Modest Fe shielding (5 cm – 20 cm) reduces efficiency but correlations still visible
- **MCNP5** default
  - –No correlations at large angles
  - –Small effect at 0° due to requirement that each cell fire only once per fission event
  - –Amount of shielding does not affect the conclusions

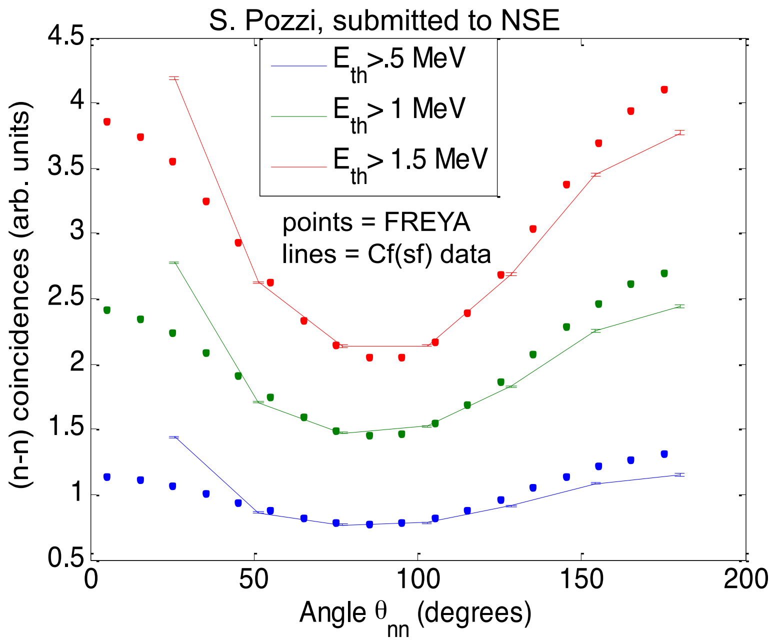


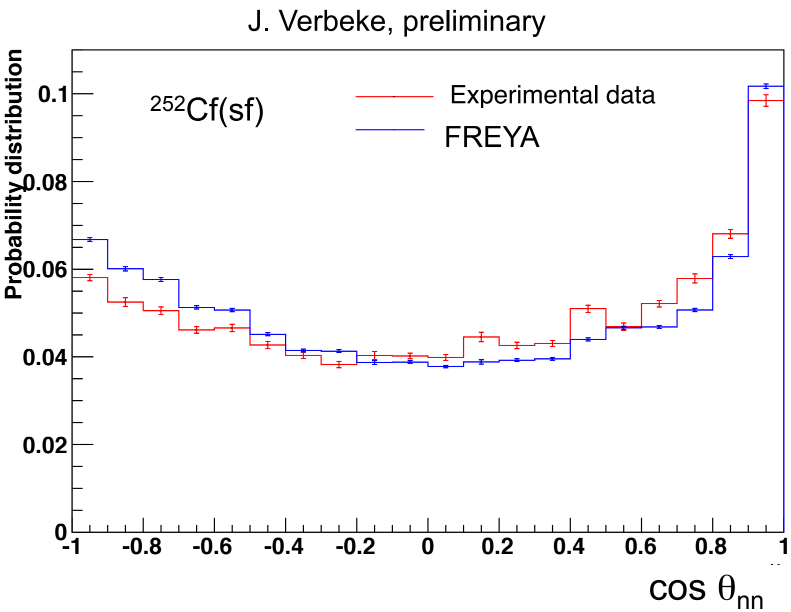


Comparison of FREYA to ^{252}Cf(sf) n-n Correlation Data

FREYA favorably compared to neutron-neutron angular correlation data on 252Cf(sf)

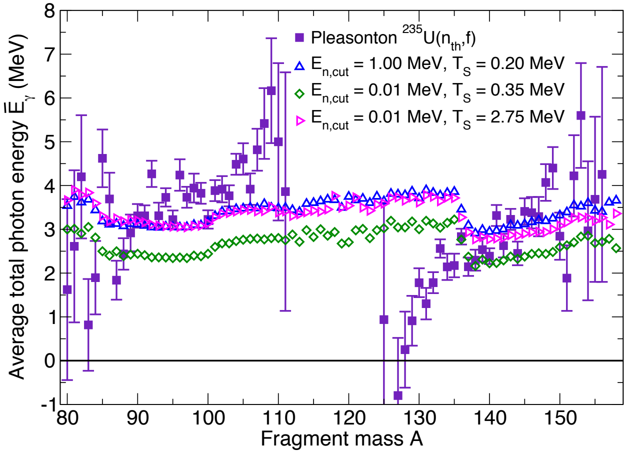
The difference between the **FREYA** calculation and Pozzi's data is due to detector cross talk in the data, not included in the calculation

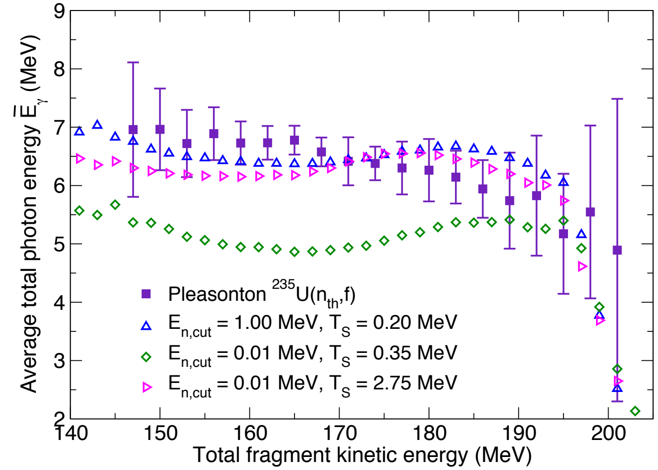




Photon Results: ^{235}U(n,f), Pleasonton et al.

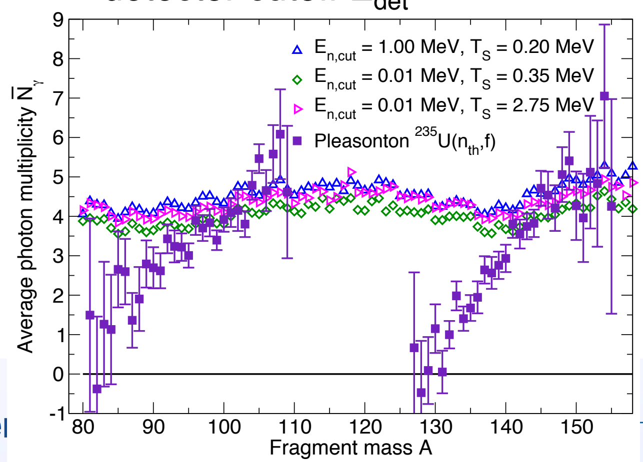
Data suggest relatively high fragment angular momentum, 6-10ħ, from earlier studies

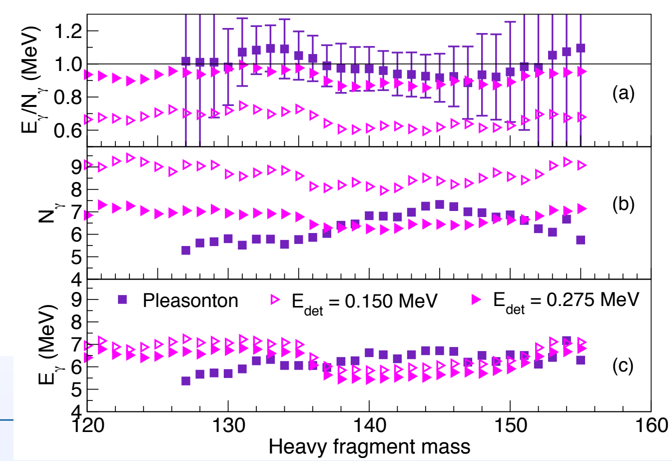




N_γ not sensitive to T_S (angular momentum), sensitive to detector cutoff E_{det}

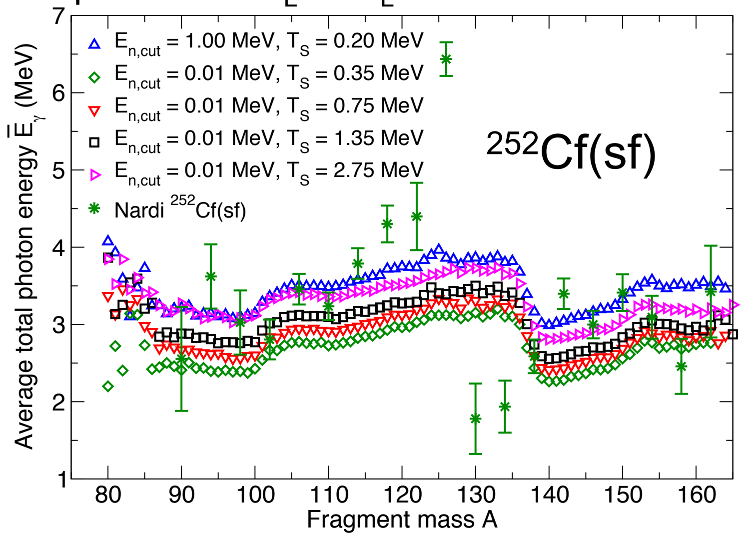
Changing E_{det} has small effect on E_γ but larger on N_γ, higher E_{det} agrees with measured E_γ/N_γ

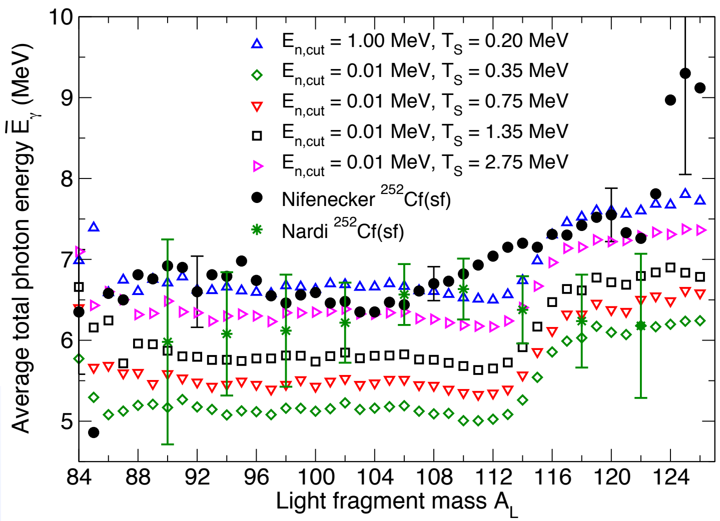




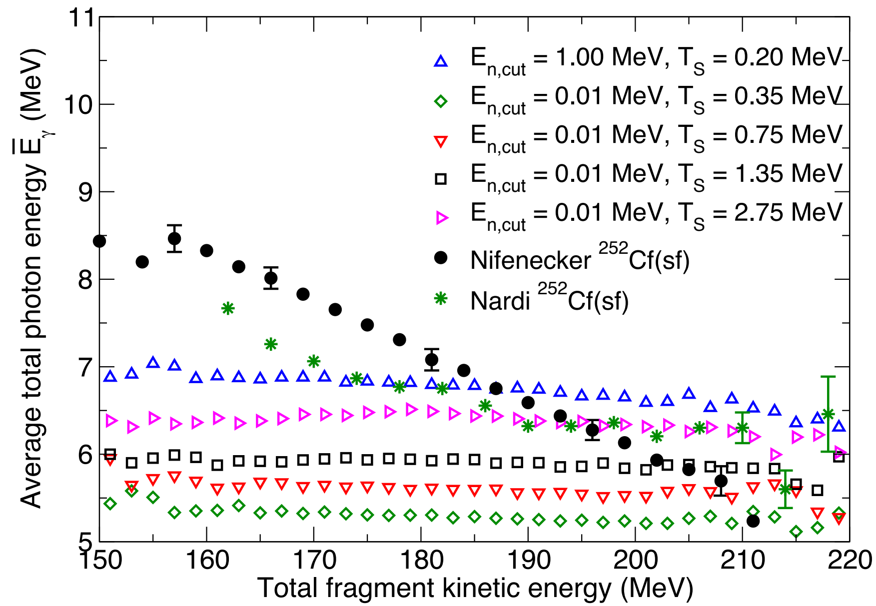
Photon Results: ^{252}Cf(sf), Nardi et al. and Niefenecker et al.

$E_\gamma(A)$ shows a change in slope similar to Nardi data but at higher A, but not as large a change, independent of A_L for A_L<112





Calculated E_γ dependence on TKE is almost flat for Cf, very different from behavior of ν(TKE)
Nifenecker data decrease linearly,
Nardi data decrease and flatten

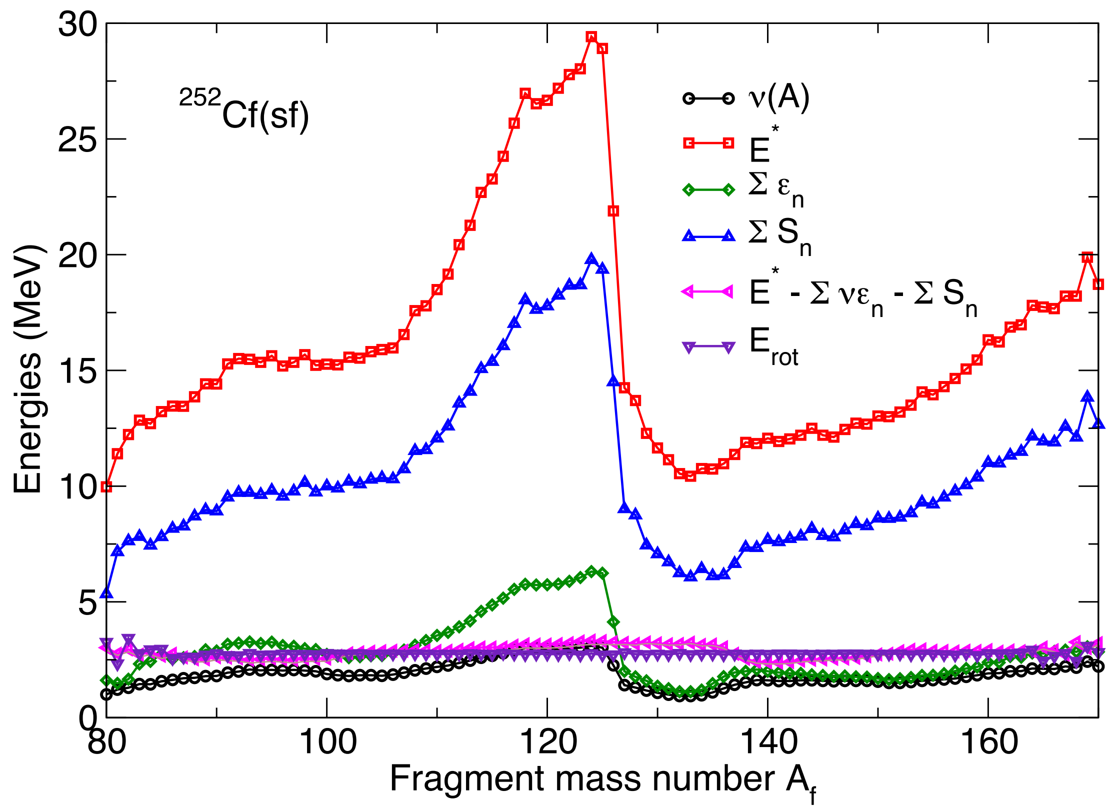


Where does the fragment excitation energy go?

FREYA now does statistical neutron emission, then photon emission – first statistical and then yrast photons

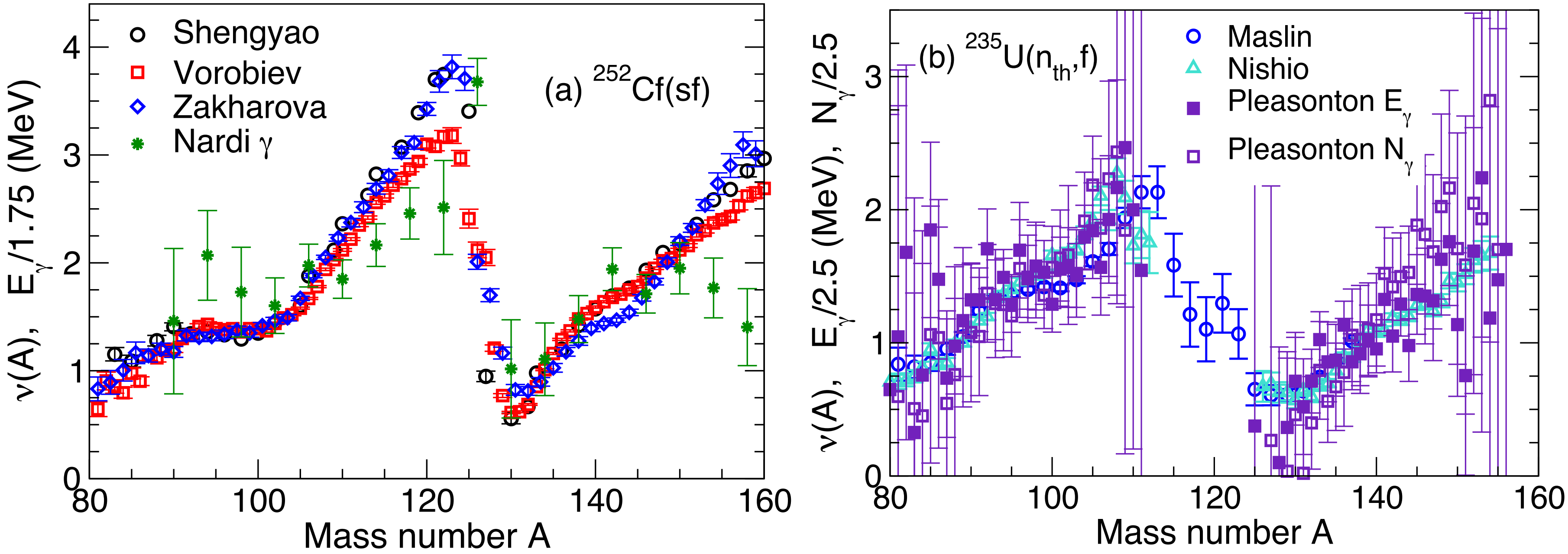
Initial excitation energy (red) goes into separation energy S_n (summed, blue) and neutron kinetic energy en (summed, green, multiplied by ν(A), black) for each neutron – what's left (magenta) can go to photon emission

The rotational energy (purple) goes to the emission of yrast photons



Trends in neutron and photon A dependence similar

Both 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 ν(A), within large uncertainties



Photon-neutron correlations not well understood

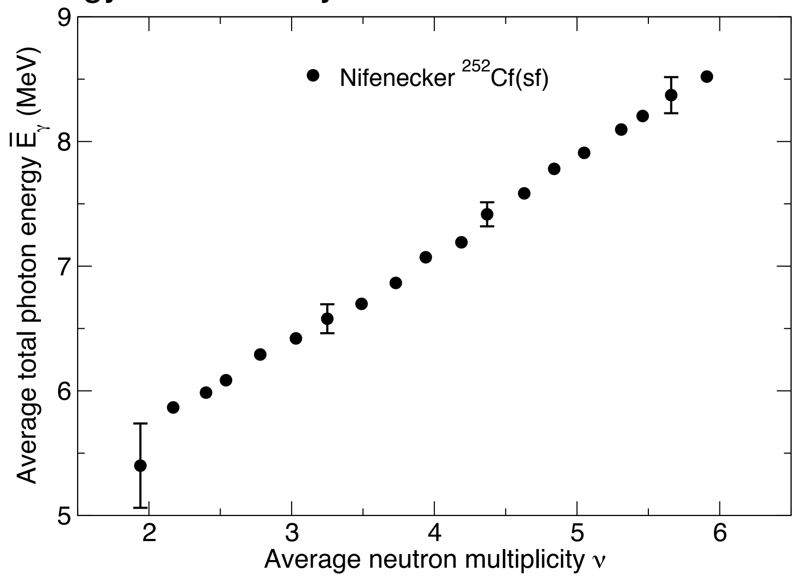
Nifenecker et al. proposed that the total average photon energy increased linearly with neutron multiplicity, not inconsistent with sawtooth-like behavior of photon emission vs. A but with relatively poor statistics

Frehaut observed an increase in both E_γ and $\nu(A)$ with E_n in ^{232}Th(n,f), ^{235}U(n,f) and ^{237}Np(n,f), consistent with increase of excitation energy with incident neutron energy

These observations were turned into an assumption that E_γ increases with ν in all circumstances, due to important competition between neutron and photon emission – a strong positive correlation, somewhat counterintuitive in event-by-event models

Some expanded versions of average fission models hardwire this in to match existing data

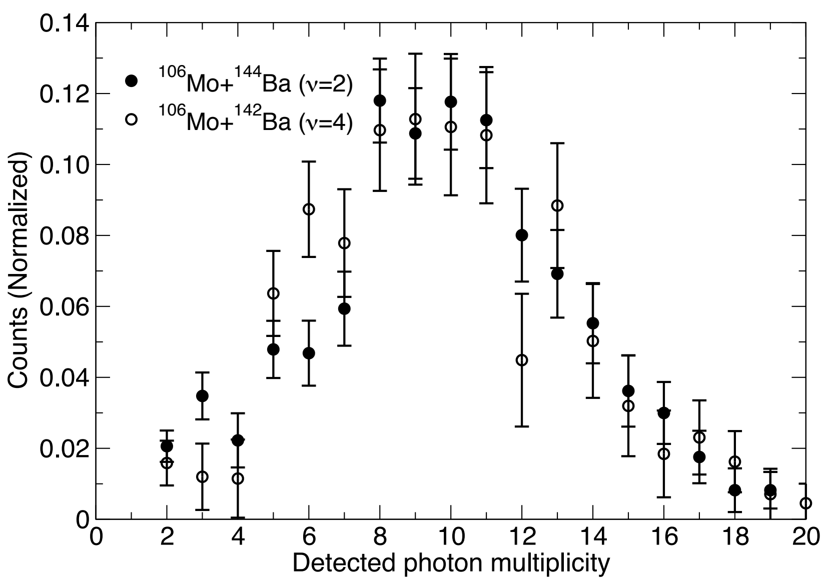
They expect that this (and sawtooth-like behavior of $E_\gamma(A)$ and $N_\gamma(A)$) comes from strong linear dependence of spin on fragment excitation energy – essentially to the exclusion of statistical photon emission



Measured neutron-photon multiplicity correlation

LiBerACE collaboration obtained photon multiplicity distribution for 2 and 4 neutrons emitted from two specific fragments, ^{106}Mo and ^{144}Ba/^{142}Ba, to look for correlations

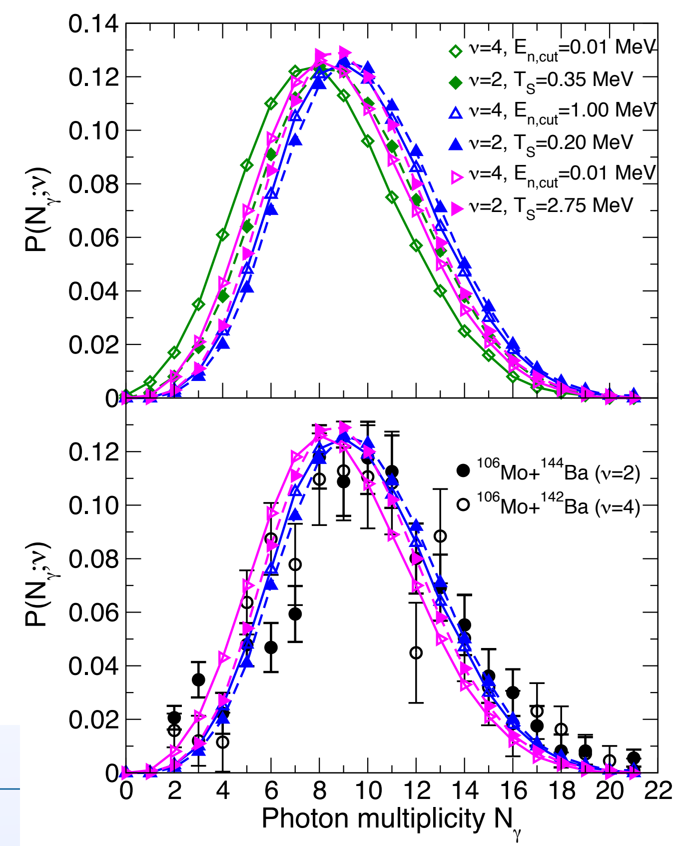
Their results, while exhibiting little correlation between neutron and photon emission, certainly do not show Nifenecker's positive correlation



Each emitted neutron shifts average $P(N_\gamma;\nu)$ to lower N_γ, shift more pronounced for lower T_S

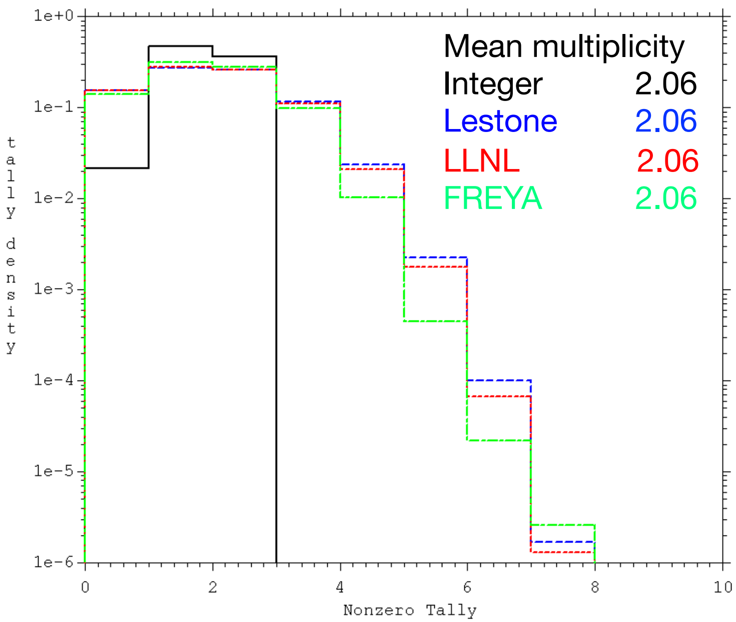
LiBerACE data favors higher T_S, smaller backward shift

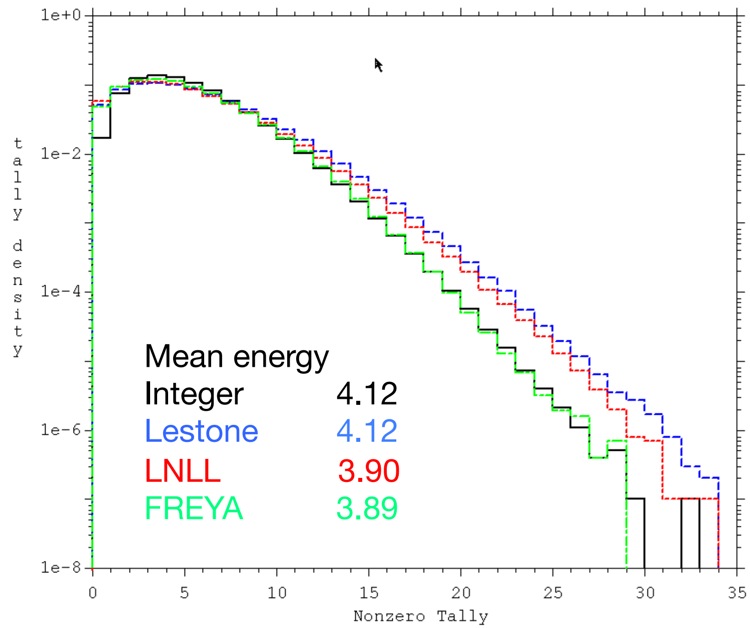
Neither event-by-event calculation nor LiBerACE data agree with Nifenecker's positive correlation



Integration of FREYA into MCNP I: Energy Correlation

- Neutron source (^{235}U) in sphere, tally crossings and energy of crossings of sphere surface
- Average neutron multiplicities should agree although multiplicity distributions differ
- Total neutron energy per fission should have a higher tail for uncorrelated treatments
- Large multiplicities sampling from same energy distributions give higher total energies
- Compare integer sampling, multiplicity treatment by Lestone, LLNL fission library and FREYA
- Results courtesy of Mike James (LANL), runs done using MCNPX

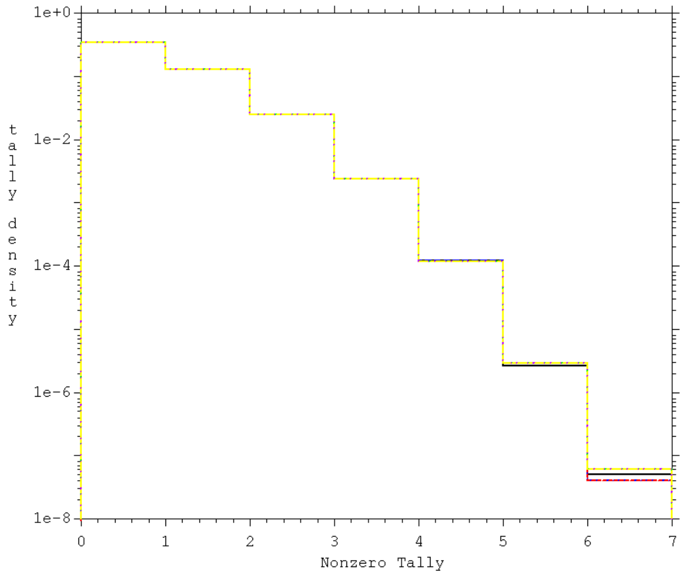




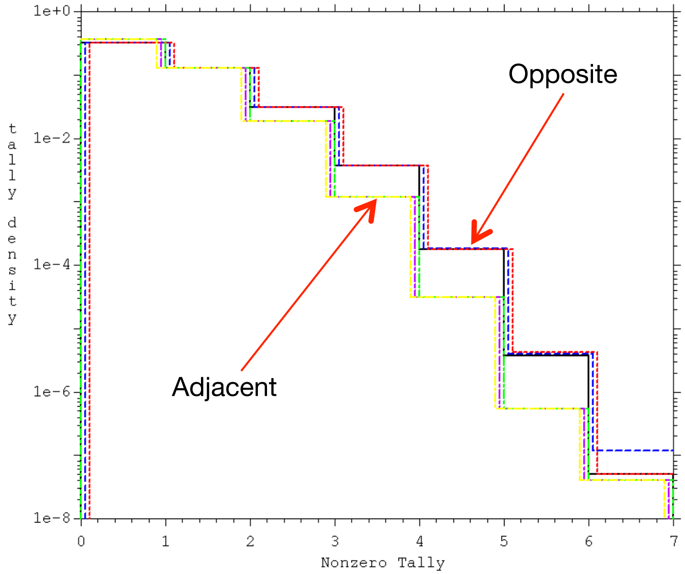
Integration of FREYA into MCNP II: Angular Correlations

- Neutron source (^{235}U) in cube, tally on opposite and adjacent cube faces
- If neutron emissions are correlated back-to-back, opposite faces should have higher multiplicities than adjacent faces
- Compare integer sampling, multiplicity treatment by Lestone, LLNL fission library and FREYA
- Results courtesy of Mike James (LANL), runs done using MCNPX

LLNL fission library is isotropic and uncorrelated opposite and adjacent tallies are identical



Results with FREYA show that opposite tallies larger than adjacent ones (x-axis offsets are for clarity)



Integration of FREYA into MCNP III: Timing

- FREYA is currently run as an option in the LLNL fission library
- While the library is rather slow relative to the integer sampling time, FREYA is
- Compare integer sampling, multiplicity treatment by Lestone, LLNL fission library and FREYA
- Results courtesy of Mike James (LANL), runs done using MCNPX

Treatment	Relative Execution Time (m)
Default (integer sampling)	1.15
Lestone	1.20
LLNL	2.52
FREYA	2.72

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
- Plans to incorporate **FREYA** into **MCNP6**, **FREYA1.0** with neutrons released as open source in July 2013