Event-by-Event Fission Modeling

GlobalSecurity
Anticipate • Innovate • Deliver

Ramona Vogt (LLNL), Jørgen Randrup (LBNL), & Jerome Verbeke (LLNL)

LLNL-PRES-659318

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

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 for spontaneous and neutron-induced fission
- 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 and photon results, compare to data
  - Present new results on neutron correlations
  - Describe integration of **FREYA** into transport codes

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

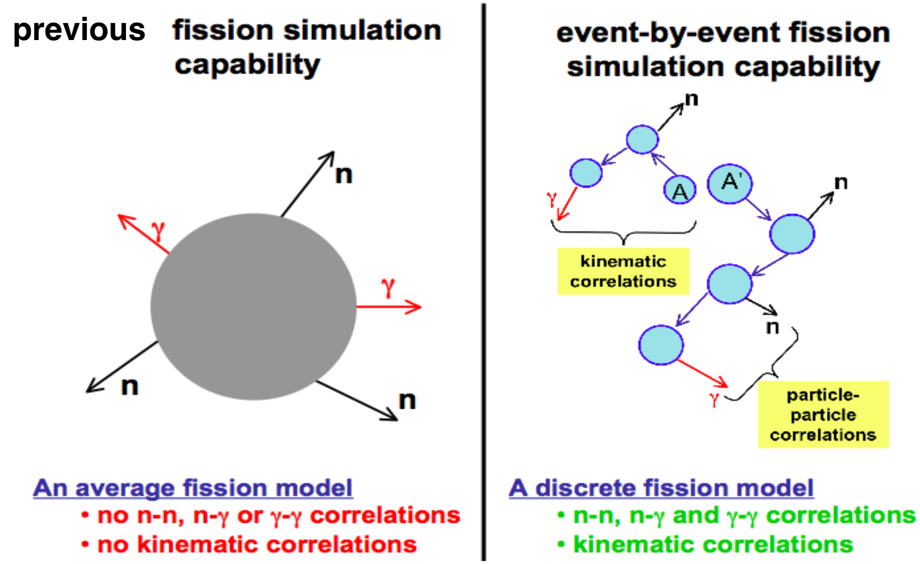
Advantage of having *samples* of complete events:

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

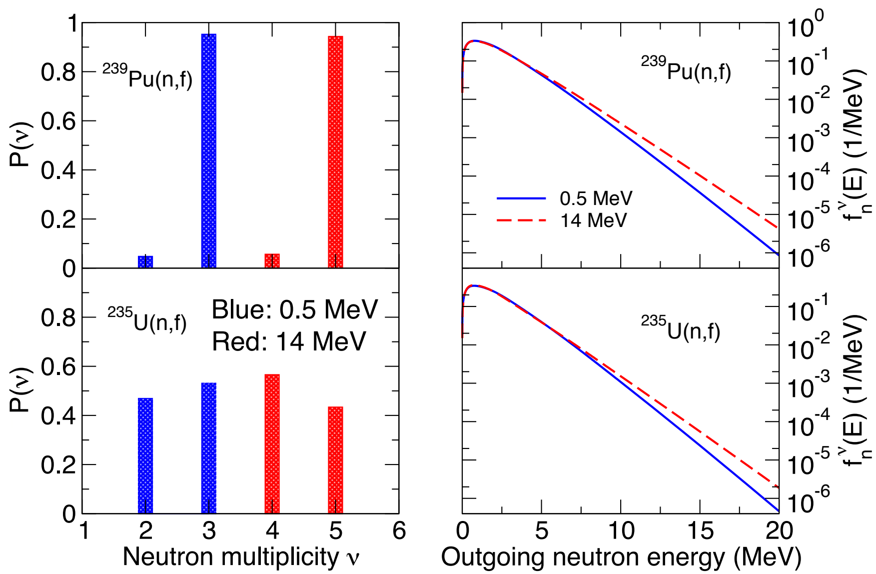
How do complete event treatments differ from traditional fission models?



- 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

- **FREYA** generates complete fission events: energy & momentum of neutrons, photons, and products in each individual fission event; correlations are automatically included

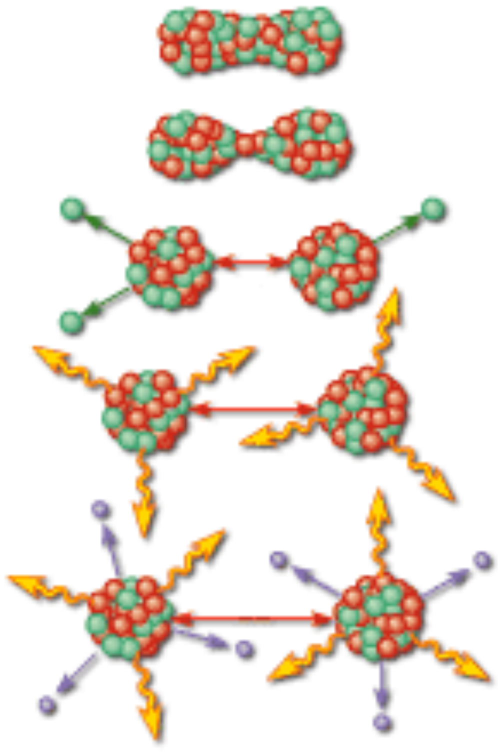
Fission model in frequently used simulation code **MCNP**:



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

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; Phys. Rev. C **89** (2014) 044601User Manual LLNL-TM-654899.
- Submitted to Comp. Phys. Comm. with J. Verbeke
- Available with LLNL fission library in Geant4, TRIPOLI, and, soon, MCNP6



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

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

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

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

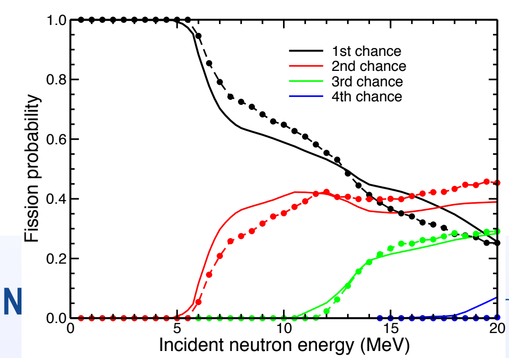
^{252}Cf ^{240}Pu

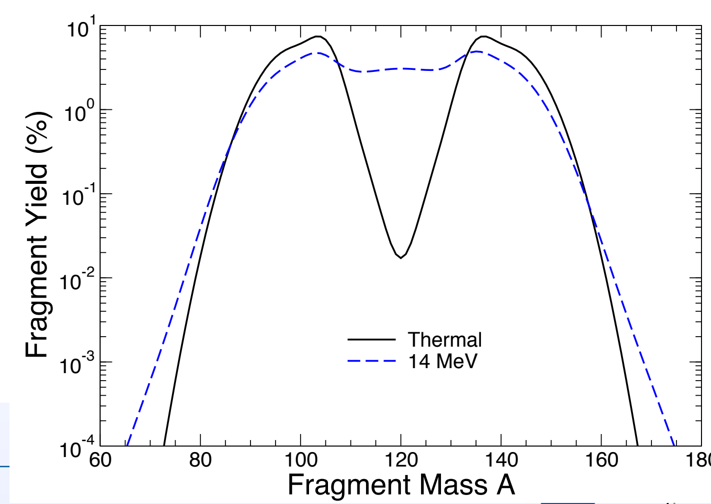
E_n = 14 MeV:

1st: 44%

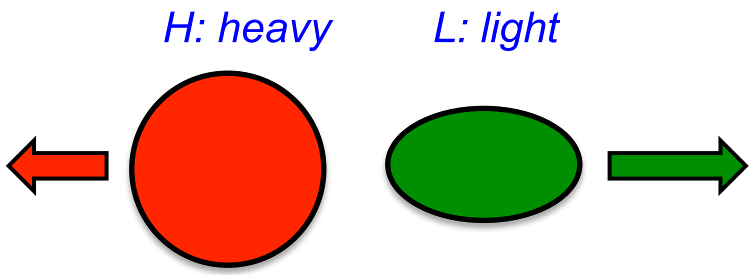
2nd: 35%

3rd: 21%





Fission fragment kinetic energies

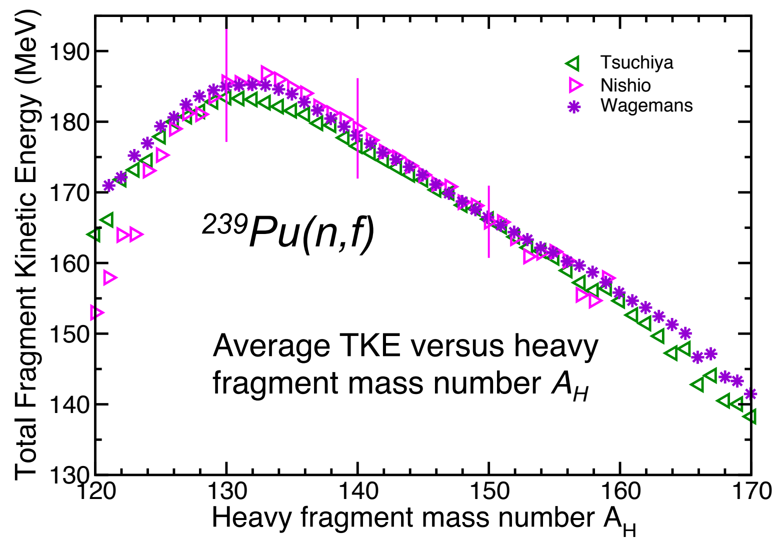


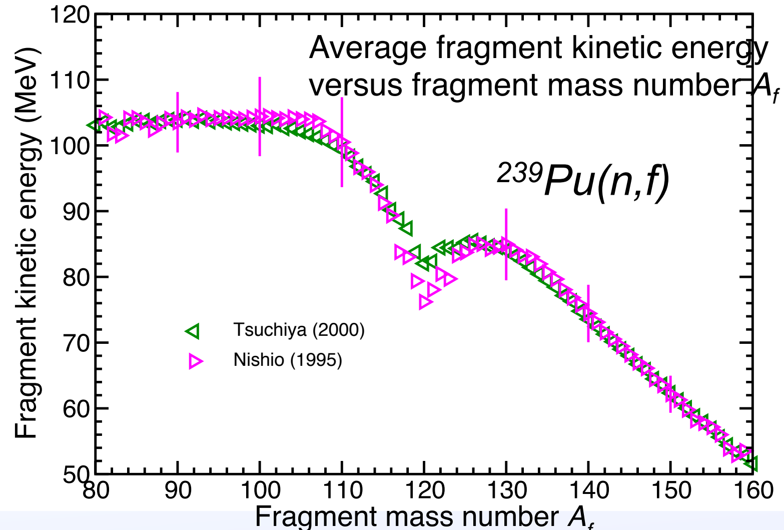
No models for *TKE(A$_f$)* exists yet, so …

we adjust TKE to exp data:

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

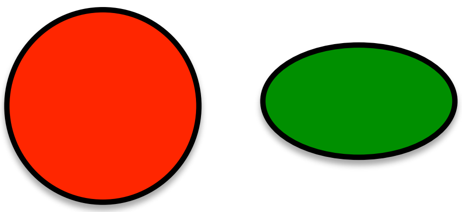
with an adjustable shift
to reproduce the mean
neutron multiplicity $<\nu>(E_{\mathrm{n}})$





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?*

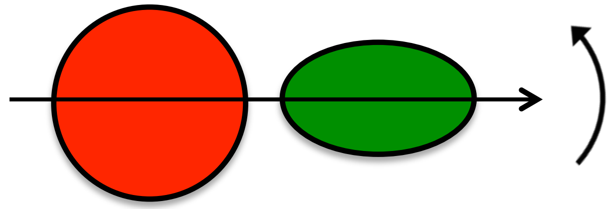
Fragment momenta then follow from energy & momentum conservation:

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

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

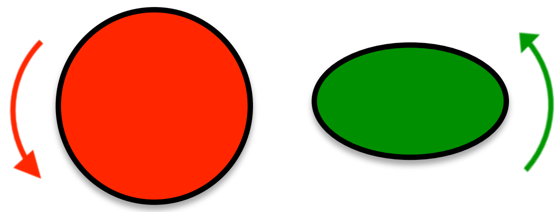
Angular momentum at scission: Rigid rotation plus fluctuations

Rigid rotation:



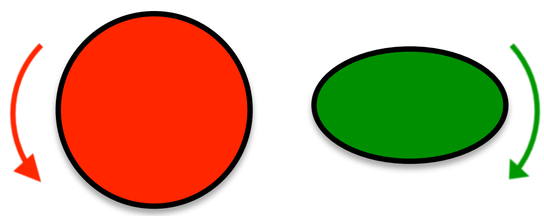
$\mathbf{S}_i = (\mathcal{I}_i/\mathcal{I})\mathbf{S}_0 + \delta\mathbf{S}_i$

Wriggling:



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

Bending:

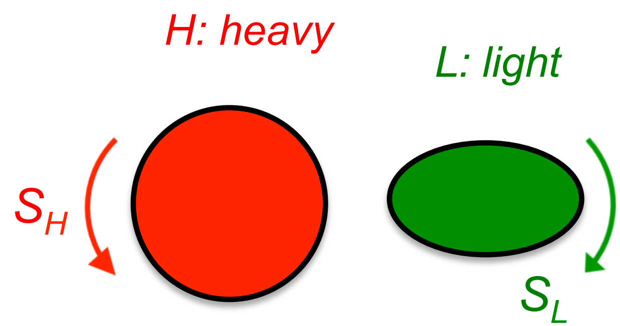


$\mathcal{I}_- = \mathcal{I}_\mathrm{H}\mathcal{I}_\mathrm{L}/(\mathcal{I}_\mathrm{H}+\mathcal{I}_\mathrm{L})$

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

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)*

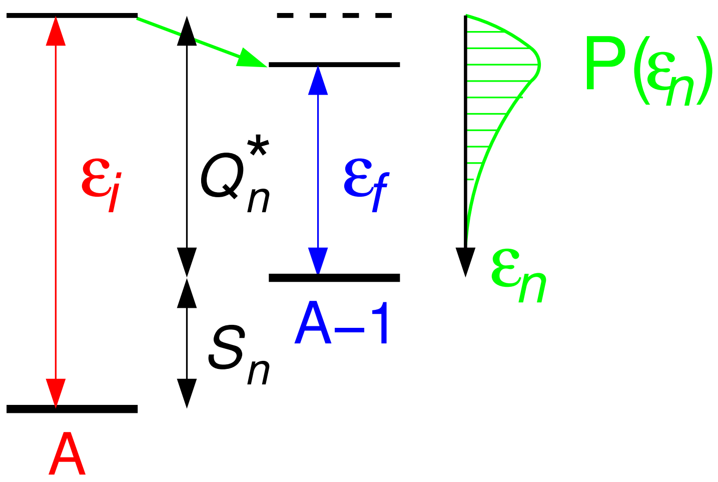
Fluctuating angular momentum components of fragments,
$\delta S_L^k = (\mathcal{I}_L/\mathcal{I}_+)s_+^k + s_-^k$; $\delta S_H^k = (\mathcal{I}_H/\mathcal{I}_+)s_+^k - s_-^k$;
Total angular momenta of fragment i are then $\mathbf{S}_i' = \mathbf{S}_i + \delta\mathbf{S}_i$
with orbital angular momentum $\mathbf{L}' = \mathbf{L} - \delta\mathbf{S}_L - \delta\mathbf{S}_H$*; 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



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

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

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

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

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

$$\epsilon + \varepsilon_f = M_i^* - M_f^{\rm gs} - m_{\rm n} = Q_{\rm n}^* = \begin{cases} \varepsilon_f^{\rm max} \\ \epsilon^{\rm max} \end{cases}$$

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

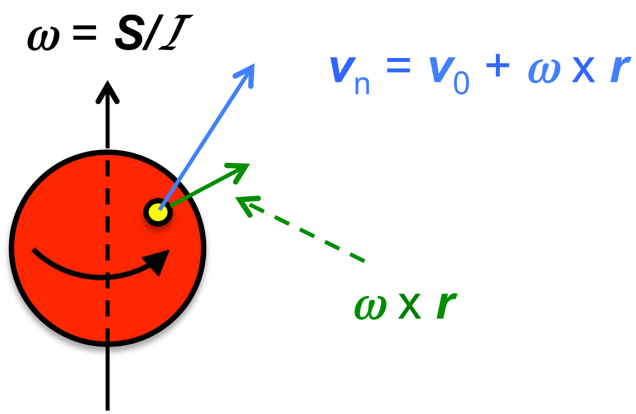
$$d^3\boldsymbol{p} \sim \sqrt{\epsilon}\, d\epsilon\, d\Omega$$

(non-relativistic)

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

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

Neutron evaporation from rotating fragments



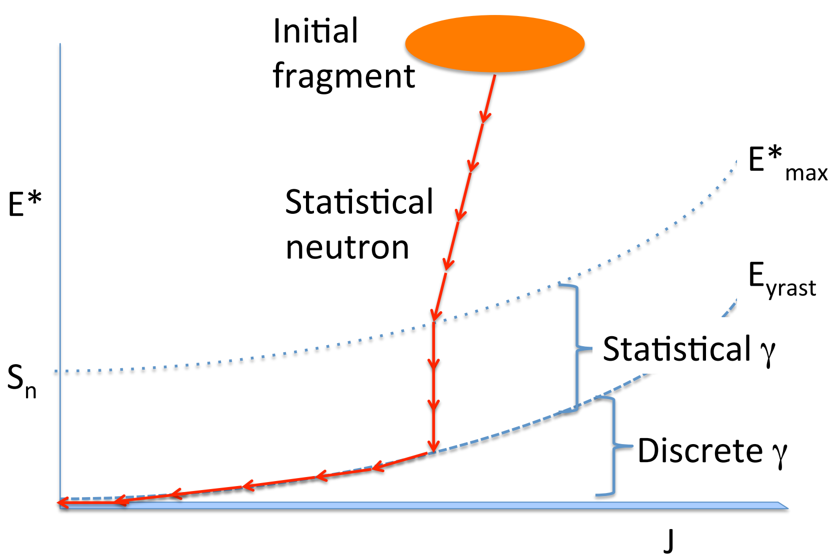
$$\boldsymbol{S}' = \boldsymbol{S} - \boldsymbol{r} \times \boldsymbol{p}_n$$

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 …

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

(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

External parameters in FREYA which can be adjusted to data

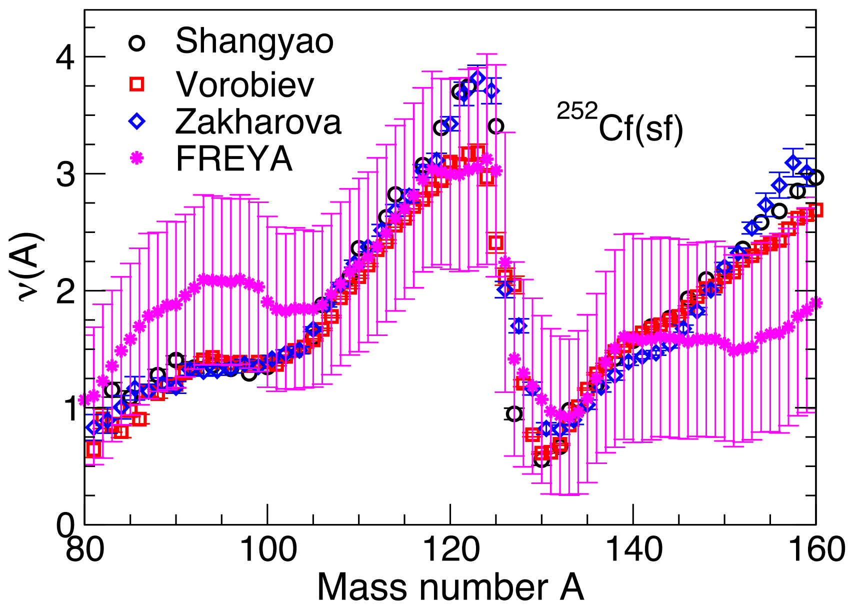
- In addition to isotope-specific inputs such as Y(A) and TKE(A_H), there are also intrinsic parameters such as nuclear masses (Audi and Wapstra for experimentally-measured masses, supplemented by masses calculated by Moller, Nix, Myers and Swiatecki), barrier heights, pairing energies and shell corrections
- 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

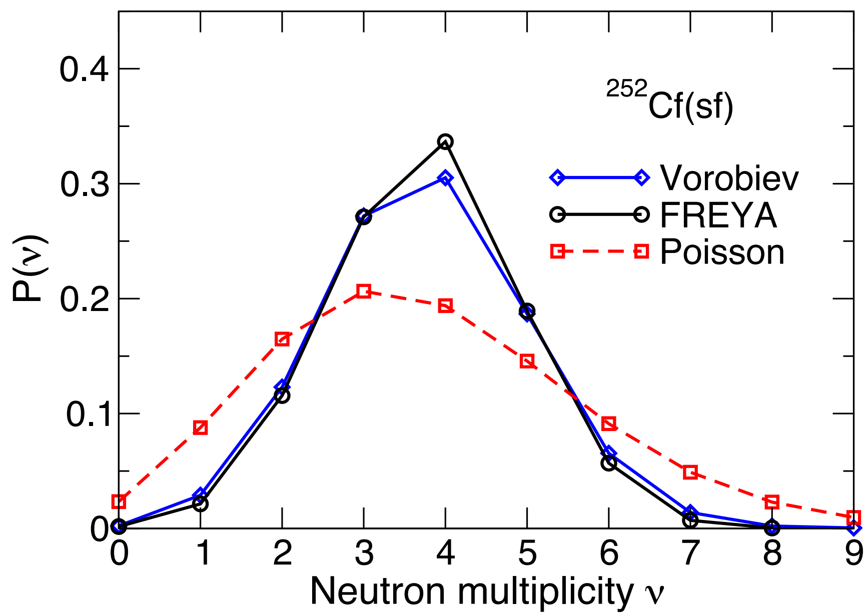
Neutron observables: $\nu(A)$ and multiplicity distribution, $P(\nu)$

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

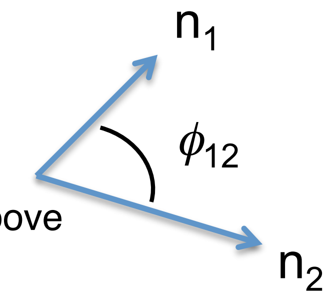
$\nu(A)$ calculation shows dispersion in Z for a given mass (**FREYA** 'error bars')

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





Two-neutron angular correlations reflect emitter source

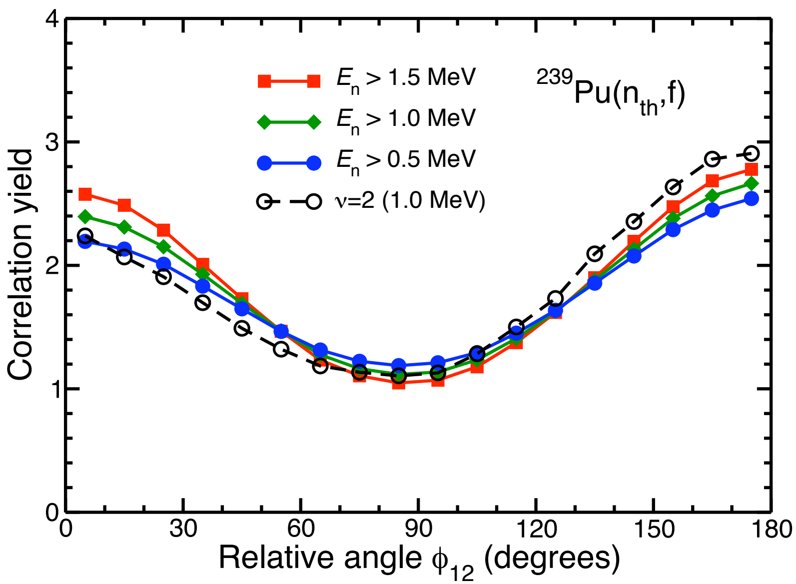


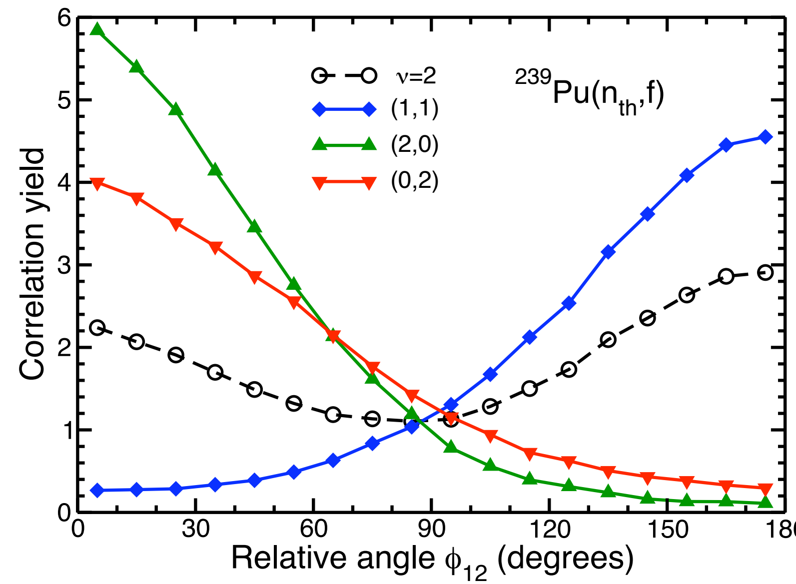
Correlations of neutrons with energies above a specified threshold energy

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



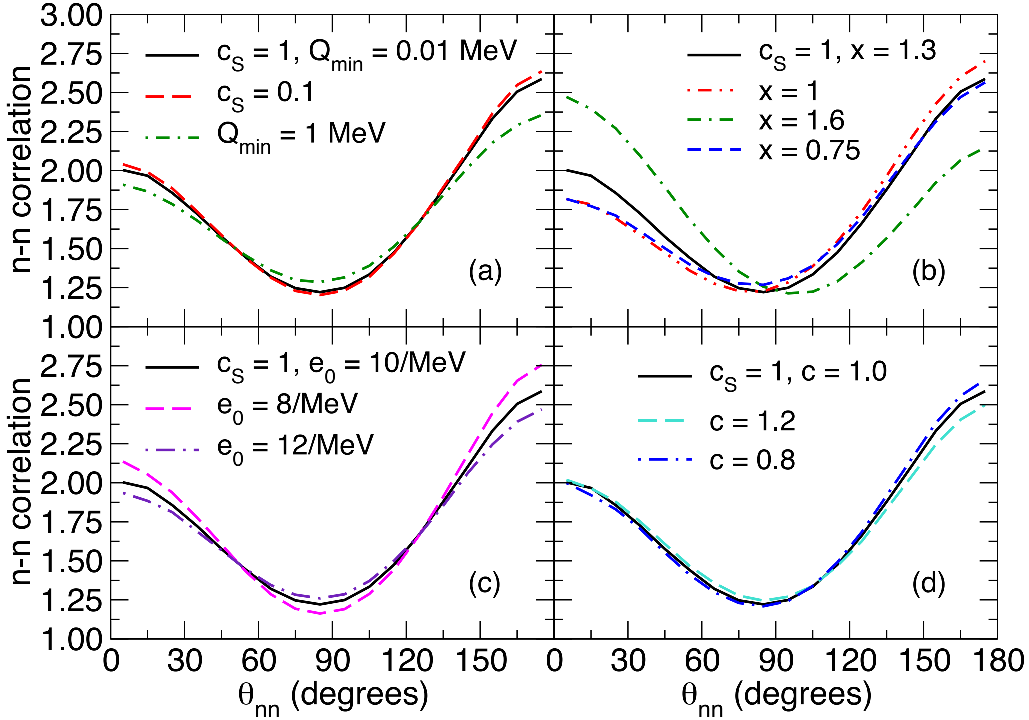


Sensitivity of correlations to input parameters

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 θ_{nn} = 0° while leaving that at 180° unchanged; x > 1.3 (giving more excitation to light fragment) produces a significantly stronger correlation at θ_{nn} = 0°

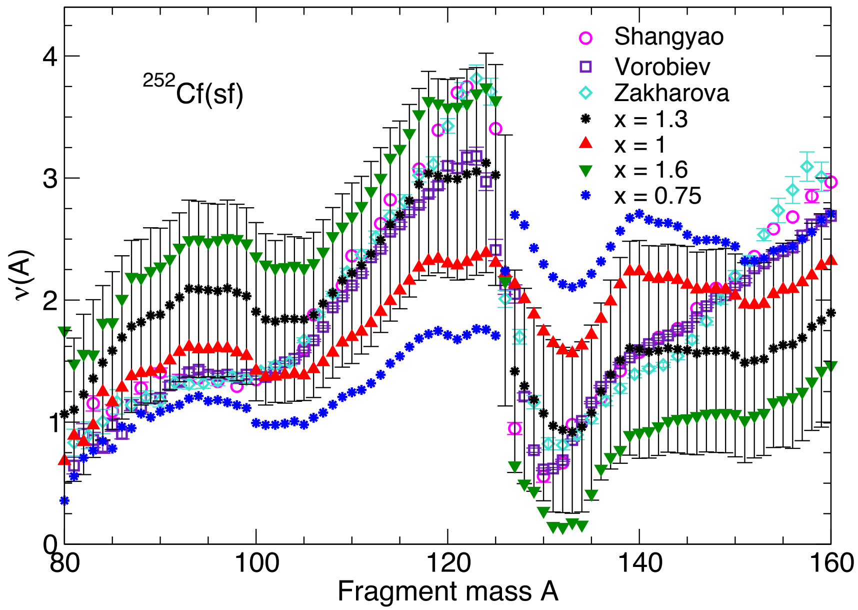
Correlation shape is relatively robust with respect to model parameters

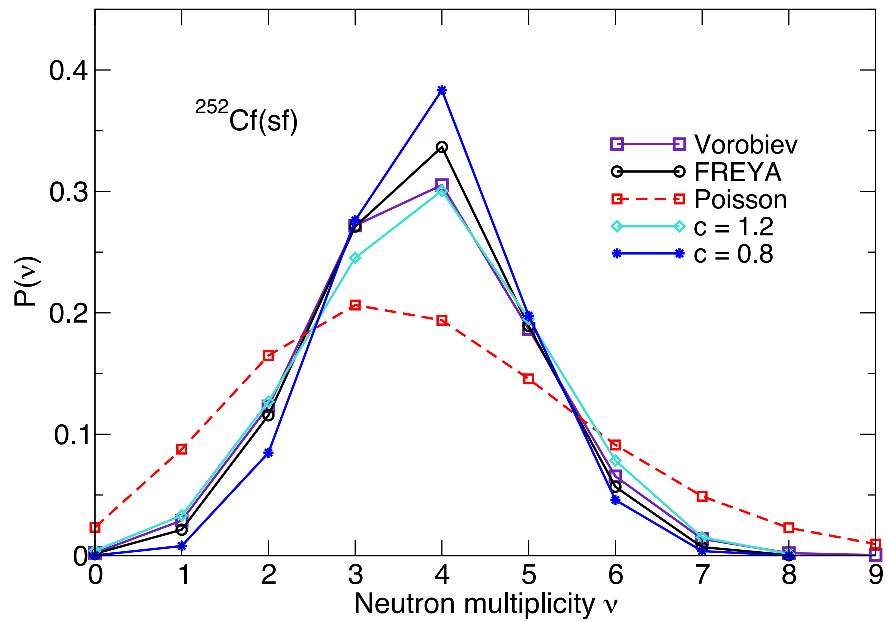


Effect of changing input parameters on other observables

(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

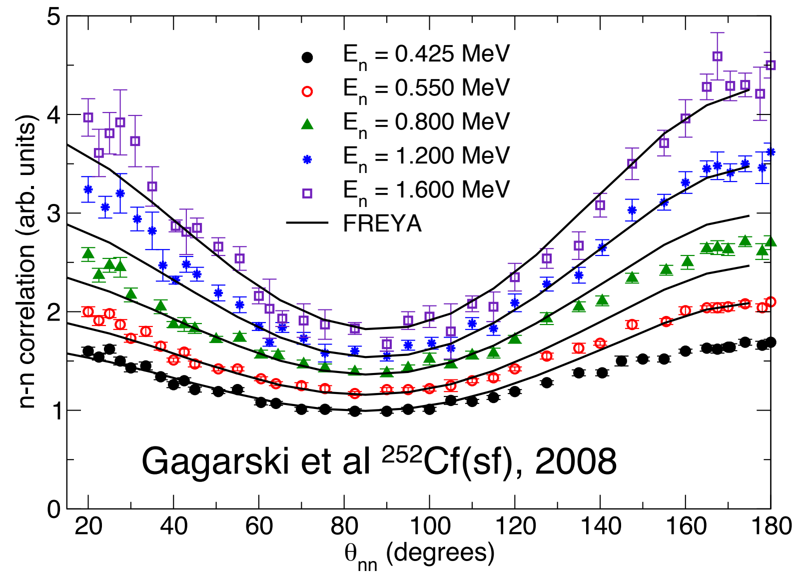
(Right) changing the width of the thermal distributions reduces the agreement of **FREYA** with the Vorobiev P(ν) data, increasing c makes P(ν) too broad, decreasing c makes it too narrow

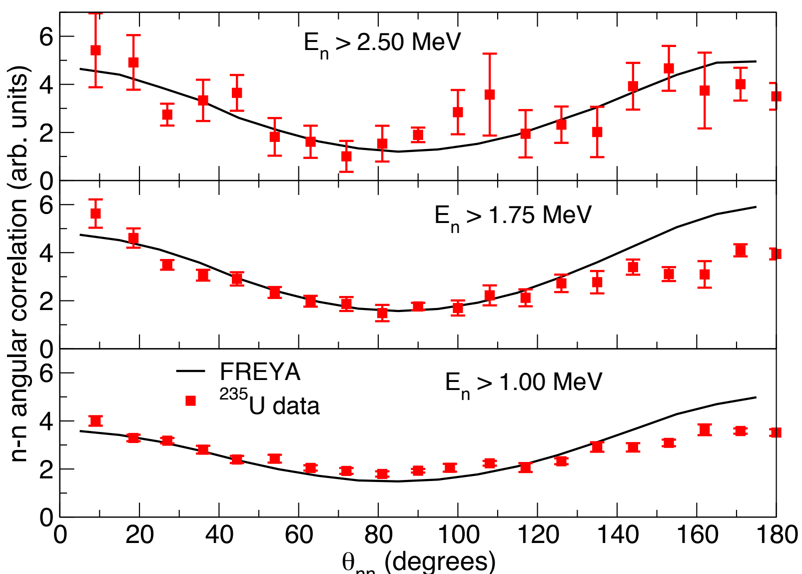




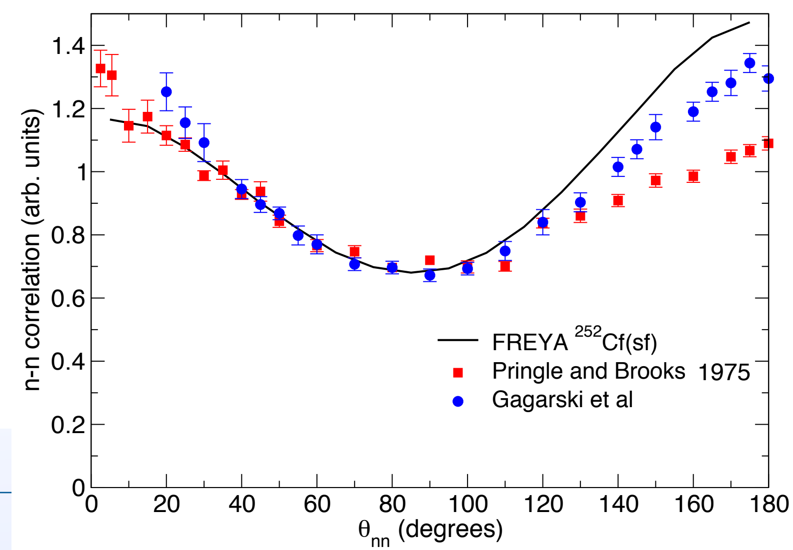
Default version of FREYA gives rather good agreement with angular correlation data

- 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

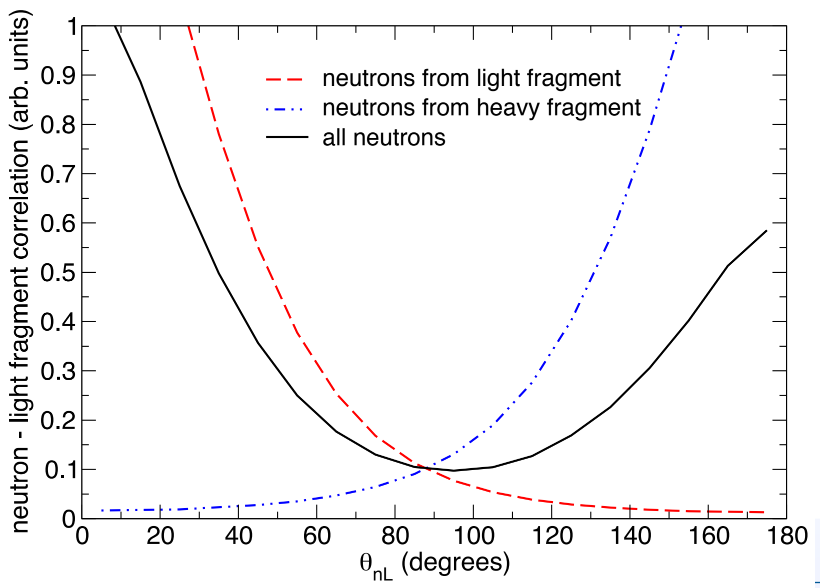


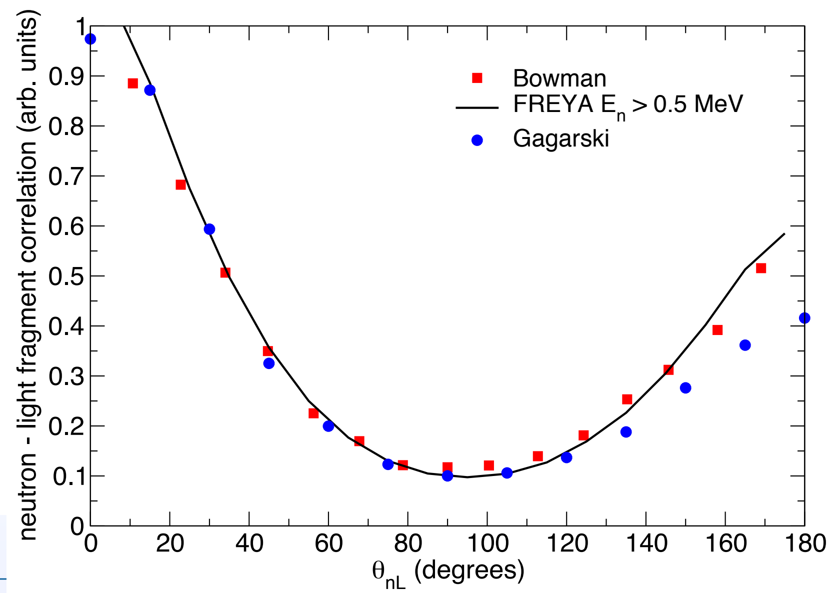
Correlation between neutron and light fragment

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

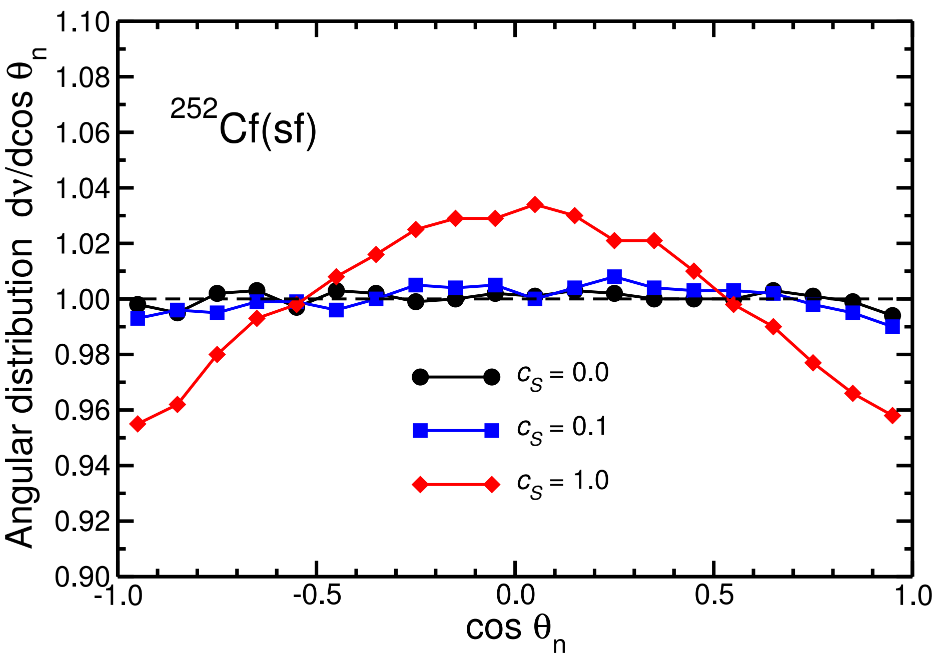
Angular distribution of neutrons evaporated from rotating nucleus acquires oblate shape – rotational boost enhances emission in plane perpendicular to angular momentum of emitter centrifugal effect quantified by 2nd Legendre moment

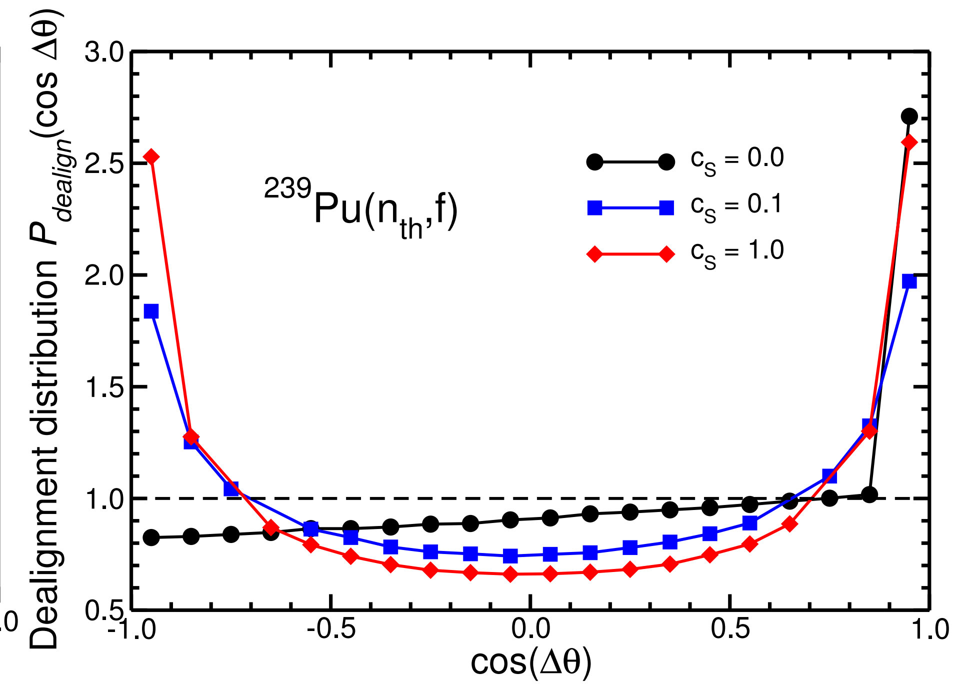
$$\langle P_2(\cos\theta)\rangle = \langle P_2(\boldsymbol{p}\cdot\boldsymbol{S}/|\boldsymbol{p}||\boldsymbol{S}|)\rangle$$

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

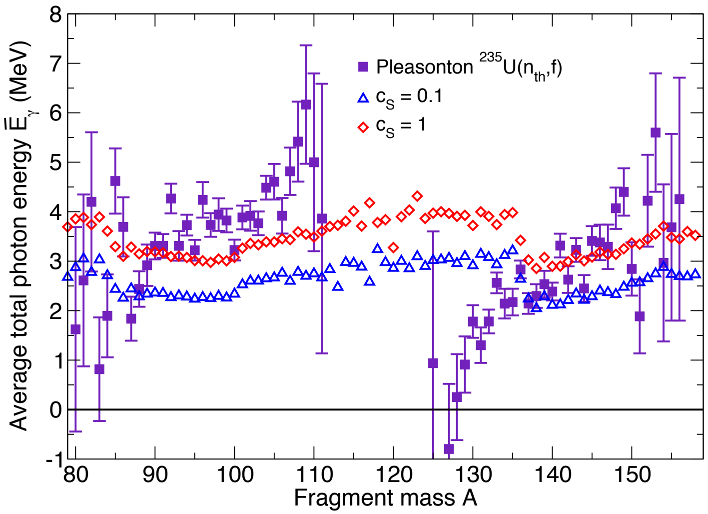
angle between initial angular momentum of compound nucleus and fragment after evaporation is the dealignment angle $\Delta\theta$ ($\boldsymbol{S}_i'\cdot\boldsymbol{S}_0 = S_i'S_0\cos\Delta\theta$)

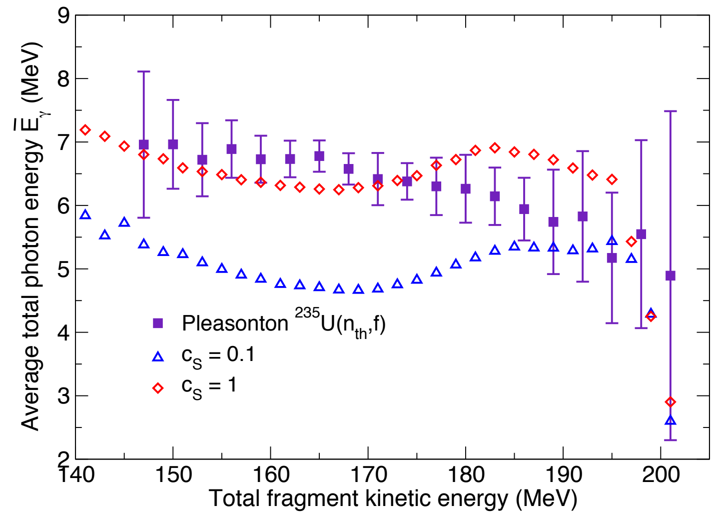


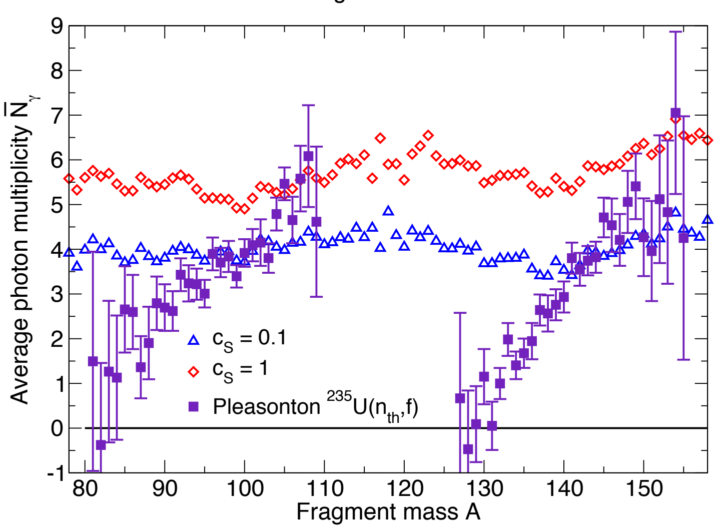


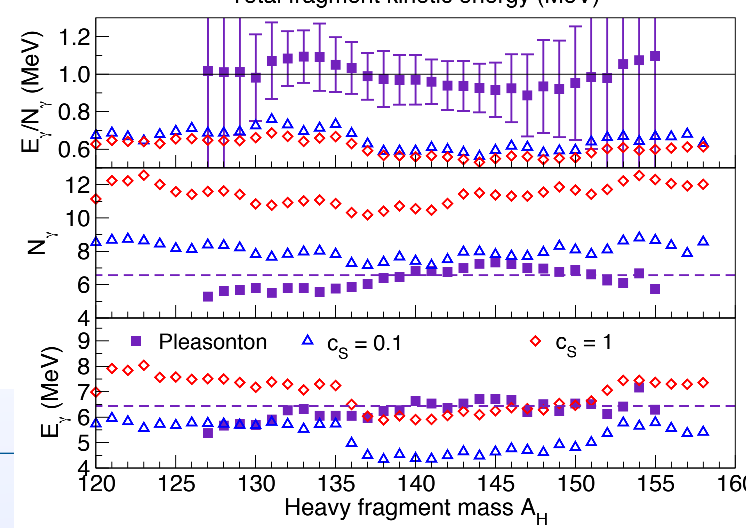
Photon Results: ^{235}U(n,f), Pleasonton et al.

Employing same values of c_S as for ^{252}Cf(sf), we see similar results: multiplicity relatively good with c_S = 0.1 but rather good agreement with energy for c_S = 1, increasing Q_{min} hardens gamma spectra
We are looking into ways to improve Eγ/Nγ in **FREYA**



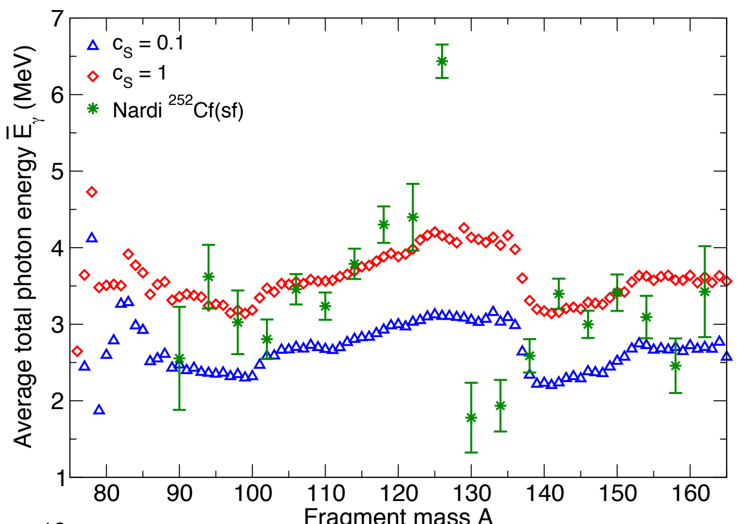


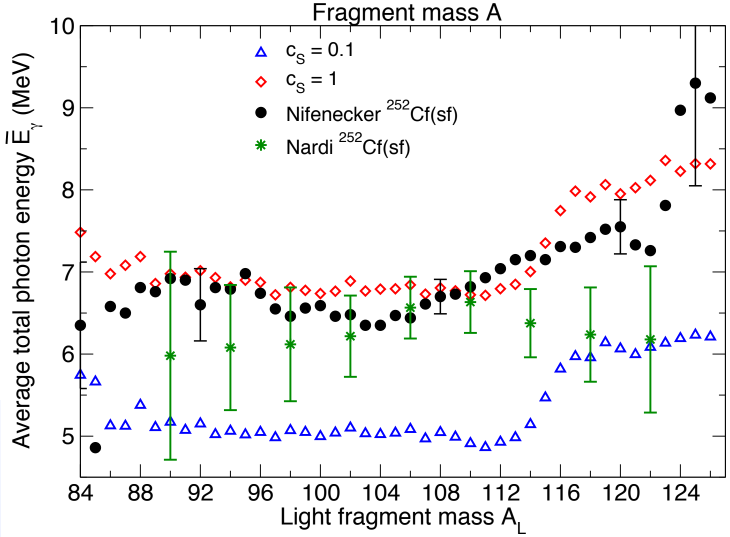




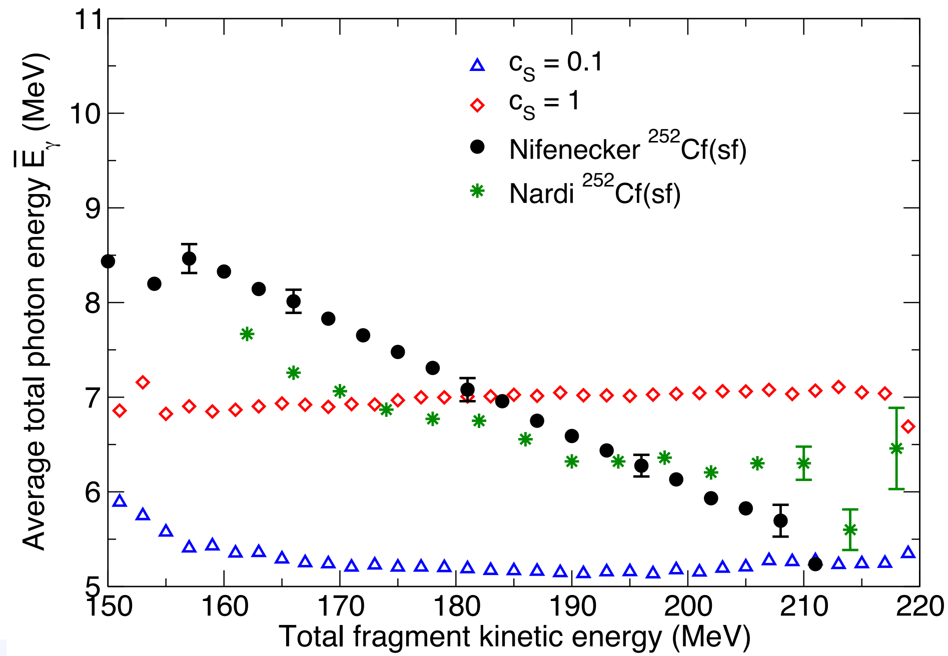
Photon Results: ^{252}Cf(sf), Nardi et al. and Niefenecker et al.

(Top) $E_\gamma(A)$ shows sawtooth-like shape similar to Nardi data with smaller, less sharp tooth at A ~ 135
(Bottom) $E_\gamma(A_L) + E_\gamma(A_H)$ vs A_L 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)
Which decreases linearly with TKE
Nifenecker data decrease linearly,
Nardi data decrease and flatten for TKE > 190 MeV



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
- 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