Covariances between fission observables coming from theory

Ramona Vogt (LLNL & UC Davis)

With J. Randrup (LBNL) & P. Talou (LANL)

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Creating an ensemble of yield functions

- Performed least-square analysis of three types of data
  - Mass yields as a function of A, Y(A)
  - Average total kinetic energy as a function of heavy fragment mass, TKE(A_H)
  - Width of TKE distribution, σ_{TKE}, as a function of A_H
- Generated best mean value as well as covariance matrix containing uncertainties and correlations, as outlined below
- A total of 15,000 yield functions were generated for input into FREYA to study consequences of varying the input on neutron observables

$$Y(\mathrm{TKE}|A) \propto \exp\left[-\frac{[\mathrm{TKE} - \overline{\mathrm{TKE}}(A)]^2}{2\sigma^2_{\mathrm{TKE}(A)}}\right]$$

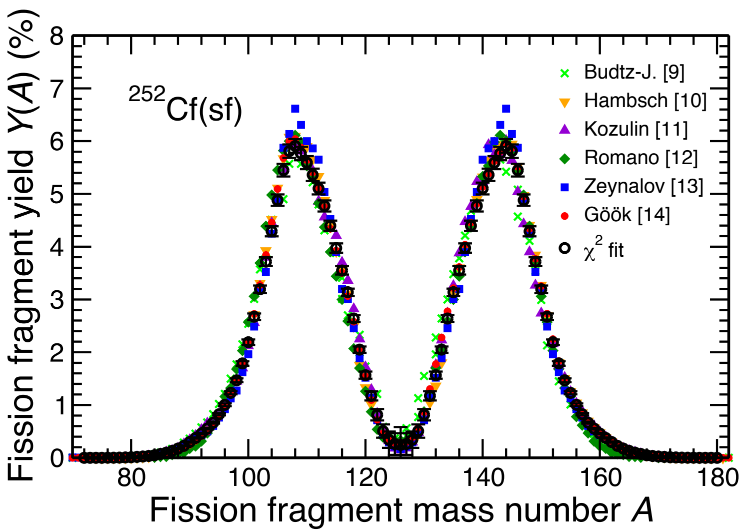
$$\int Y(Z|A)\, dZ = 1$$

$$Y(A) = \int Y(\mathrm{TKE}|A)\, d\mathrm{TKE}$$

$$Y(A, Z, \mathrm{TKE}) = Y(\mathrm{TKE}|A)\, Y(Z|A)$$

Mass and charge yields for ^{252}Cf(sf)

Data Type	First Author	Year	EXFOR Entry	Reference
$Y(A)$	Göök	2014	-	Phys. Rev. C **90**, 064611
	Zeynalov	2011	23118-002	J. Korean Phys. Soc. **59**, 1396
	Romano	2010	14259-008	Phys. Rev. C **81**, 014607
	Kozulin	2008	41581-003	Inst. and Exp. Techniques **51**, 44
	Hambsch	1997	22780-002	Nucl. Phys. **A617**, 347
	Budtz-Jørgensen	1988	23175-002	Nucl. Phys. **A490**, 307

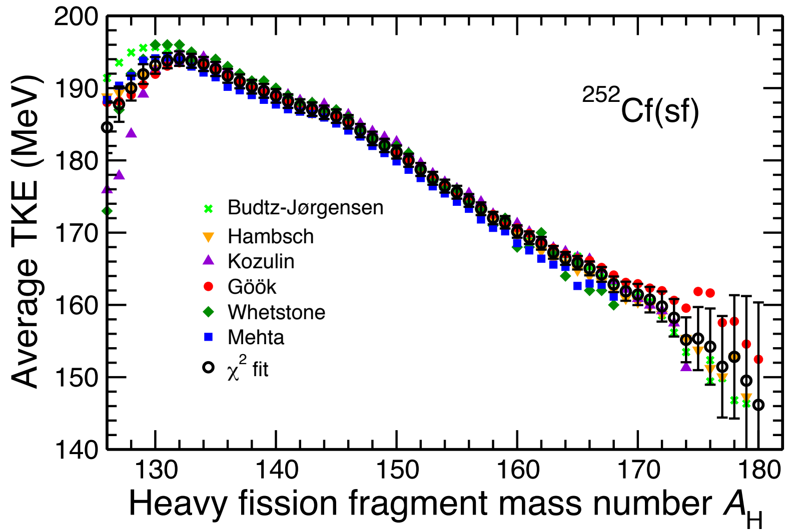


Uncorrelated uncertainties of 0.5-3% added to each point of different sets, also allowed for normalization uncertainties

Charge distribution Y(Z|A) determined from Wahl systematics

Average total kinetic energy vs. heavy fragment mass

Data Type	First Author	Year	EXFOR Entry	Reference
$\langle TKE\rangle(A)$	Göök	2014	-	Phys. Rev. C **90**, 064611
	Kozulin	2008	41581-004	Inst. and Exp. Techniques **51**, 44
	Hambsch	1997	22780-003	Nucl. Phys. **A617**, 347
	Budtz-Jørgensen	1988	23175-003	Nucl. Phys. **A490**, 307
	Mehta	1973	23213-008	Phys. Rev. C **7**, 373
	Whetstone	1963	14101-003	Phys. Rev. **131**, 1232



1% normalization uncertainty and
0.5% statistical uncertainty added to all sets

1% uncertainty on TKE ~1.5-2 MeV abs. norm.

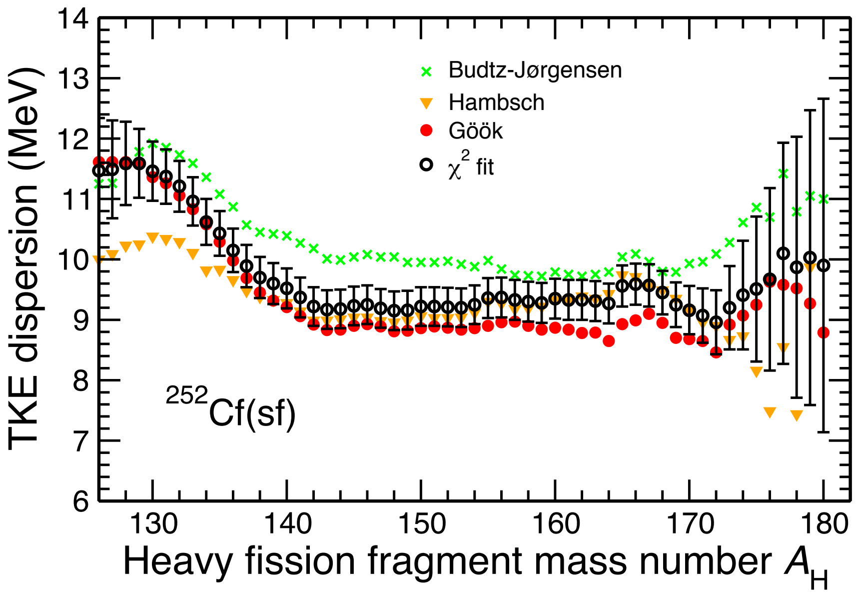
Additional uncertainties added at A's near symmetry and very asymmetric splits:

$$\delta y_i = 0.002\; y_i \exp((132 - A_i)/2)\;,\quad A_H < 132$$
$$\delta y_i = 0.001\; y_i \exp((A_i - 160)/4)\;,\quad A_H > 160$$

$$y_i \equiv \overline{\mathrm{TKE}}(A_i)$$

Width of TKE(A_H) less well determined

Data Type	First Author	Year	EXFOR Entry	Reference
$\sigma_{TKE}(A)$	Göök	2014	-	Phys. Rev. C **90**, 064611
	Hambsch	1997	22780-003	Nucl. Phys. **A617**, 347
	Budtz-Jørgensen	1988	23175-003	Nucl. Phys. **A490**, 307



Fewer data sets, with significant differences between them

A 4% normalization uncertainty and a 1% statistical uncertainty added to all sets

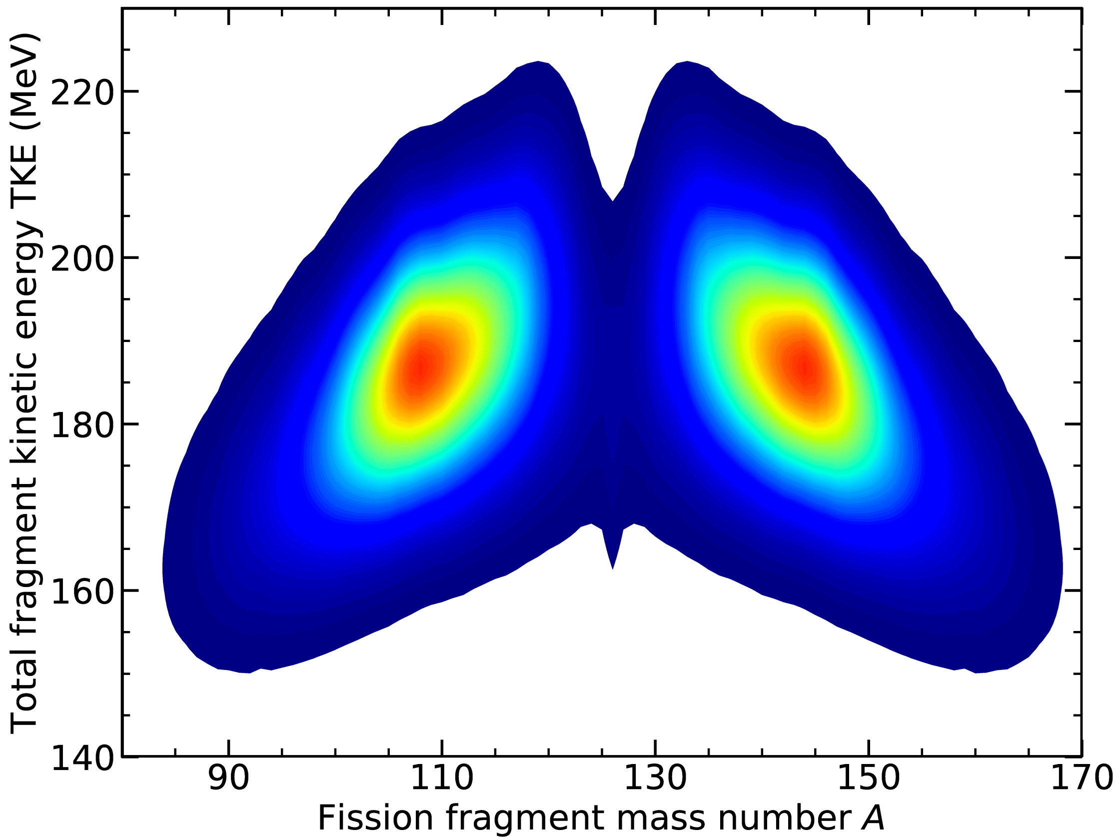
Statistical uncertainties on data grow for symmetric and very asymmetric splits:

$$\delta y_i = 0.002\ y_i \exp((140 - A_i)/2)\ ,\quad A_H < 140$$
$$\delta y_i = 0.001\ y_i \exp((A_i - 165)/4)\ ,\quad A_H > 165$$

$$y_i \equiv \sigma_{\mathrm{TKE}(A_i)}$$

Example of typical yield function

Contour plot with projection on the A-TKE plane



Event selection

- FREYA modified from standard version to take Y(A,Z,TKE) as input
- Initial nucleus has mass number A_0 and charge Z_0
- Joint yield function is normalized to unity:

$$\sum_A \sum_Z \int Y(A,Z,\mathrm{TKE})\, d\mathrm{TKE} = 1$$

- First, mass of one fragment is selected, followed by its charge

$$P_A(A) = \sum_Z \int Y(A,Z,\mathrm{TKE})\, d\mathrm{TKE} \qquad P_Z(Z;A) = \frac{1}{P_A(A)} \int Y(A,Z,\mathrm{TKE})\, d\mathrm{TKE}$$

$$\sum_A P_A(A) = 1 \qquad \sum_Z P_Z(Z;A) = 1$$

- TKE selected from probability distribution

$$P_{\mathrm{TKE}}(\mathrm{TKE};A,Z) = \frac{Y(A,Z,\mathrm{TKE})}{P_Z(Z;A)}$$

$$\int P_{\mathrm{TKE}}(\mathrm{TKE};A,Z)\, d\mathrm{TKE} = 1$$

Event generation

- Mass and charge of complementary fragments are $A' = A_0 - A$, $Z' = Z_0 - Z$, Q value calculated and total excitation energy obtained:

$$
\begin{aligned}
E^*(A, Z, \mathrm{TKE}) &= Q(A, Z) - \mathrm{TKE} \\
Q(A, Z) &= M(A_0, Z_0) - M(A, Z) - M(A', Z')
\end{aligned}
$$

- Excitation energy split between rotational and intrinsic, $E^* = E_{rot} + E_{int}$
- Intrinsic excitation energy split between fragments, first by statistical partitioning by level densities to E_L' and E_H', then by favoring the light fragment giving it an additional energy, $E_L^* = xE_L'$, $E_H^* = E_{int} - E_L'$
- Standard FREYA allows further fluctuations affecting neutron multiplicity distribution but because TKE width is fixed, this is not done in this study
- Finally, TKE is adjusted by parameter dTKE to give evaluated value of average neutron multiplicity, 3.765

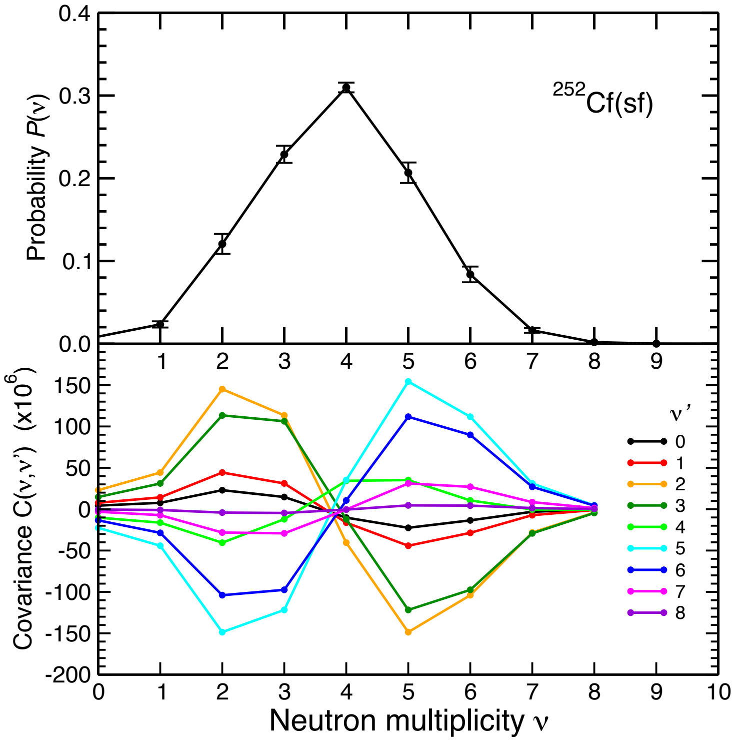
Calculation of observables

- Take ensemble of yield functions and run FREYA for each given yield function, calculate results ensemble average
- For comparison, results are also shown for generating the observables by reusing the average yield function the same number of times
  - In this case, there are no ensemble fluctuations, only statistical ones
- Compare results for averaging over the entire ensemble and reusing the same yield function equally many times

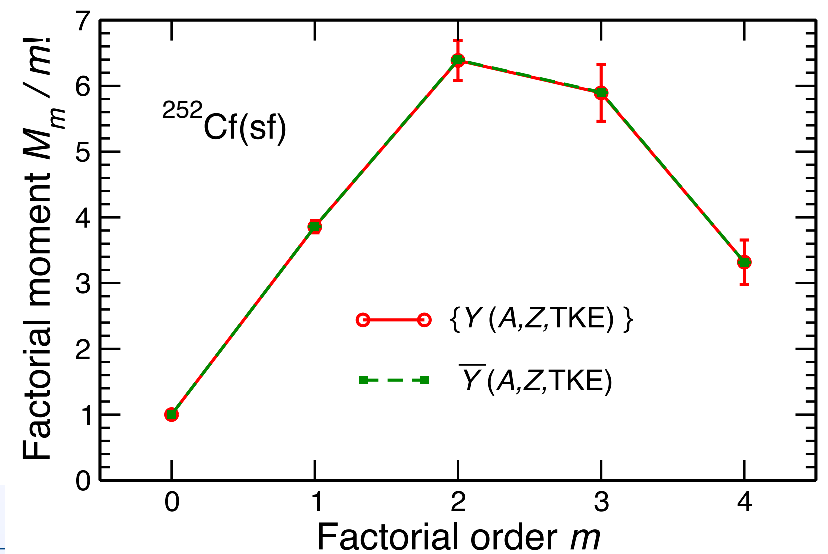
Neutron multiplicity P(ν) and moments

Uncertainties on P(ν) result from ensemble fluctuations (top)
Covariances (bottom) relate probability of ν for given ν’

$$
\begin{aligned}
\prec P_n(\nu) \succ &= \sum_{i=1}^{N} W_i P_n^{(i)}(\nu) \\
C_{nn}(\nu,\nu') &= \prec P_n(\nu) P_n(\nu') \succ - \prec P_n(\nu) \succ \prec P_n(\nu') \succ \\
&= \sum_{i=1}^{N} W_i P_n^{(i)}(\nu) P_n^{(i)}(\nu') - \prec P_n(\nu) \succ \prec P_n(\nu') \succ \\
M_n^{(i)} &\equiv \sum_{\nu} \nu(\nu-1)\cdots(\nu-n+1) P_n^{(i)}(\nu)
\end{aligned}
$$



Uncertainty in moments averaged over all yield functions larger than those reusing the same yield functions equally many times



Prompt fission neutron spectrum and covariances

Results averaged over all multiplicities

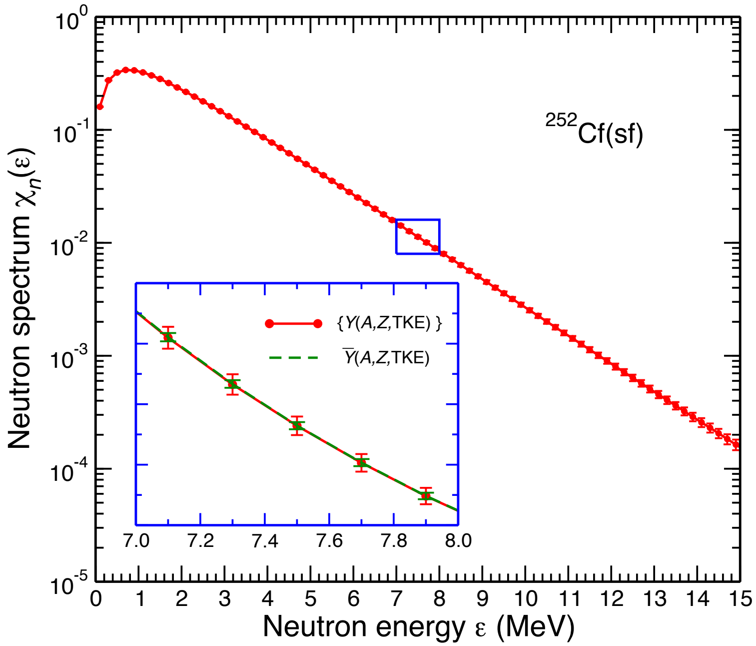
Inset illustrates that the yield functions introduce larger uncertainties than sampling same yield function N times

$$\chi_n(\epsilon) = \frac{1}{\overline{\nu}}\frac{d\nu}{d\epsilon}$$

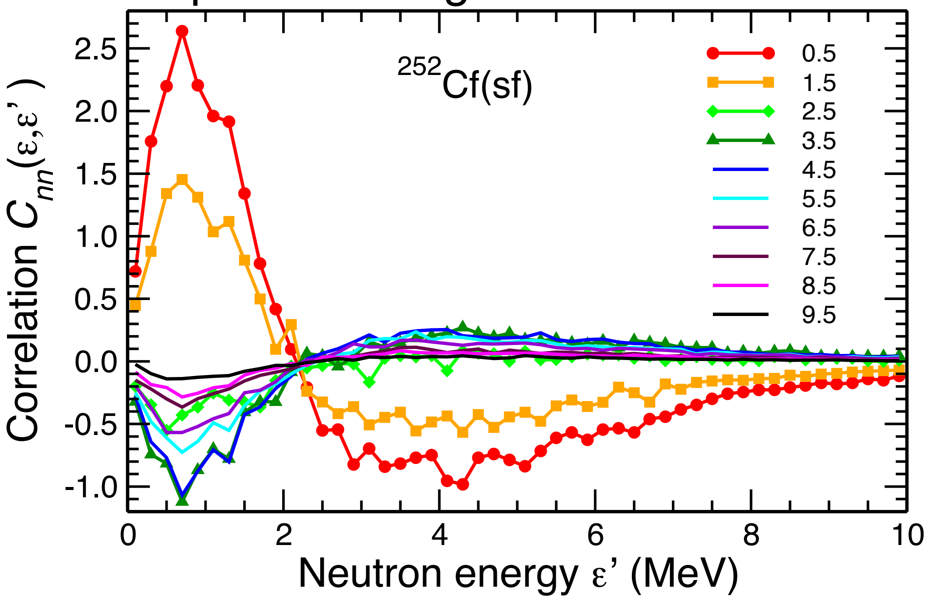
$$\prec \chi_n(\epsilon) \succ = \sum_{i=1}^{N} W_i \chi_n^{(i)}(\epsilon)$$

$$C_{nn}(\epsilon,\epsilon') = \sum_{i=1}^{N} W_i \chi_n^{(i)}(\epsilon)\chi_n^{(i)}(\epsilon') - \prec \chi_n(\epsilon) \succ \prec \chi_n(\epsilon') \succ$$

Prompt fission neutron spectrum



Covariance between different spectral energies



Neutron-neutron correlations

- Only events producing at least two neutrons contribute to the two-neutron directional distribution

$$\overline{P}_{nn}(\hat{\mathbf{p}},\hat{\mathbf{p}}') = \frac{1}{K}\sum_{k=1}^{K} P_{nn}^{(k)}(\hat{\mathbf{p}},\hat{\mathbf{p}}')$$

- Cosine of opening angle between two neutron directions

$$\cos\theta(\hat{\mathbf{p}}_1,\hat{\mathbf{p}}_2) = \hat{\mathbf{p}}_1\cdot\hat{\mathbf{p}}_2 = \sin\vartheta_1\sin\vartheta_2 cos(\phi_1-\phi_2)$$

- Distribution as a function of angle with normalization

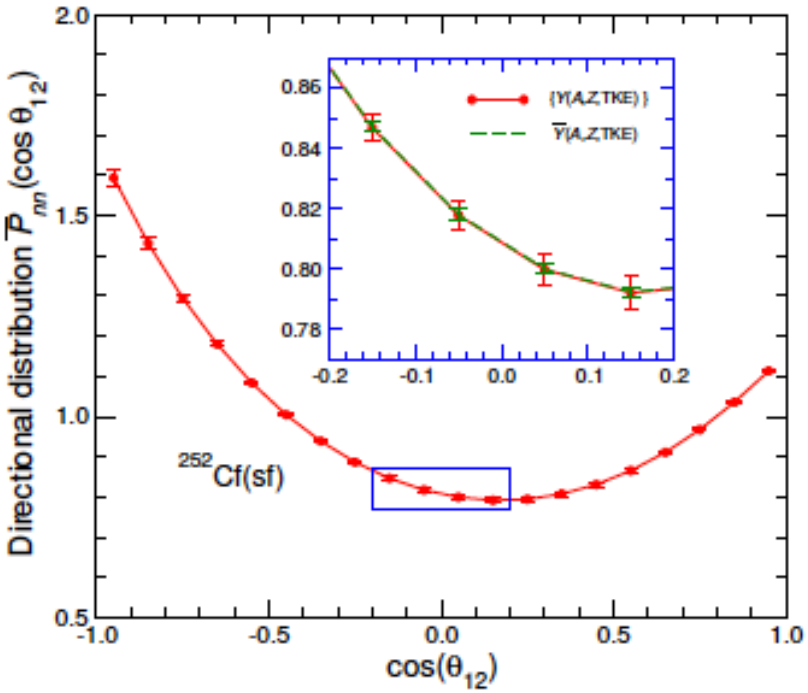
$$\begin{aligned}\overline{P}_{nn}(\cos\theta_{12}) &= \int d^2\hat{\mathbf{p}}\int d^2\hat{\mathbf{p}}'\overline{P}_{nn}(\hat{\mathbf{p}},\hat{\mathbf{p}}')\delta(\cos\theta(\hat{\mathbf{p}}_1,\hat{\mathbf{p}}_2)-\cos\theta_{12})\\ \int d\cos\theta_{12}\overline{P}_{nn}(\cos\theta_{12}) &= \langle\nu(\nu-1)\rangle\end{aligned}$$

Directional distribution with variance

- Distribution shown in figure, variance shown in error bars, ensemble of distributions compared to sampling from same initial distribution the same number of times

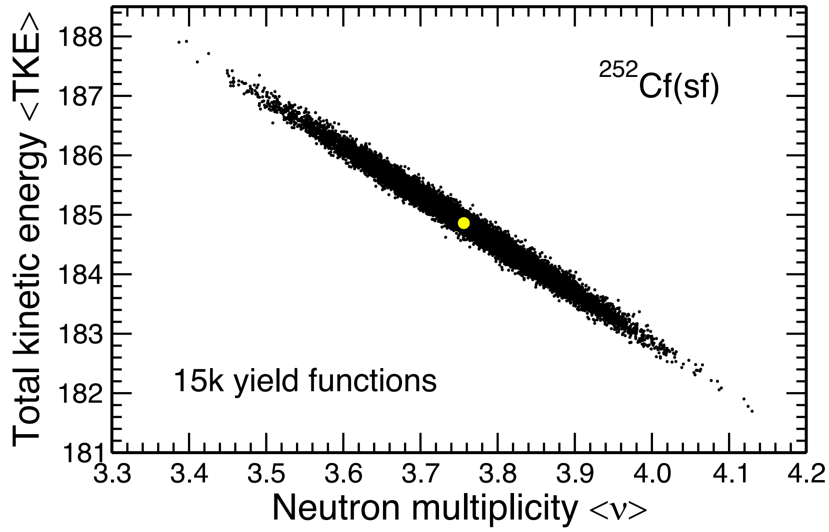
$$\prec \overline{P}_{nn}(\cos\theta_{12}) \succ = \sum_{i=1}^{N} W_i \overline{P}_{nn}^{(i)}(\cos\theta_{12})$$

$$\prec \overline{P}_{nn}(\cos\theta_{12}^2) \succ - (\prec \overline{P}_{nn}(\cos\theta_{12}) \succ)^2$$
$$= \sum_{i=1}^{N} W_i [\overline{P}_{nn}^{(i)}(\cos\theta_{12})]^2 - \left[\sum_{i=1}^{N} W_i \overline{P}_{nn}^{(i)}(\cos\theta_{12})\right]^2$$

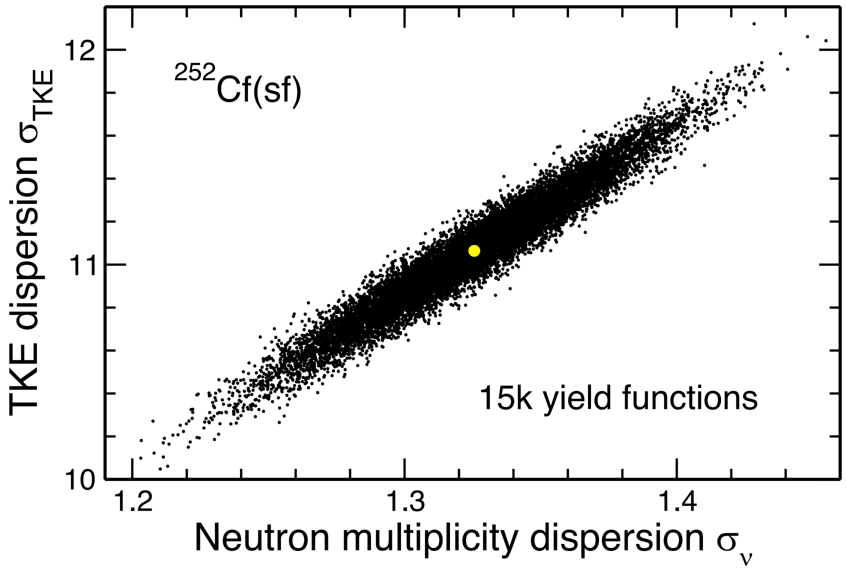


Correlations between neutron multiplicity and TKE

Larger TKE reduces available excitation energy and thus reduces the neutron multiplicity



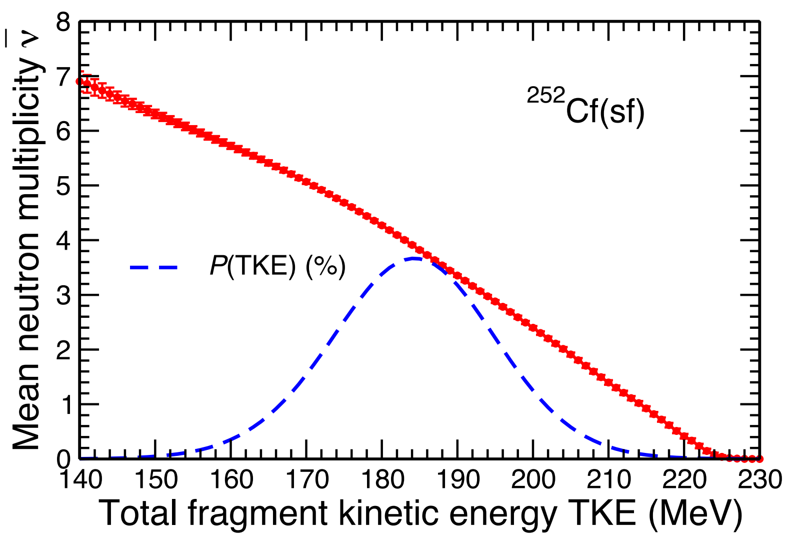
Increasing the fluctuations (dispersion) in TKE also increases fluctuations in the neutron multiplicity



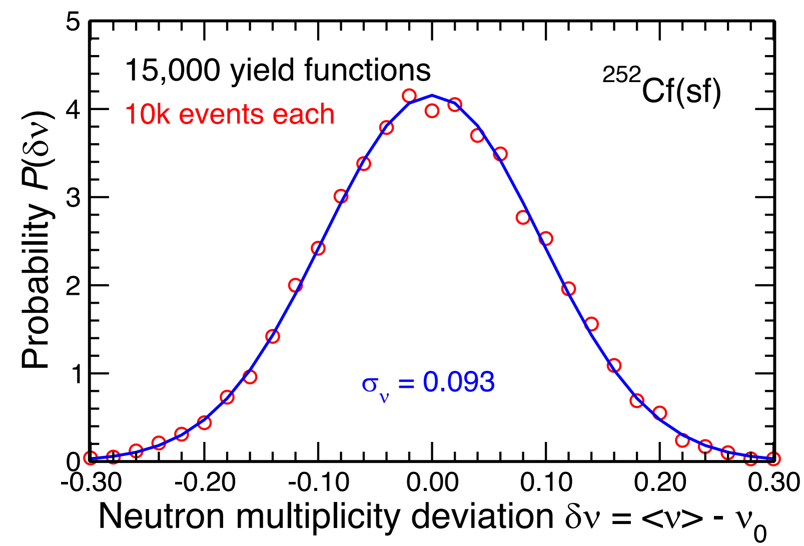
Known average neutron multiplicity, TKE, and their dispersions indicated by yellow dots on the plots

TKE distribution and effect on neutron multiplicity

Distribution of average TKE (unit normalized) obtained by sampling all 15K yield functions with different numbers of events



Distribution of deviations from the known mean value of <ν>.
The dispersion of the resulting Gaussian fit is shown.



Deviations from mean ν much larger than evaluated dispersion, σ_o = 0.015,
To bring results closer to mean value of ν, we introduce a biased weight

Bias of average TKE imposed by $\bar{\nu}$

Width of average TKE distribution obtained from specific values of imposed bias width in weight of individual yield functions
”max” obtained for $\sigma_0 \rightarrow \infty$; “min” for $\sigma_0 \rightarrow 0$; experimental uncertainty close to 0

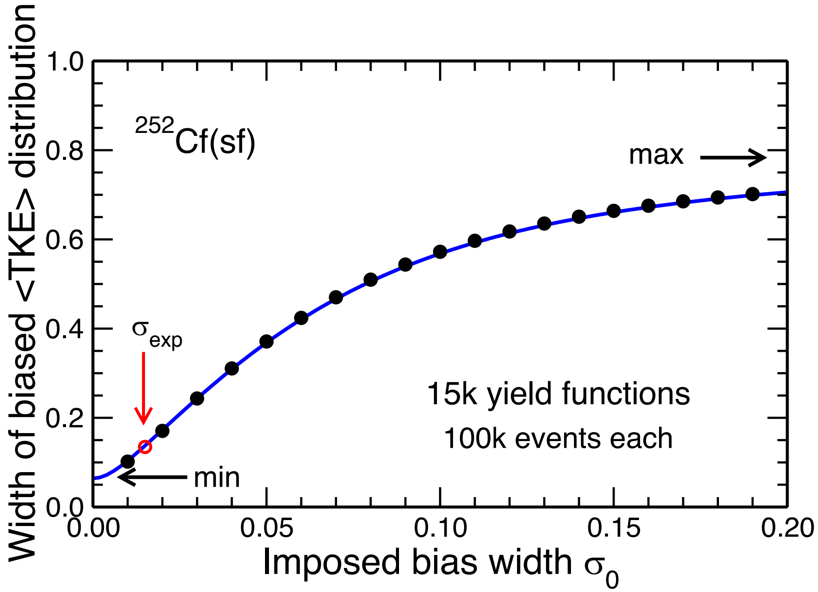
Using the experimental uncertainty on ν reduces the width of TKE to 17.2% of its Unbiased value, showing that the widths of ν and TKE are tightly correlated

$$W_i = \exp[-(\overline{\nu}^{(i)} - \nu_0)^2/2\sigma_0^2]$$

Biased weight W_i leads to
biased weight of TKE distribution, σ_K

$$\overline{\sigma}_K^2 = \sigma_K^2 - \frac{\sigma_{\nu K}^2}{\sigma_\nu^2 + \sigma_0^2}$$

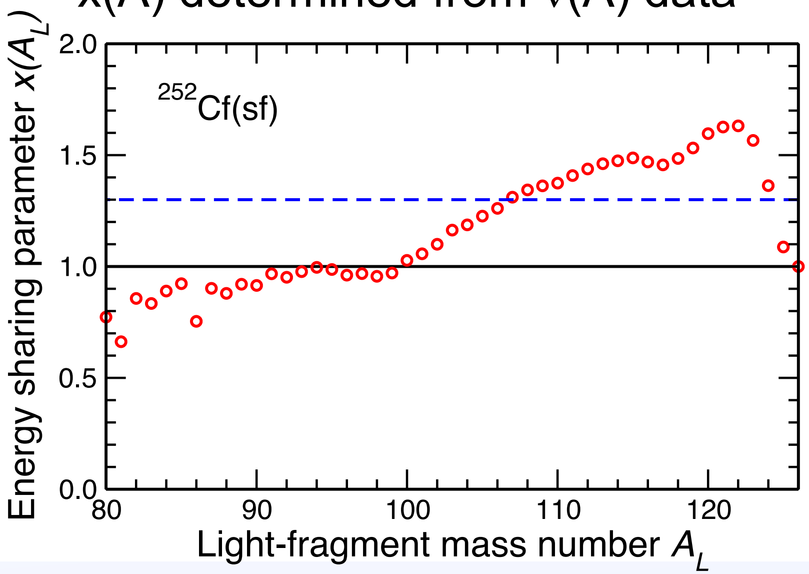
$$\begin{aligned}
\sigma_K^2 &= \prec \delta K^2 \succ = \prec (\overline{\mathrm{TKE}} - \prec \overline{\mathrm{TKE}} \succ)^2 \succ \\
\sigma_\nu^2 &= \prec \delta \nu^2 \succ = \prec (\overline{\nu} - \prec \overline{\nu} \succ)^2 \succ \\
\sigma_{\nu K} &= \prec \delta\nu\delta K \succ = \prec (\overline{\nu} - \prec \overline{\nu} \succ)(\overline{\mathrm{TKE}} - \prec \overline{\mathrm{TKE}} \succ) \succ
\end{aligned}$$



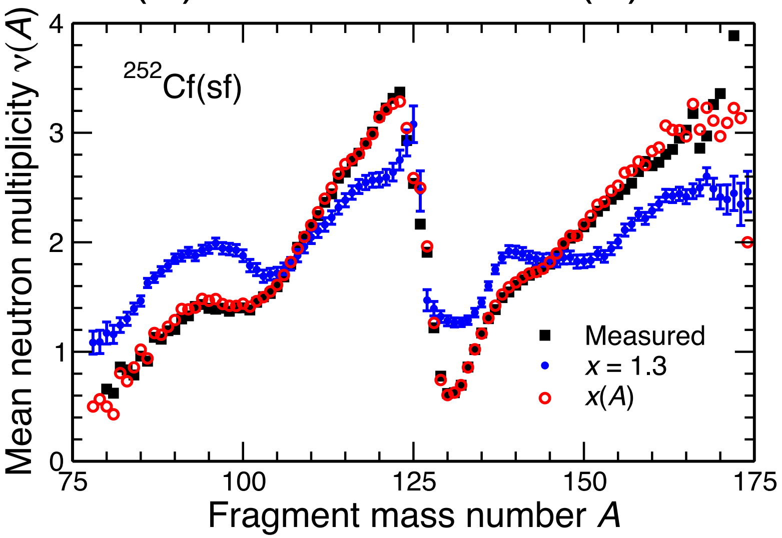
Sensitivity to input parameter *x*

FREYA uses a single valued parameter, x, to divide up the excitation energy between light and heavy fragments, other codes like **CGMF** and **FIFRELIN** use a mass dependent “x” parameter, $R_T(A)$ in **CGMF**, determined from data, to partition excitation energy. We also examined how results would change if such a method were adopted in **FREYA**.

x(A) determined from ν(A) data

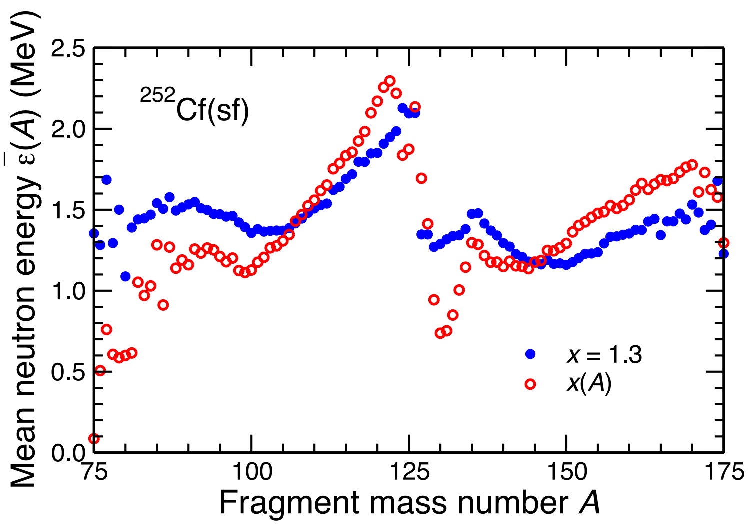


ν(A) with fixed x and x(A)

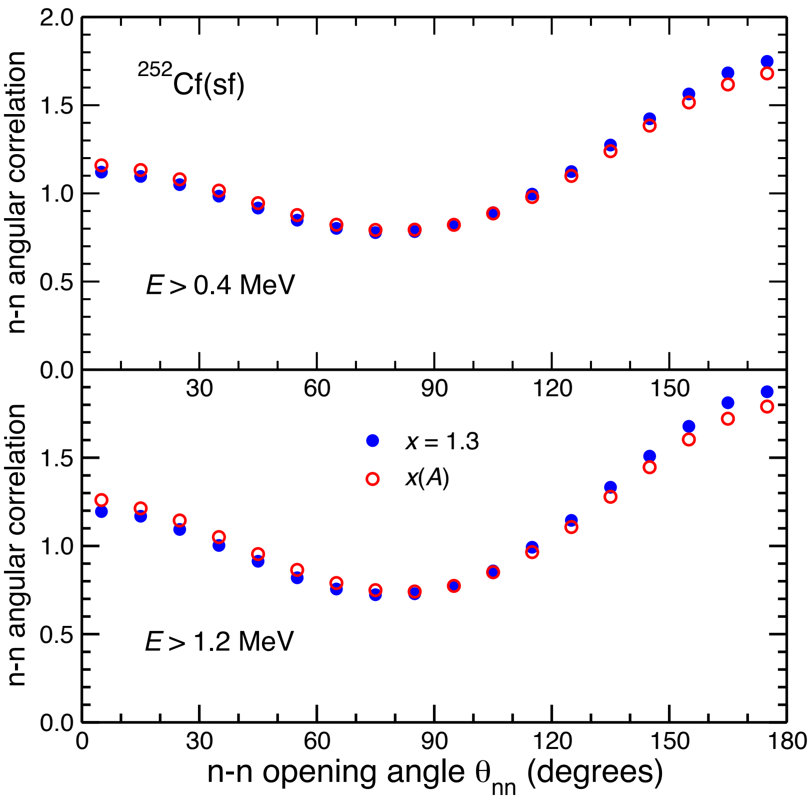


Sensitivity of observables to *x* variations

Kinetic energy per neutron



neutron-neutron angular correlation



ν(A) and ε(A) are significantly changed by the way *x* is calculated but the changes to the n-n correlations are much smaller, other observables essentially unaffected by x changes

Sensitivity to other parameter variations

- In standard FREYA, *c* controls width of variance in statistical excitation energy; changing *c* from 1 to 1.5 changes neutron multiplicity by 1.5%; in reality, average neutron multiplicity provides tightest constraint on *c*

- Rotational fluctuations controlled by parameter c_S, varying this parameter can have a large effect on neutron multiplicity because giving more energy to photon emission reduces neutron multiplicity and vice versa; within uncertainties of recent optimization, neutron multiplicity can vary by 2%

- Varying the asymptotic level density parameter as represented by e_0 can change neutron multiplicity because increasing e_0 increases fragment temperature, hardening the neutron spectrum and decreasing multiplicity; within uncertainties on e_0, multiplicity can change by 2.7%

- Individual variations need to be taken in context of all observables, thus true variations in multiplicity are more tightly constrained and will not be so large

Summary

- We have studied sensitivity of neutron observables to input fission fragment yields and input parameters
  - The sensitivity to the input yields is generally small
  - We can set tighter constraints on TKE than given by the data
  - Parameter sensitivity important but large excursions in parameter space are constrained by optimizations
- **FREYA** available from http://nuclear.llnl.gov//simulation/ and CPC code library
- User manuals also available online

FREYA references

- **FREYA** developed in collaboration with J. Randrup (LBNL); neutron-transport code integration by J. Verbeke (LLNL); available in MCNP6.2
- **FREYA** journal publications: Phys. Rev. C **80** (2009) 024601, 044611; **84** (2011) 044621; **85** (2012) 024608; **87** (2013) 044602; **89** (2014) 044601; **90** (2014) 064623; **96** (2017) 064620; version 1.0 in Comp. Phys. Comm. **191** (2015) 178; version 2.0.2 in Comp. Phys. Comm. **222** (2018) 263.
- Invited book chapter, R. Vogt and J. Randrup, “Nuclear Fission”, Chapter 5 of ‘100 Years of Subatomic Physics’, World Scientific, 2013
- Review in Eur. Phys. J. A **54** (2018) 9
- Contributed to (and coauthored) papers on neutron polarization in photofission, Mueller *et al,* Phys. Rev. C **89** (2014) 034615; neutron-gamma correlations, Wang *et al*, Phys. Rev. C **93** (2016) 014606, Marcath *et al*, Phys. Rev. C **97** (2018) 044622, Marin et al, arxiv:1907.01483; neutron-neutron correlations, Schuster et al, Phys. Rev. C **100** (2019) 014605; Verbeke *et al*, Phys. Rev. C **97** (2018) 044601; Pozzi *et al,* Nucl. Sci. Eng. **178** (2014) 250.
- Isotopes currently included: spontaneous fission of ^{252}Cf, ^{244}Cm, ^{238,240,242}Pu, ^{238}U and neutron-induced fission of ^{233,235,238}U(n,f), ^{239,241}Pu(n,f) for $E_n \leq 20$ MeV