A Method for Generation of Fission Yield Covariance Matrices

Eric F. Matthews
UC Berkeley

Motivation

- The 1994 fission yield evaluation by England and Rider does not include information on covariances between fission yields. [1]
- Covariances between fission yields affect a number of important applications:
  - Forensics and safeguards calculations
  - Reactor antineutrino rates
  - Reactor inventory, decay heat, and poisoning

[1] – Evaluation and Compilation of Fission Product Yields – T.R. England and B.F. Rider (1994)

Previous Work

- Pigni et al. – 2013
  - Variance estimation with Wahl systematics
- Schmidt – 2013
  - Parameters perturbation in the GEF code
- Leray et al. – 2017
  - Parameters perturbation in the GEF code
- Kawano and Chadwick – 2013
  - Bayesian method for ^{239}Pu FPY

Previous Work

- Pigni et al. – 2013
  - Variance estimation with Wahl systematics
- Schmidt – 2013
  - Parameters perturbation in the GEF code
- Leray et al. – 2017
  - Parameters perturbation in the GEF code
- Kawano and Chadwick – 2013
  - Bayesian method for ^{239}Pu FPY

- Work by Pigni, Schmidt, and Kawano presented in WPEC Subgroup 37
- Work by Pigni, Schmidt, and Leray relies on an underlying model of fission and parameter uncertainties.
- Results of these work are not readily accessible due in part to ENDF format limitations.

Motivation

- The goal of this work is to generate a set of covariance matrices for the fissioning systems of the England and Rider evaluation **with as little fission model bias/uncertainty as possible.**
- This method seeks to use simple conservation rules in order to constrain a sample space for Monte-Carlo bootstrapping.
- The resulting covariance matrix will predominantly reflect the evaluated uncertainties in the independent fission yields.
- Once these matrices are generated, making them available online will be a priority.

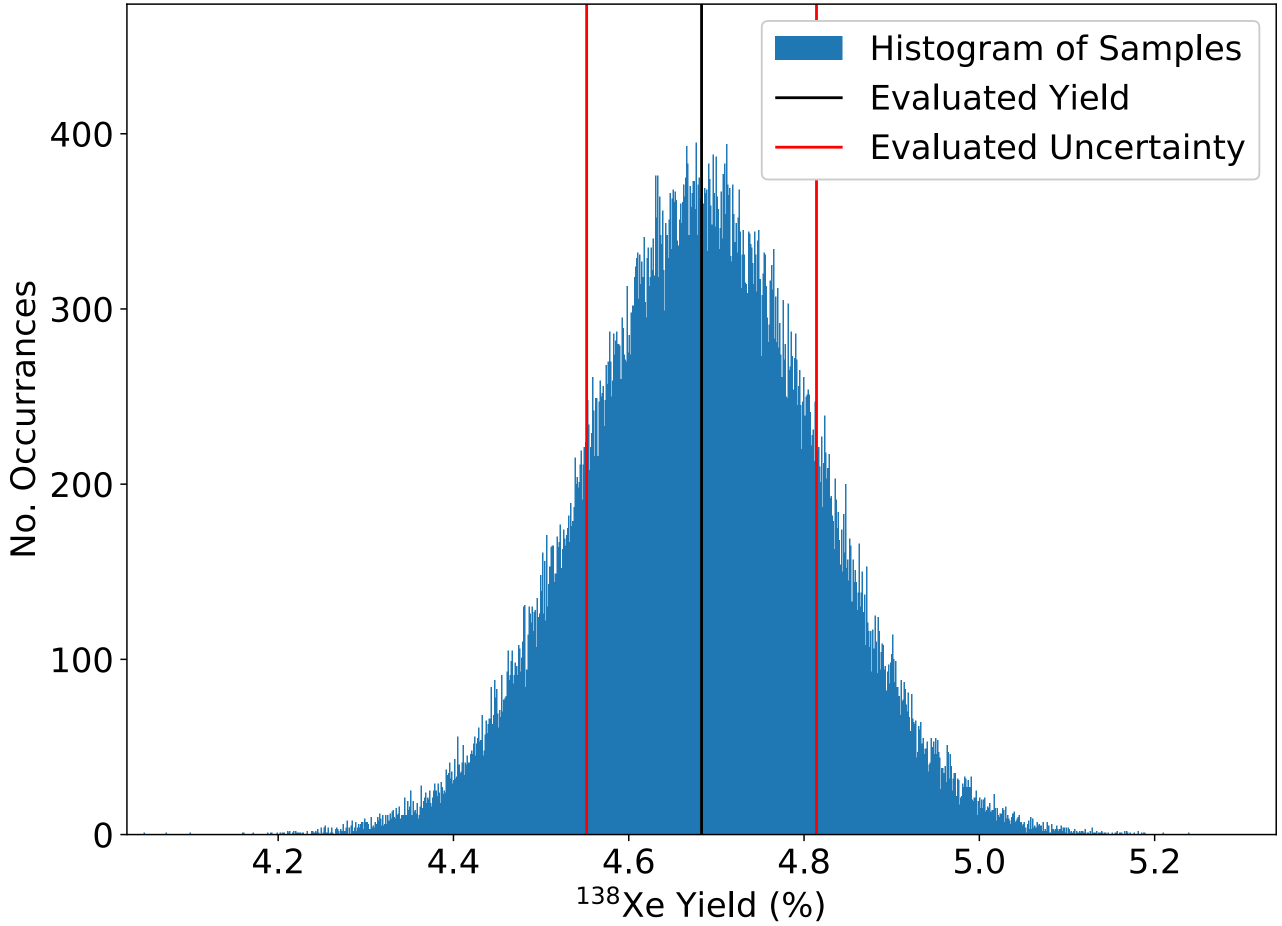
Bootstrapping

- Bootstrapping is a Monte-Carlo method for uncertainty estimation and propagation.
- Given a dataset with characterized uncertainty; one builds a new series of datasets by resampling the original one.
  - This can be used to assess uncertainties and covariance in an output calculation by varying the input data.
  - It could also be used to assess covariances between the values in the original dataset.

Field specific resource: “An introduction to bootstrap for nuclear physics” – A. Pastore (2019)

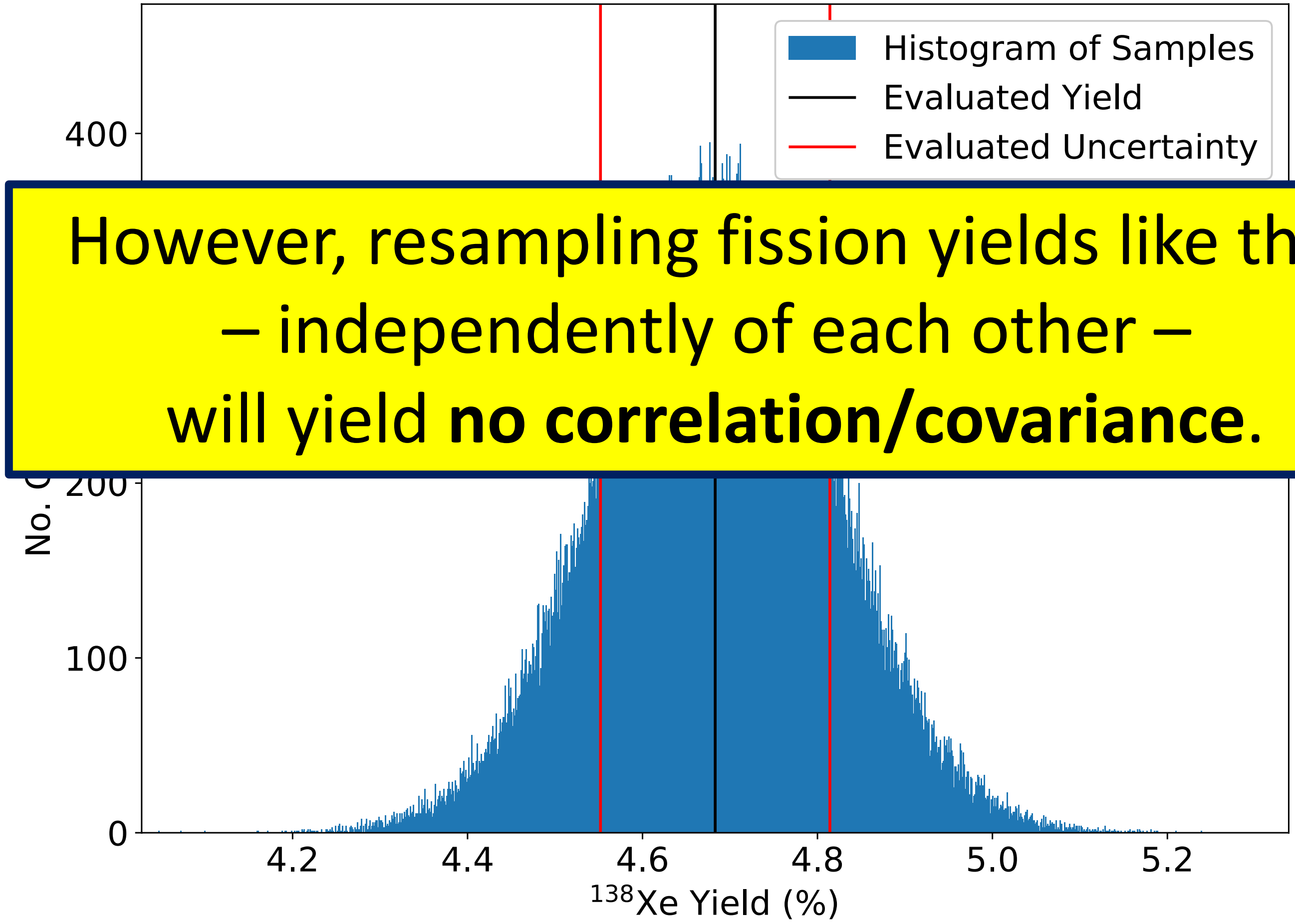
Bootstrapping

- Covariances between fission yields can be generated by statistically resampling fission yields about their evaluated uncertainties:



Bootstrapping

- Covariances between fission yields can be generated by statistically resampling fission yields about their evaluated uncertainties:



However, resampling fission yields like this – independently of each other – will yield **no correlation/covariance**.

Conserved Relationships

- In order to obtain correlation, conserved quantities can be enforced upon a set of resampled fission yields [1]:

Total Yield:

$$\sum_i Y_i = 2$$

[1] - Generation of Fission Yield Covariances to Correct Discrepancies in the JEFF Fission Yield Library – L. Fiorito et al. (2015) - https://www.oecd-nea.org/science/wpec/sg37/Meetings/2015_May/SG37_8_LF.pdf

Conserved Relationships

- In order to obtain correlation, conserved quantities can be enforced upon a set of resampled fission yields [1]:

Total Yield:

$$\sum_i Y_i = 2$$

Total Charge:

$$\sum_i Z_i Y_i = Z_{CN}$$

[1] - Generation of Fission Yield Covariances to Correct Discrepancies in the JEFF Fission Yield Library – L. Fiorito et al. (2015) - https://www.oecd-nea.org/science/wpec/sg37/Meetings/2015_May/SG37_8_LF.pdf

Conserved Relationships

- In order to obtain correlation, conserved quantities can be enforced upon a set of resampled fission yields [1]:

Total Yield:

$$\sum_i Y_i = 2$$

Total Charge:

$$\sum_i Z_i Y_i = Z_{CN}$$

Total Mass:

$$\sum_i A_i Y_i = A_{CN} - \bar{\nu}$$

[1] - Generation of Fission Yield Covariances to Correct Discrepancies in the JEFF Fission Yield Library – L. Fiorito et al. (2015) - https://www.oecd-nea.org/science/wpec/sg37/Meetings/2015_May/SG37_8_LF.pdf

Conserved Relationships

- In order to obtain correlation, conserved quantities can be enforced upon a set of resampled fission yields [1]:

Total Yield:

$$\sum_i Y_i = 2$$

Total Charge:

$$\sum_i Z_i Y_i = Z_{CN}$$

Total Mass:

$$\sum_i A_i Y_i = A_{CN} - \bar{\nu}$$

Mass Yields:

$$\sum_i Y_i(A) = Y_m(A)$$

[1] - Generation of Fission Yield Covariances to Correct Discrepancies in the JEFF Fission Yield Library – L. Fiorito et al. (2015) - https://www.oecd-nea.org/science/wpec/sg37/Meetings/2015_May/SG37_8_LF.pdf

Conserved Relationships

- In order to obtain correlation, conserved quantities can be enforced upon a set of resampled fission yields [1]:

Total Yield:

$$\sum_i Y_i = 2$$

Total Charge:

$$\sum_i Z_i Y_i = Z_{CN}$$

Total Mass:

$$\sum_i A_i Y_i = A_{CN} - \bar{\nu}$$

Mass Yields:

$$\sum_i Y_i(A) = Y_m(A)$$

Charge Parity:

$$\sum_i Y_i(Z_1, A_i) = \sum_i Y_i(Z_{CN} - Z_1, A_i)$$

[1] - Generation of Fission Yield Covariances to Correct Discrepancies in the JEFF Fission Yield Library – L. Fiorito et al. (2015) - https://www.oecd-nea.org/science/wpec/sg37/Meetings/2015_May/SG37_8_LF.pdf

Conserved Relationships

- In order to obtain correlation, conserved quantities can be enforced upon a set of resampled fission yields [1]:

Total Yield:

$$\sum_i Y_i = 2$$

Total Charge:

$$\sum_i Z_i Y_i = Z_{CN}$$

Total Mass:

$$\sum_i A_i Y_i = A_{CN} - \bar{\nu}$$

Mass Yields:

$$\sum_i Y_i(A) = Y_m(A)$$

Charge Parity:

$$\sum_i Y_i(Z_1, A_i) = \sum_i Y_i(Z_{CN} - Z_1, A_i)$$

Mass Symmetry:

$$\sum_{A_i > \frac{A_{CN} - \bar{\nu}}{2}} Y_i(A_i) = 1$$

[1] - Generation of Fission Yield Covariances to Correct Discrepancies in the JEFF Fission Yield Library – L. Fiorito et al. (2015) - https://www.oecd-nea.org/science/wpec/sg37/Meetings/2015_May/SG37_8_LF.pdf

Conserved Relationships

- In order to obtain correlation, conserved quantities can be enforced upon a set of resampled fission yields [1]:

Total Yield:

$$\sum_i Y_i = 2$$

Total Charge:

$$\sum_i Z_i Y_i = Z_{CN}$$

Total Mass:

$$\sum_i A_i Y_i = A_{CN} - \bar{\nu}$$

Mass Yields:

$$\sum_i Y_i(A) = Y_m(A)$$

Charge Parity:

This relationship is only approximately conserved. It is debatable whether it is a valid condition. Nevertheless, it is exploited in order to help conserve the other 5 relationships.

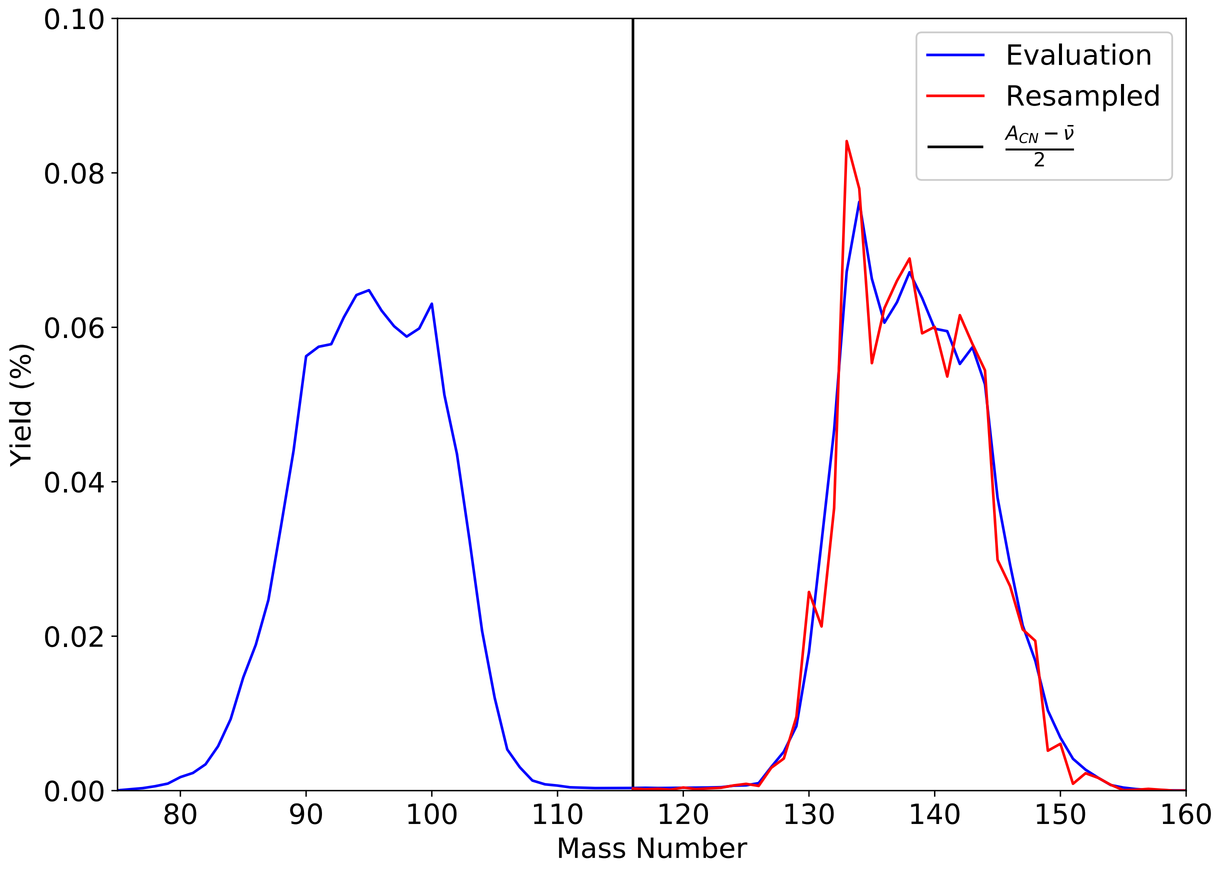
Mass Symmetry:

$$\sum_{A_i > \frac{A_{CN} - \bar{\nu}}{2}} Y_i(A_i) = 1$$

[1] - Generation of Fission Yield Covariances to Correct Discrepancies in the JEFF Fission Yield Library – L. Fiorito et al. (2015) - https://www.oecd-nea.org/science/wpec/sg37/Meetings/2015_May/SG37_8_LF.pdf

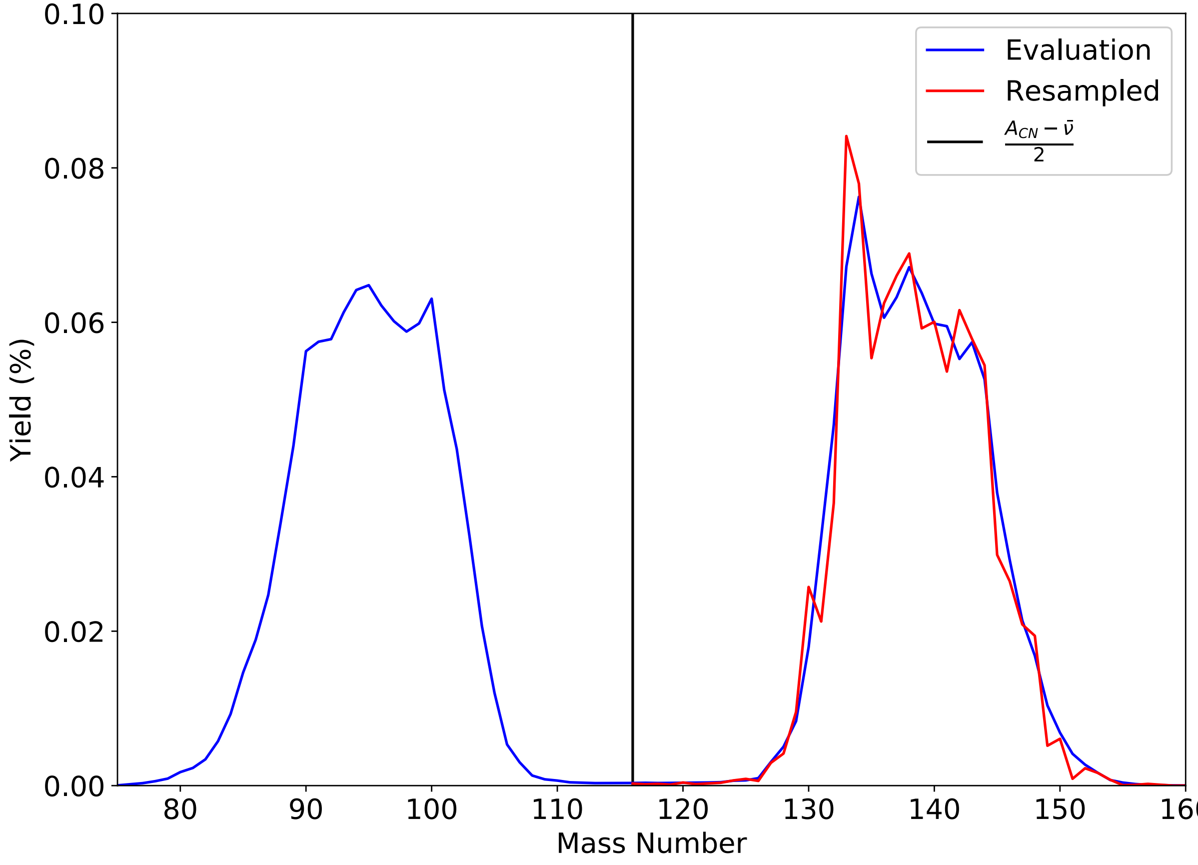
FY Covariance Matrix Generation

- The way in which a set of fission yields are resampled can be structured to conserve these relationships:
- **1)** Randomly selected the "light" or "heavy" side of the fission product spectrum to resample.
- **2)** Randomly select (weighted by uncertainty) a product in each A chain, resample its yield about its evaluated uncertainty.
- **3)** Scale all other yields in that A chain by the same percent change.



FY Covariance Matrix Generation

- The way in which a set of fission yields are resampled can be structured to conserve these relationships:
- **1)** Randomly selected the "light" or "heavy" side of the fission product spectrum to resample.
- **2)** Randomly select (weighted by uncertainty) a product in each A chain, resample its yield about its evaluated uncertainty.
- **3)** Scale all other yields in that A chain by the same percent change.



Step 3 is allowed if the Z distribution for a given A is Gaussian, which empirical data and the E&R evaluation supports [1].

[1] – Evaluation and Compilation of Fission Product Yields – T.R. England and B.F. Rider (1994)

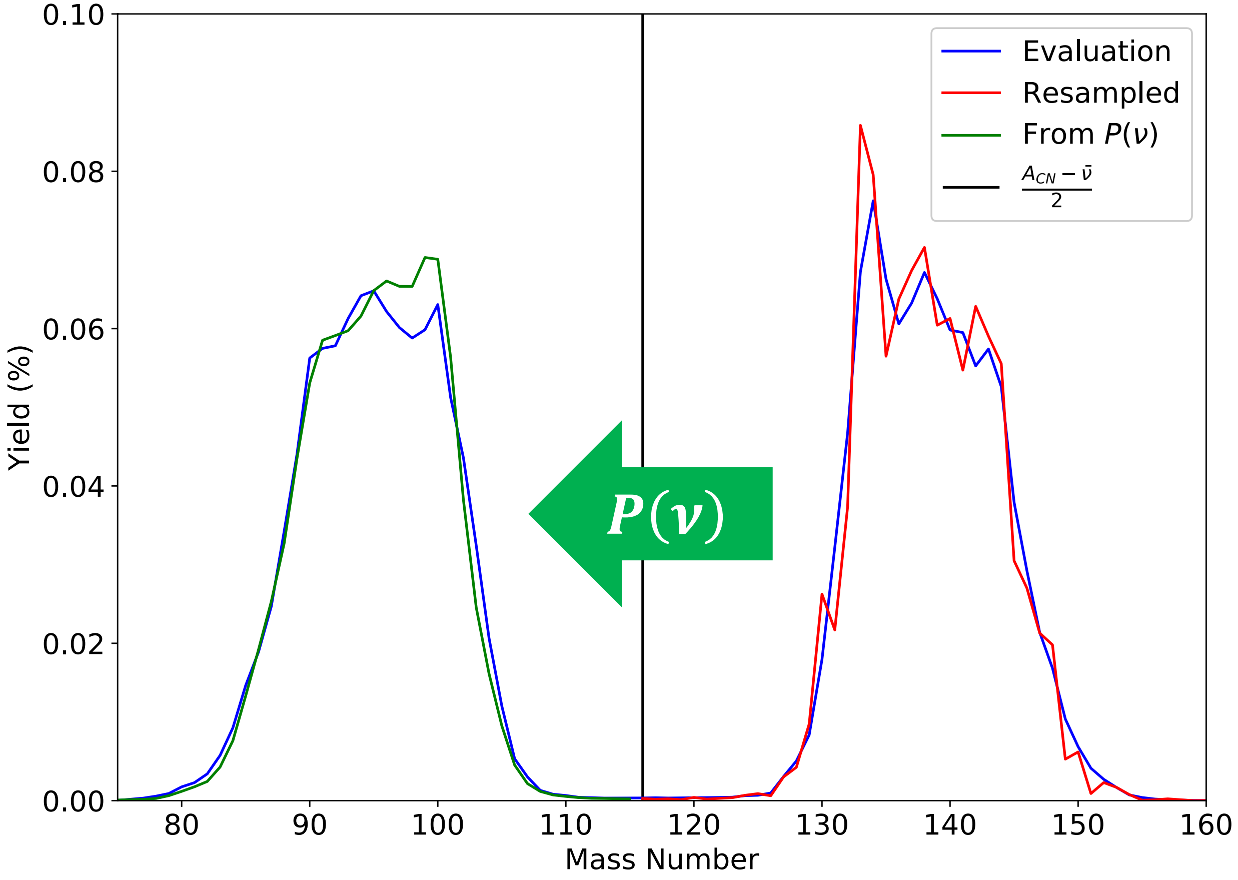
FY Covariance Matrix Generation

- **4)** Normalize the resampled yields such that they sum to 1.
- **5)** Generate the fission yields on the complementary side of the fission product spectrum using the neutron multiplicity of the compound system.

$$Y_{frac}(Z_{CN} - Z, A_{CN} - A - \nu) = P(\nu)\, Y(Z, A)$$

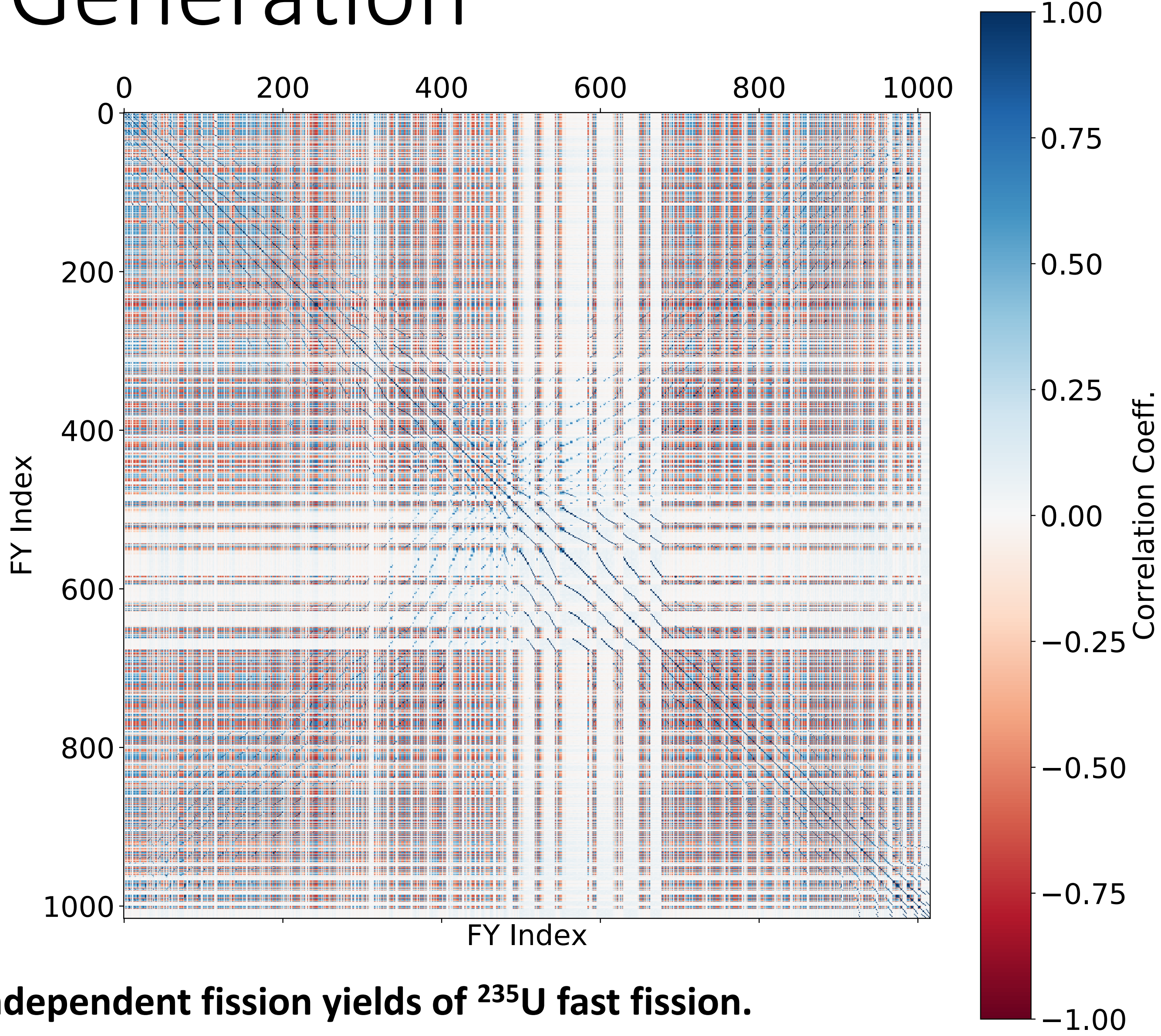
$$Y(Z_{CN} - Z, A_i) = \sum_{\nu} Y_{frac}(Z_{CN} - Z, A_i)$$

By Step 5 we've ensured all of the conservation rules are met.



FY Covariance Matrix Generation

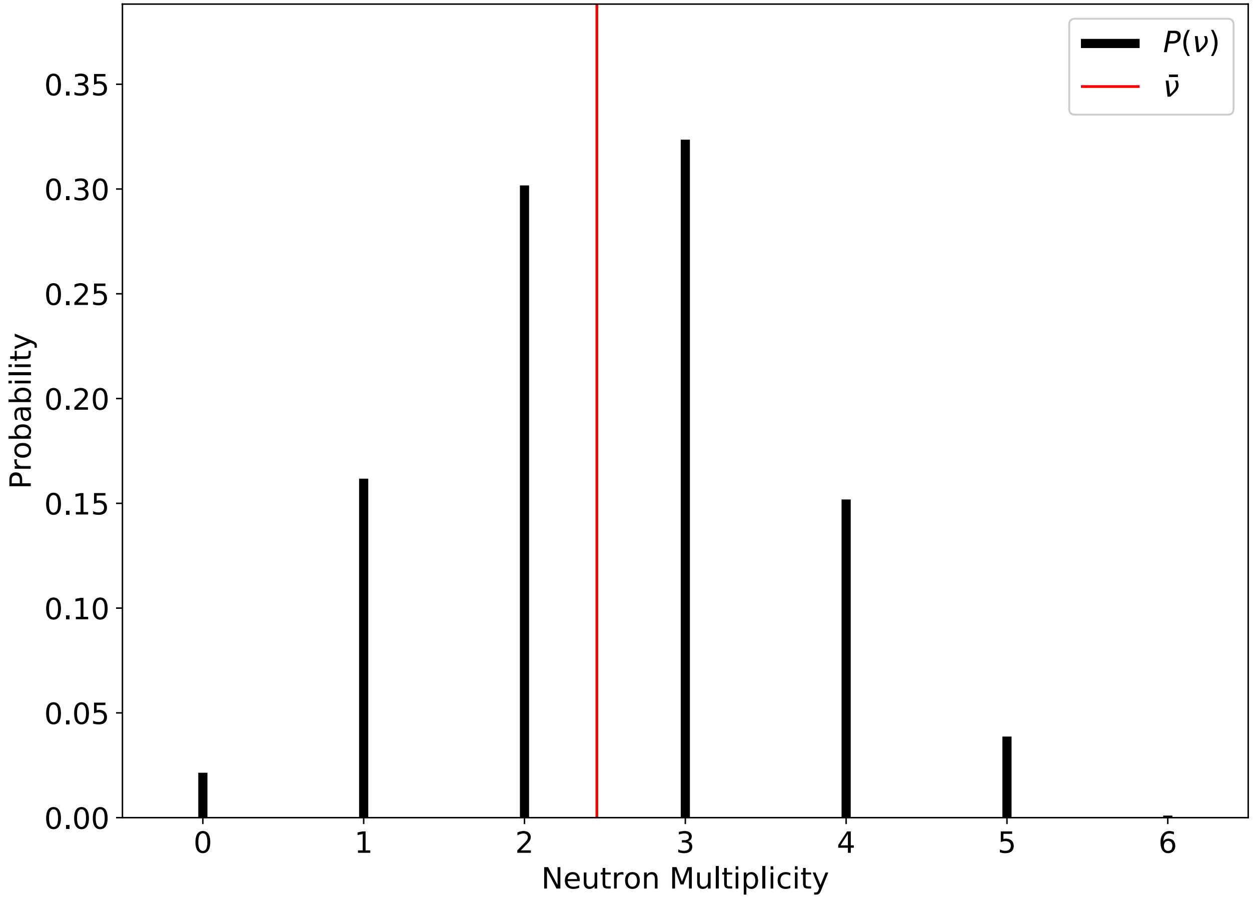
- **6)** Repeat steps 1-5) N times. Select N such that statistical noise is minimized.
- **7)** Calculate the resulting correlation matrix from the N trials.



Correlation matrix for independent fission yields of ^{235}U fast fission.

FY Covariance Matrix Generation

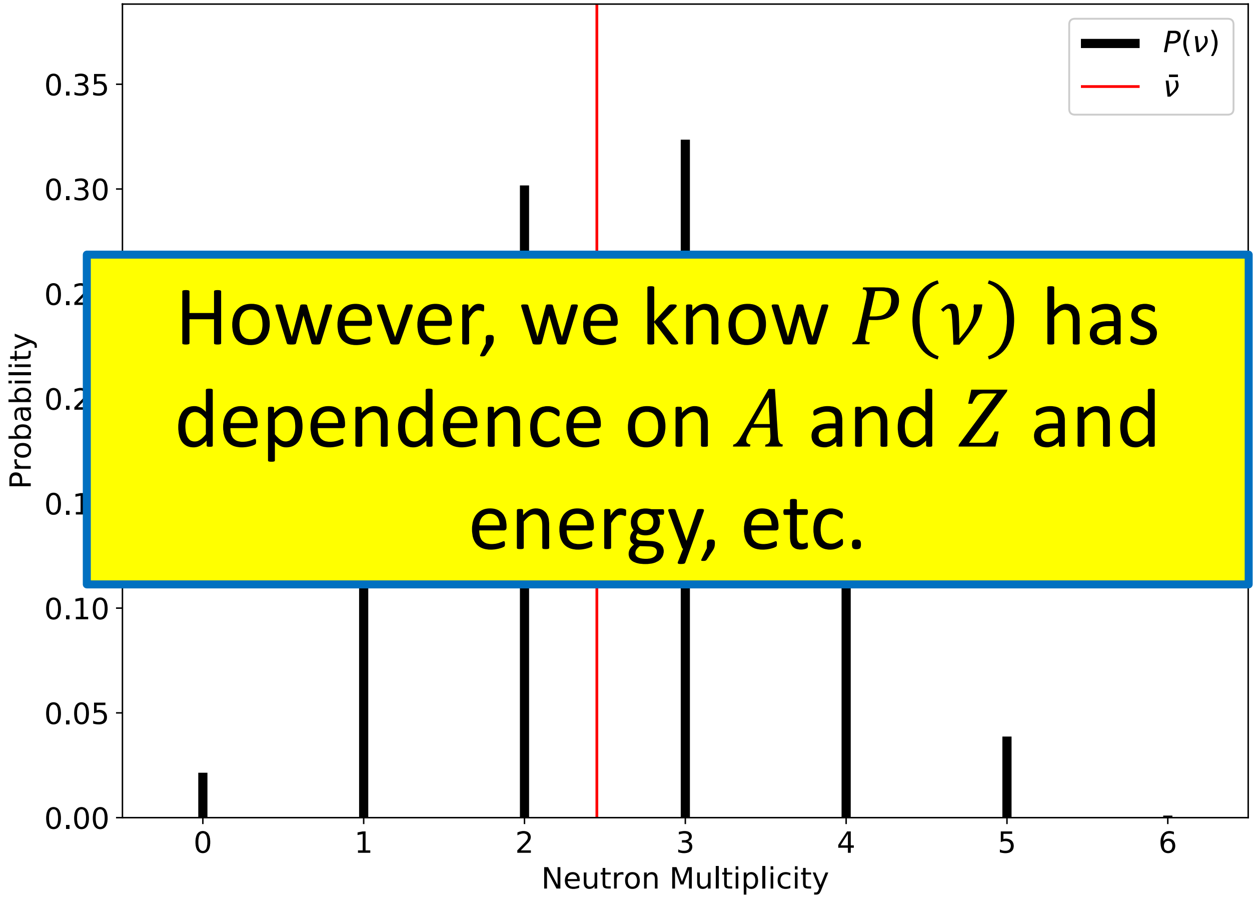
- The England and Rider evaluation does not make any mention of the neutron multiplicity distribution used for their evaluations.
- Thus we are left to assume a neutron multiplicity distribution that sufficiently matches the England and Rider evaluation.



Neutron Multiplicity for fast neutron induced fission of ^{235}U according to J.P. Lestone in LA-UR-05-0288.

FY Covariance Matrix Generation

- The England and Rider evaluation does not make any mention of the neutron multiplicity distribution used for their evaluations.
- Thus we are left to assume a neutron multiplicity distribution that sufficiently matches the England and Rider evaluation.



However, we know $P(\nu)$ has dependence on A and Z and energy, etc.

Neutron Multiplicity for fast neutron induced fission of ^{238}U according to J.P. Lestone in LA-UR-05-0288.

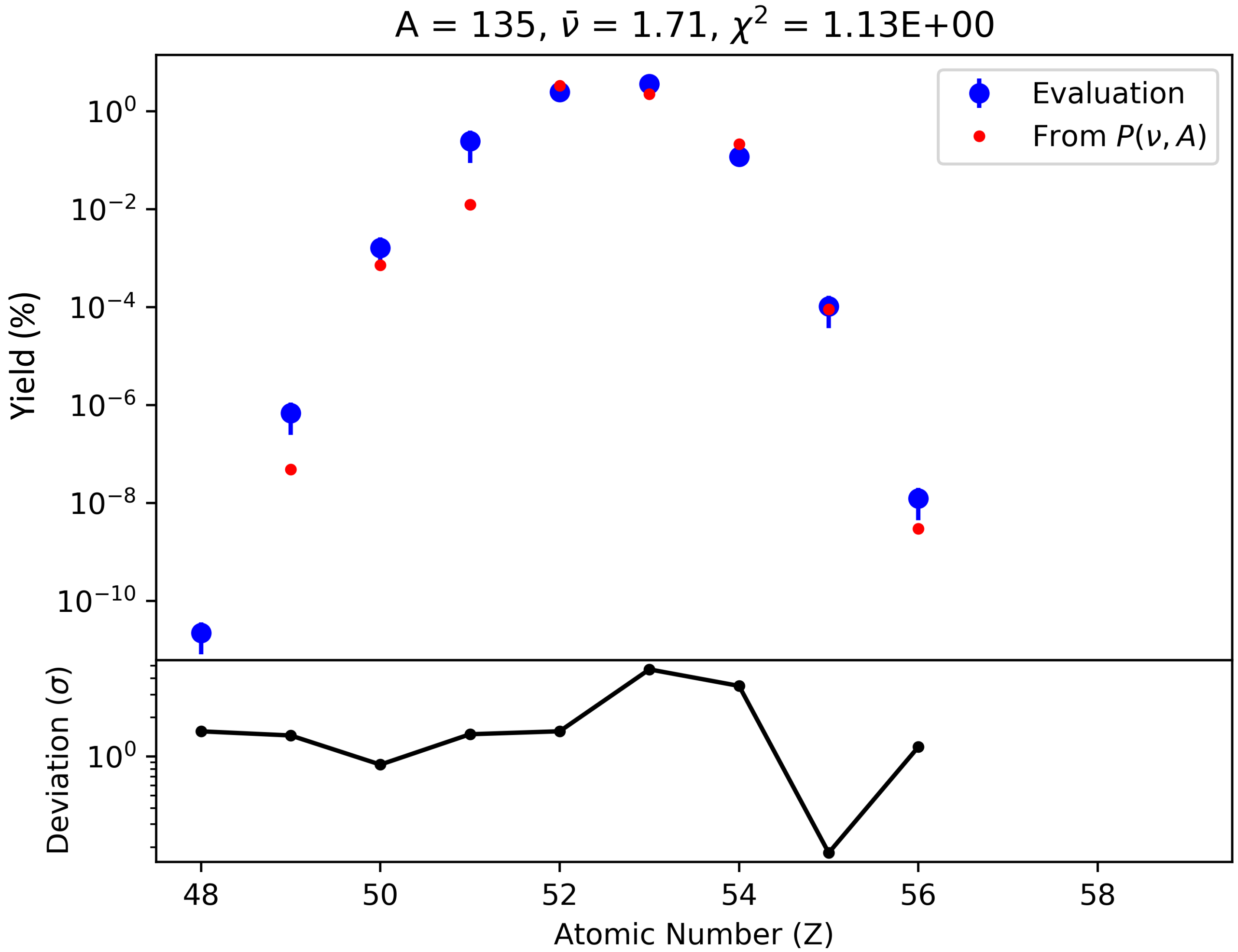
E&R Consistent $P(\nu, A)$ Data

- $P(\nu, A)$ can be fitted to the England and Rider evaluation in order to obtain the best degree of consistency.
- A truncated Gaussian is used to fit the shape of the $P(\nu)$ distribution for each A chain.
- Select $P(\nu, A)$ that minimizes χ^2 between evaluated yields and "recalculated yields", $Y'(Z, A)$

$$Y'(Z, A) = \sum_{\nu} P(\nu, A)\, Y(Z_{CN} - Z, A_{CN} - A - \nu)$$

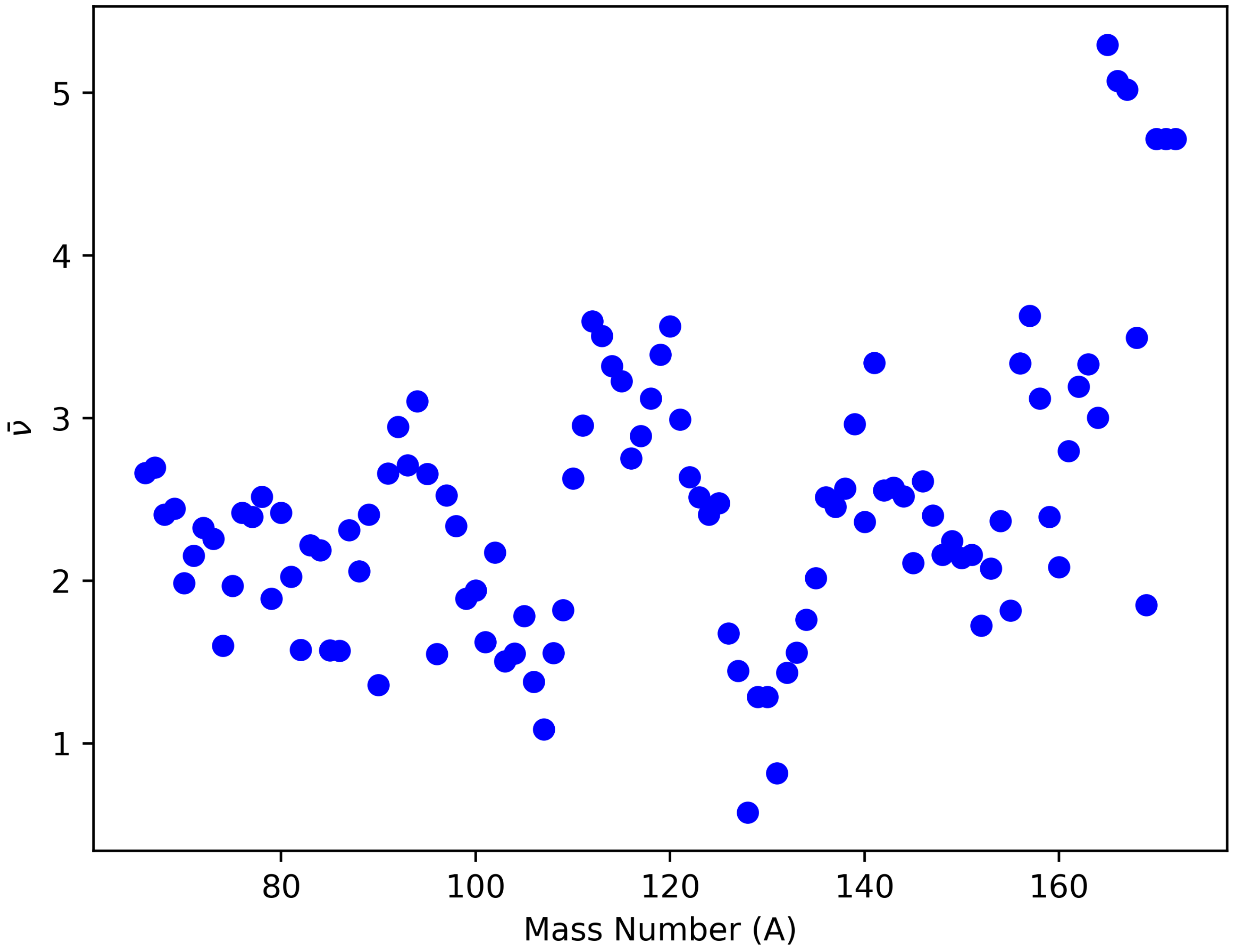
E&R Consistent $P(\nu, A)$ Data

Example:
Reproduction of evaluated yields to obtain $P(\nu, 135)$ for fast fission of ^{235}U.



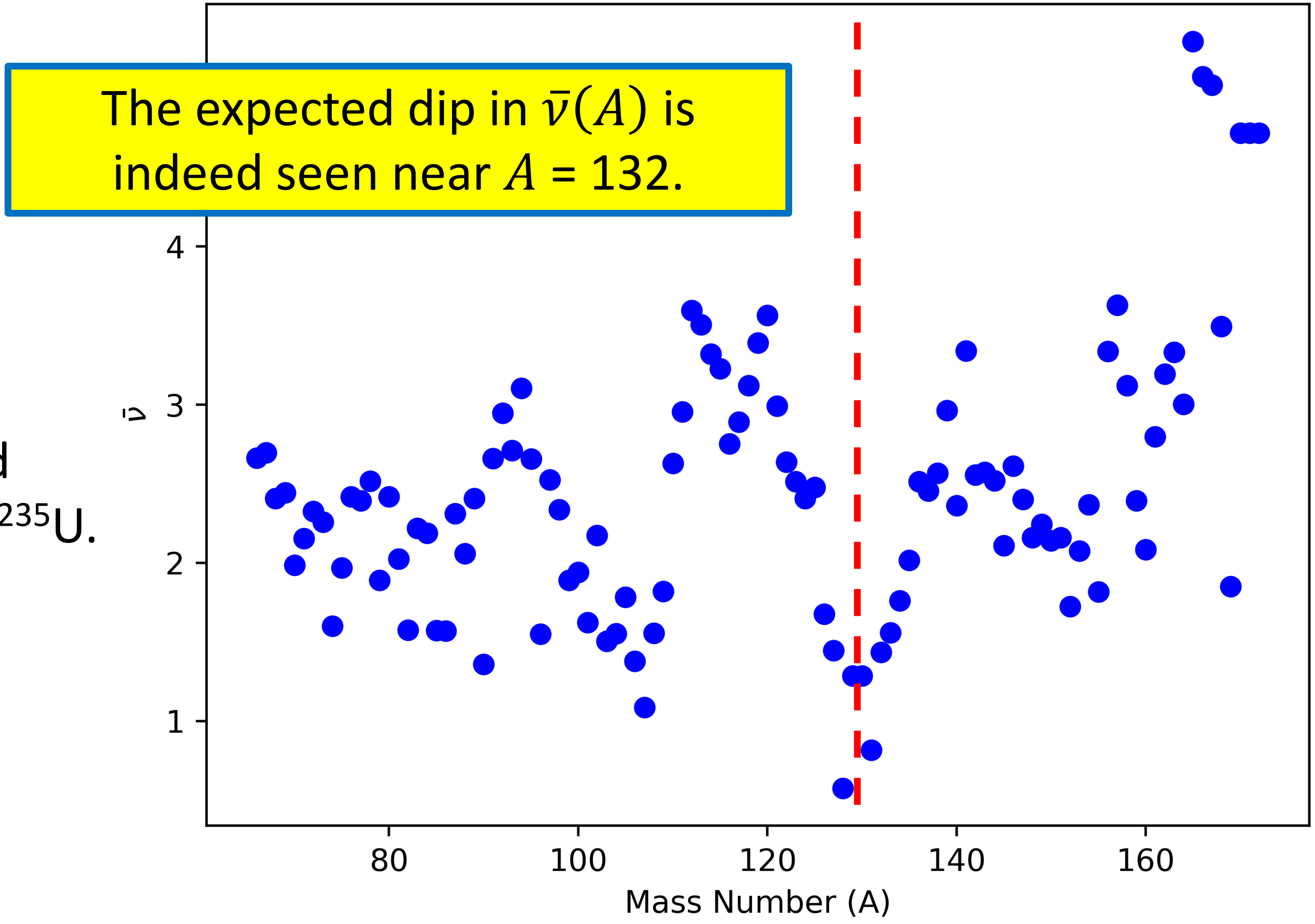
E&R Consistent $P(\nu, A)$ Data

Example:
$\bar{\nu}(A)$ obtained from fitted $P(\nu, A)$ for fast fission of ^{235}U.

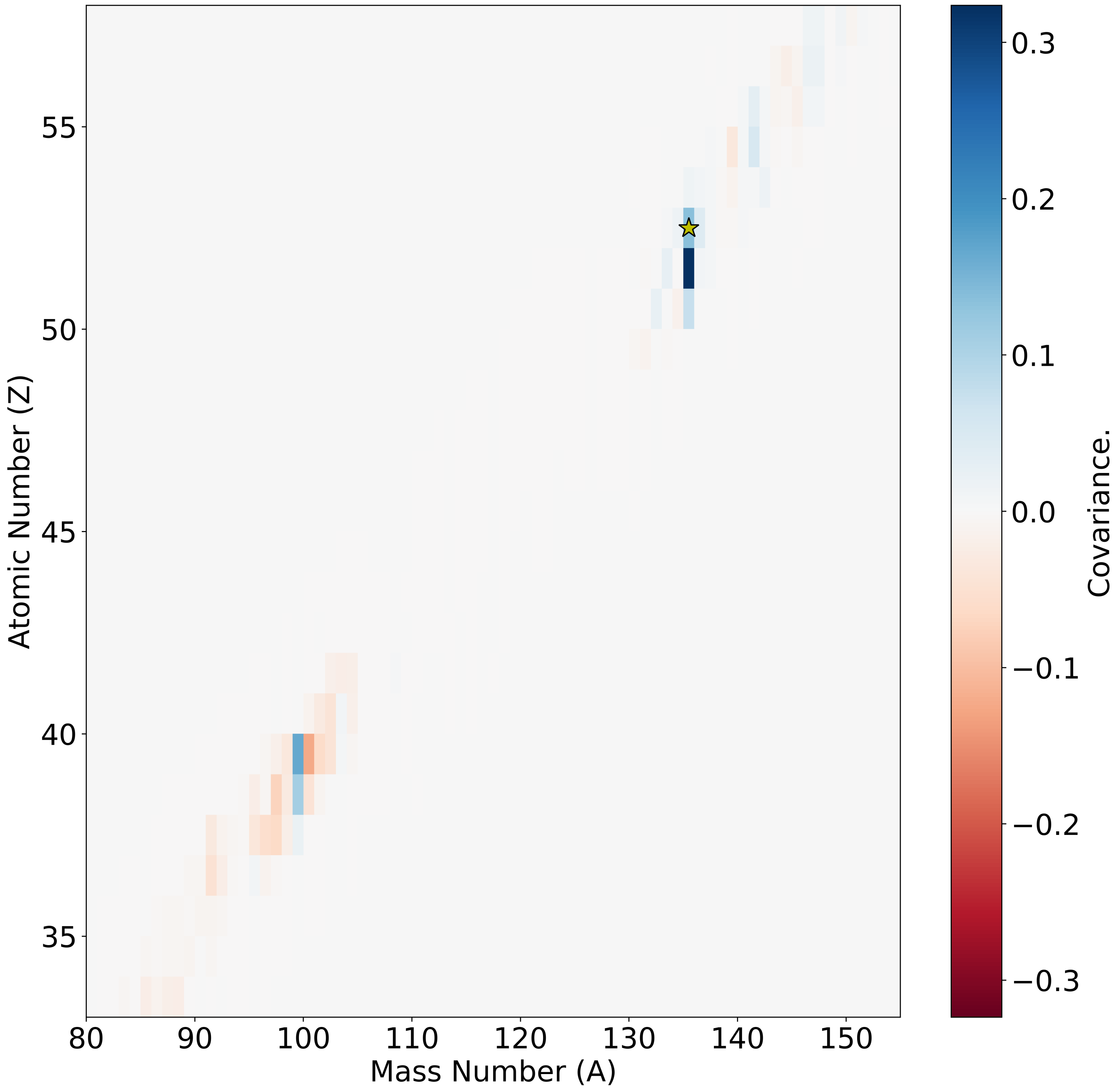


E&R Consistent $P(\nu, A)$ Data

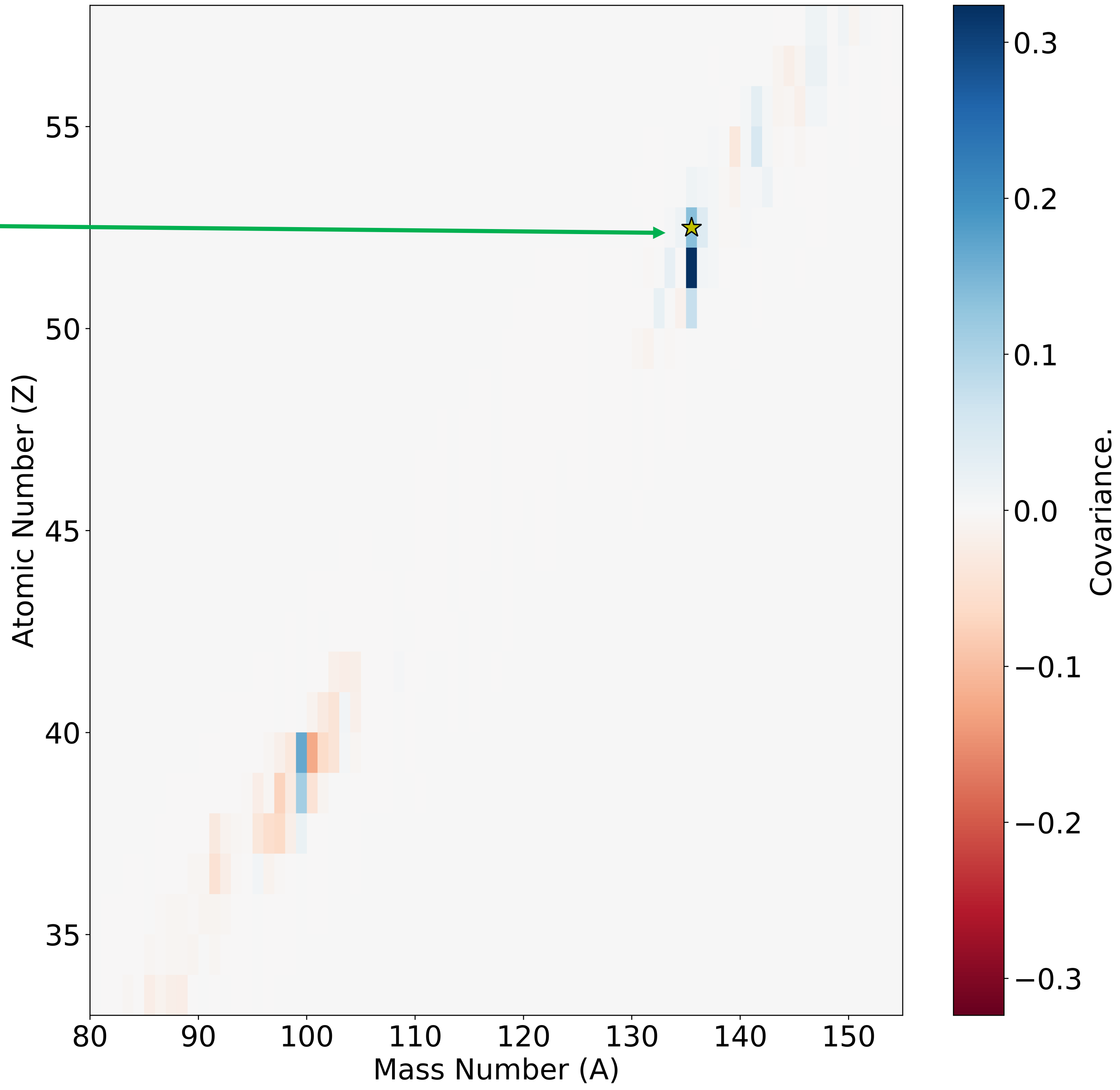
Example:
$\bar{\nu}(A)$ obtained from fitted $P(\nu, A)$ for fast fission of ^{235}U.



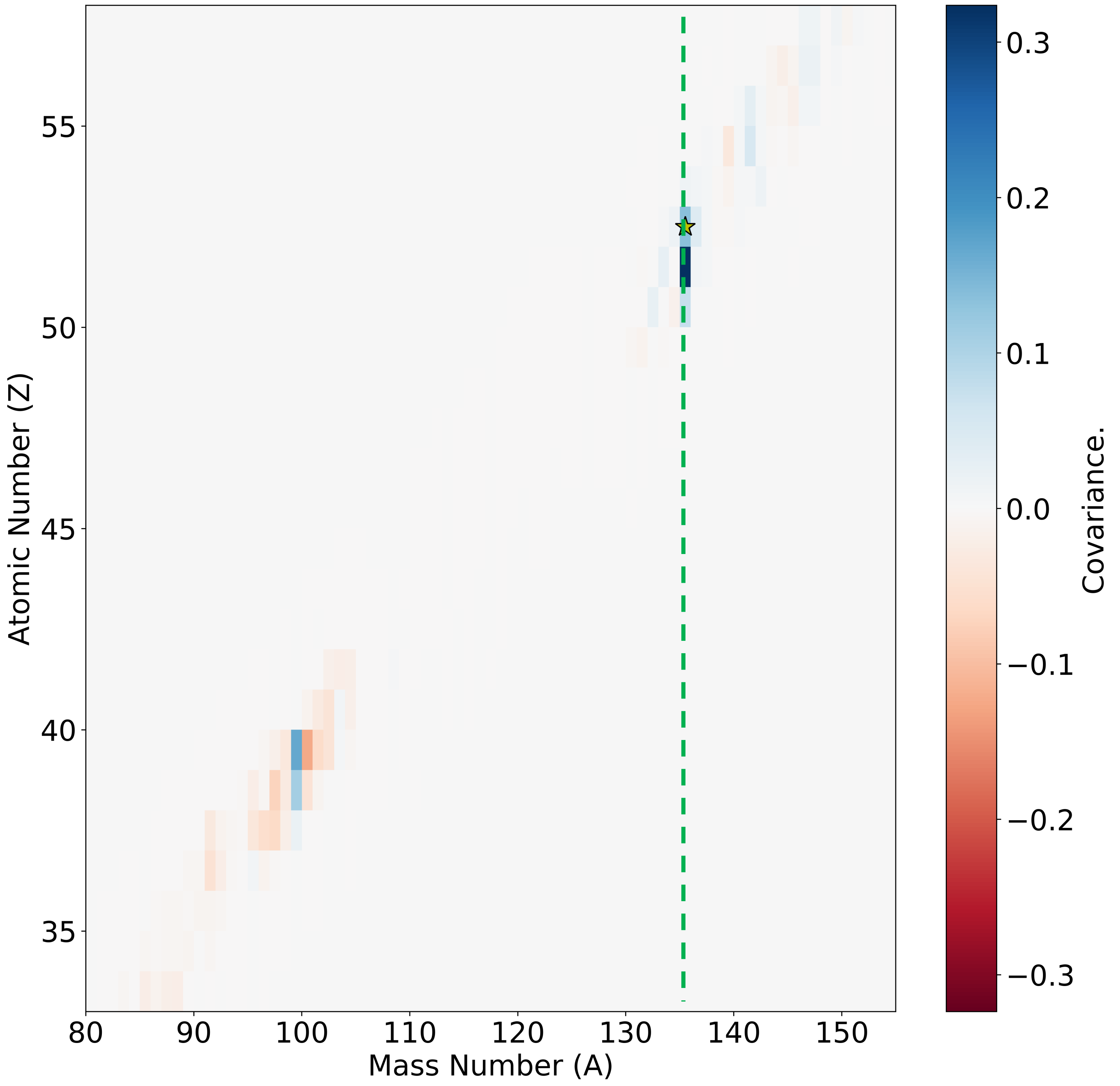
- **Example:** ^{135}Te
- Presented is the covariance between independent yields as function of Z and A and that of ^{135}Te.
- The evaluated yield for ^{135}Te is $2.47 \pm 0.57\%$



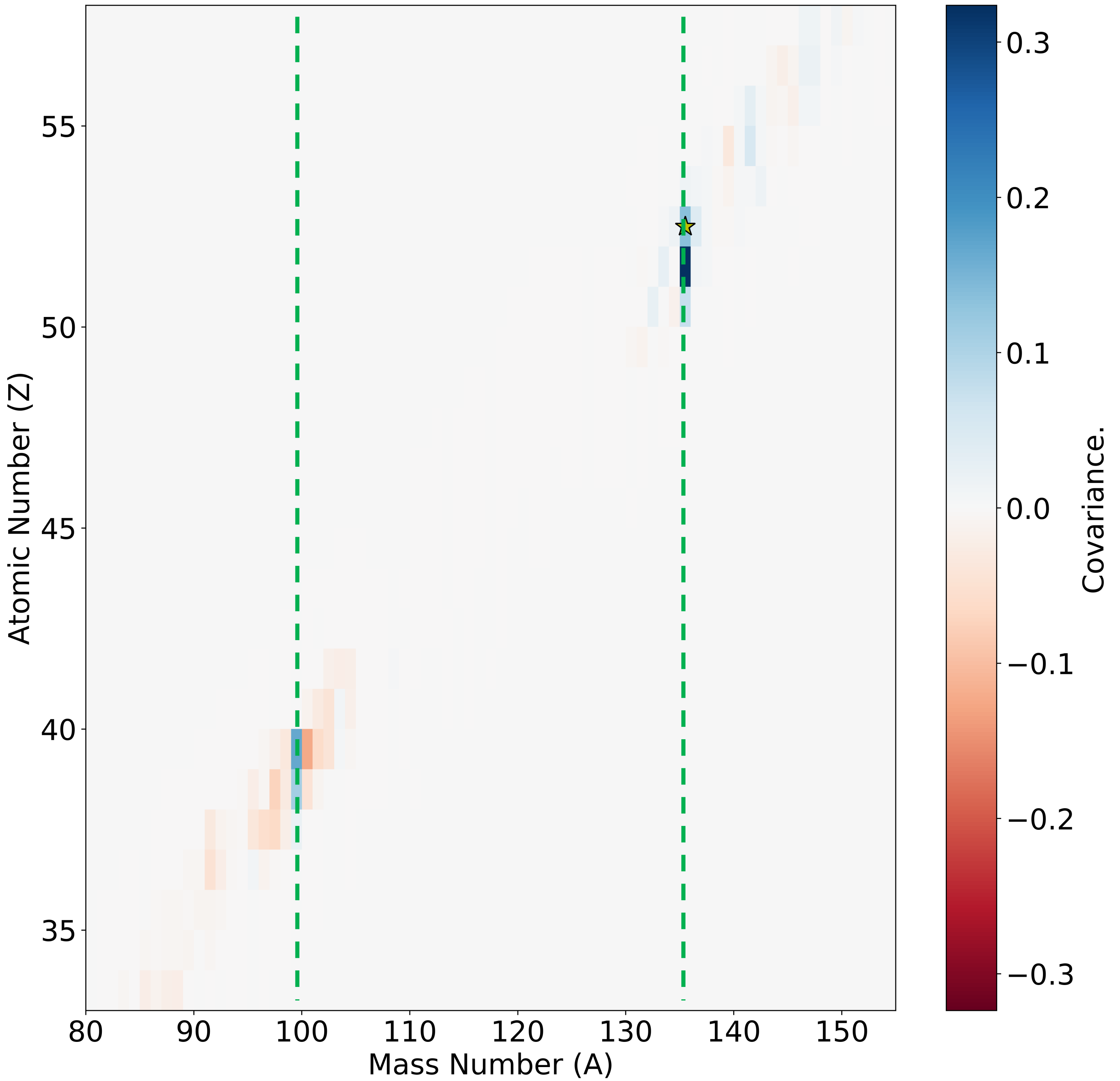
- **Features:**
- ^{135}Te is positively correlated with itself.



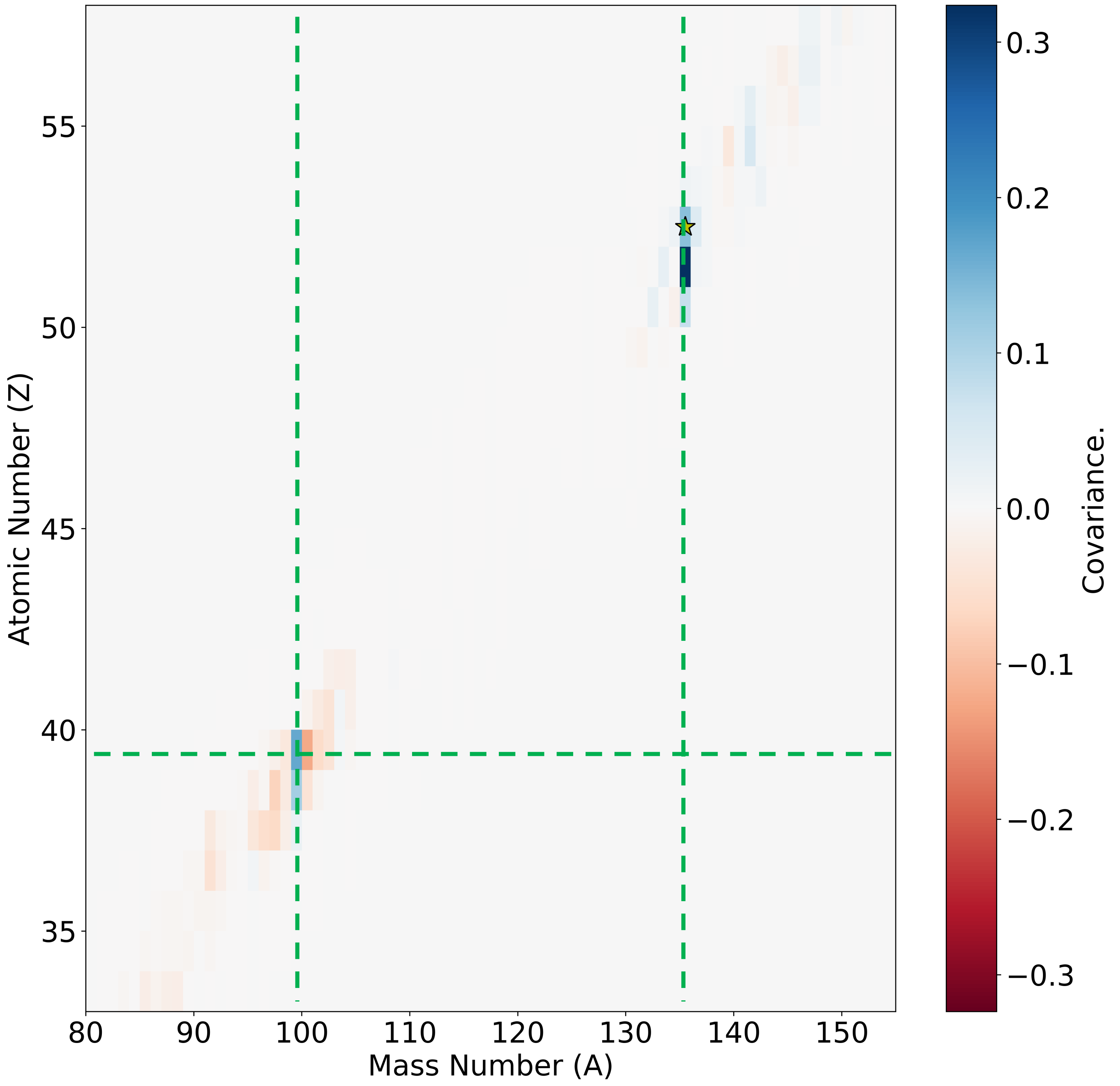
- **Features:**
- ^{135}Te is positively correlated with itself.
- Products along the A chain have positive correlation.



- **Features:**
- ^{135}Te is positively correlated with itself.
- Products along the A chain have positive correlation.
  - This positive correlation is reflected along a complementary $A = 99$ chain.



- **Features:**
- ^{135}Te is positively correlated with itself.
- Products along the A chain have positive correlation.
    - This positive correlation is reflected along a complementary $A = 99$ chain.
- Products along A chains that do not have complementary Z have negative correlation.

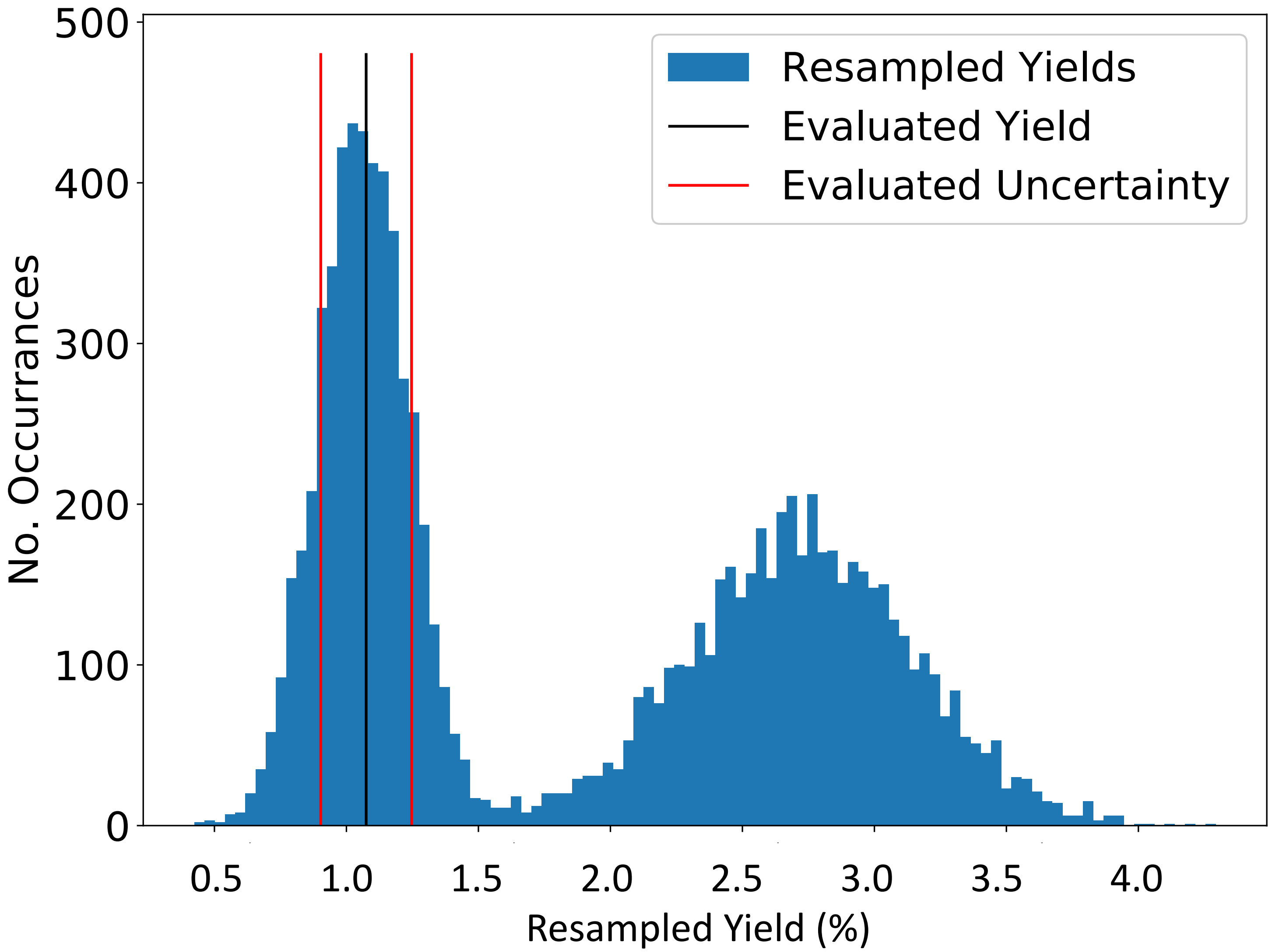


Issues and Challenges

- This choice of an A-independent $P(\nu)$ leads to bimodality in the distribution of resampled yields in this process.

<u>Example</u>: ^{132}Te

- One Gaussian from resampling starting on the heavy side and one from resampling starting on the light side.
- This simplistic $P(\nu)$ is not consistent with the neutron multiplicity of ^{132}Te.

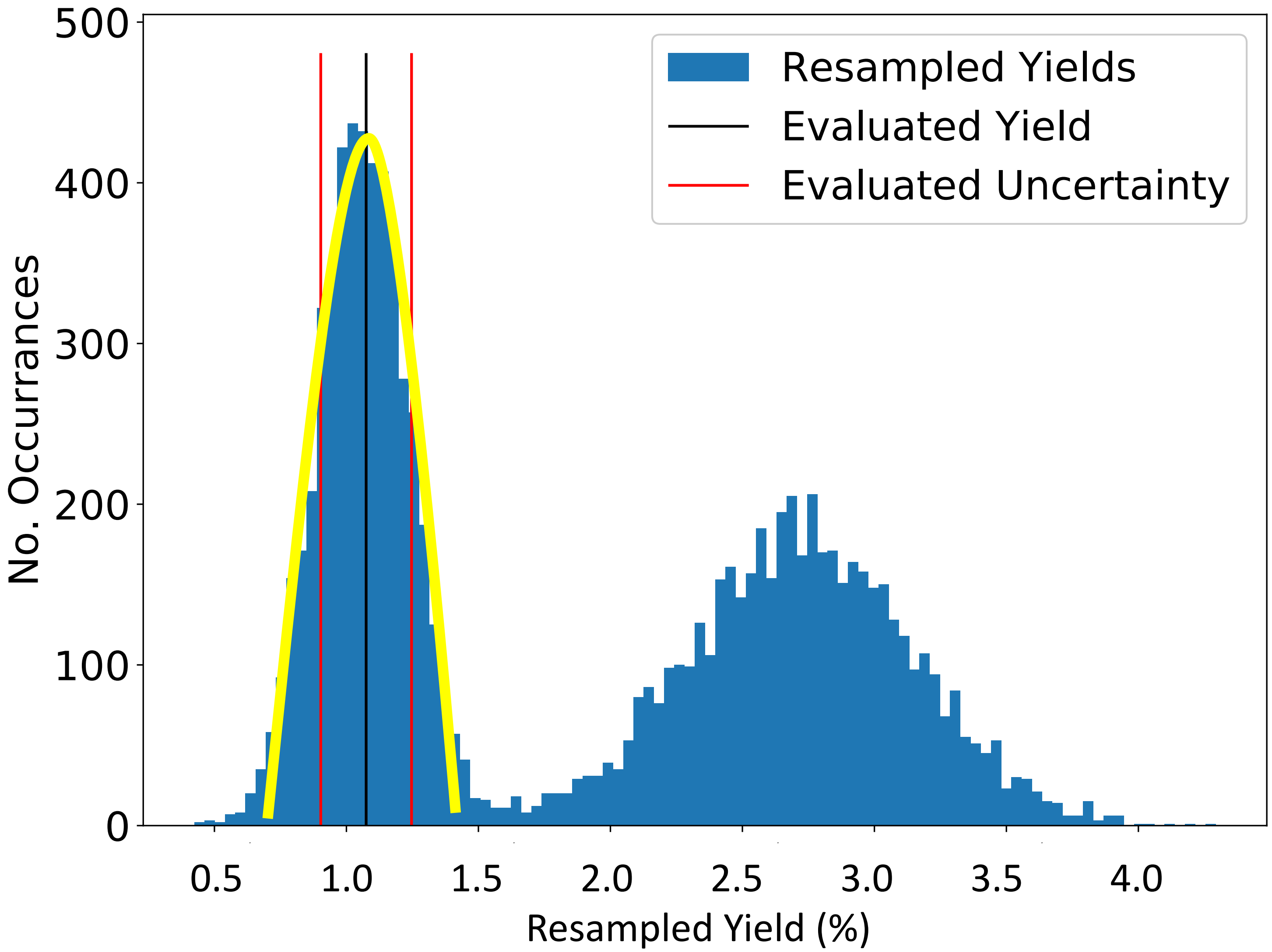


Issues and Challenges

- This choice of an A-independent $P(\nu)$ leads to bimodality in the distribution of resampled yields in this process.

Example: ^{132}Te

- One Gaussian from resampling starting on the heavy side and one from resampling starting on the light side.
- This simplistic $P(\nu)$ is not consistent with the neutron multiplicity of ^{132}Te.

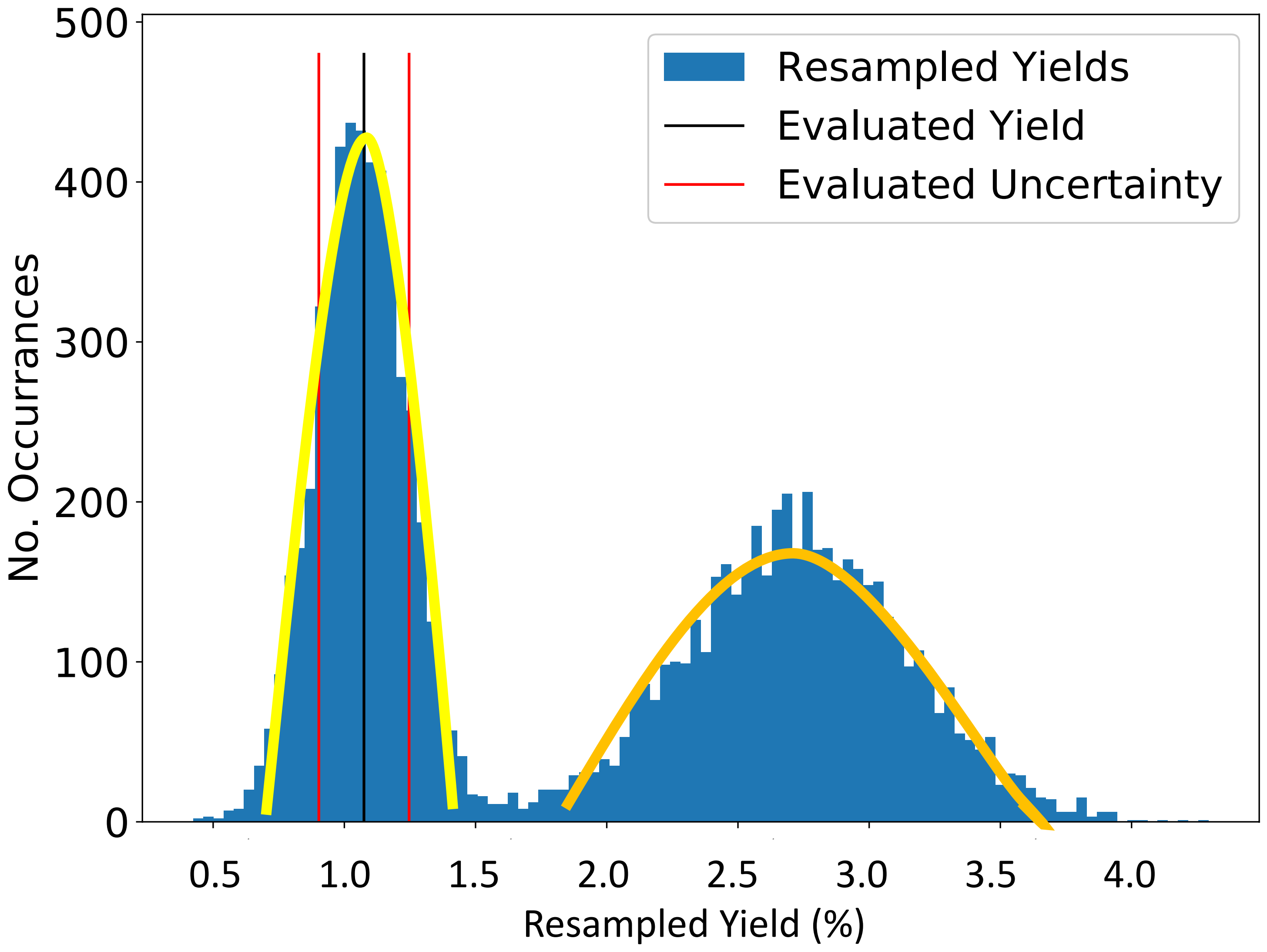


Issues and Challenges

- This choice of an A-independent $P(\nu)$ leads to bimodality in the distribution of resampled yields in this process.

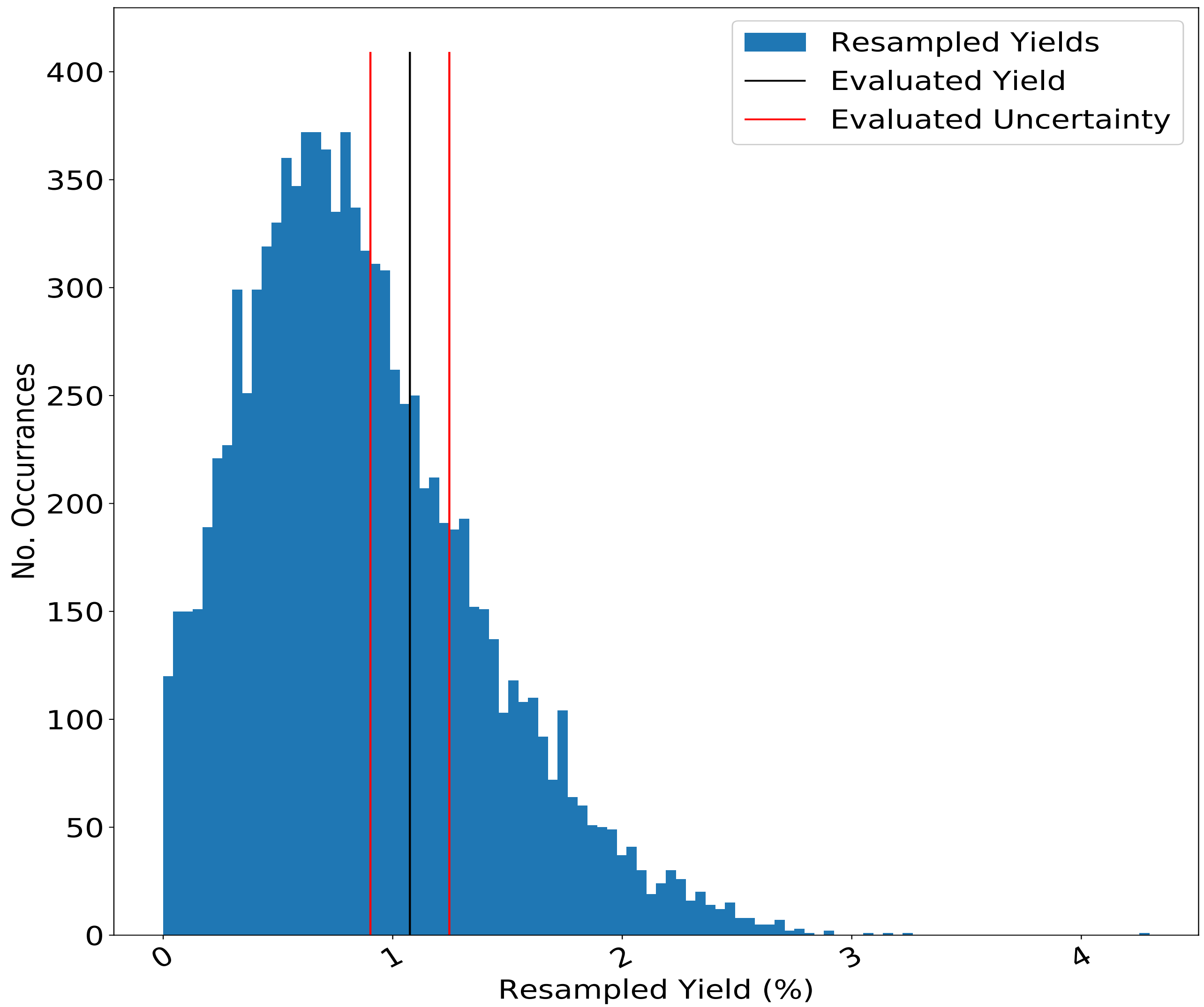
<u>Example</u>: ^{132}Te

- One Gaussian from resampling starting on the heavy side and one from resampling starting on the light side.
- This simplistic $P(\nu)$ is not consistent with the neutron multiplicity of ^{132}Te.



Issues and Challenges

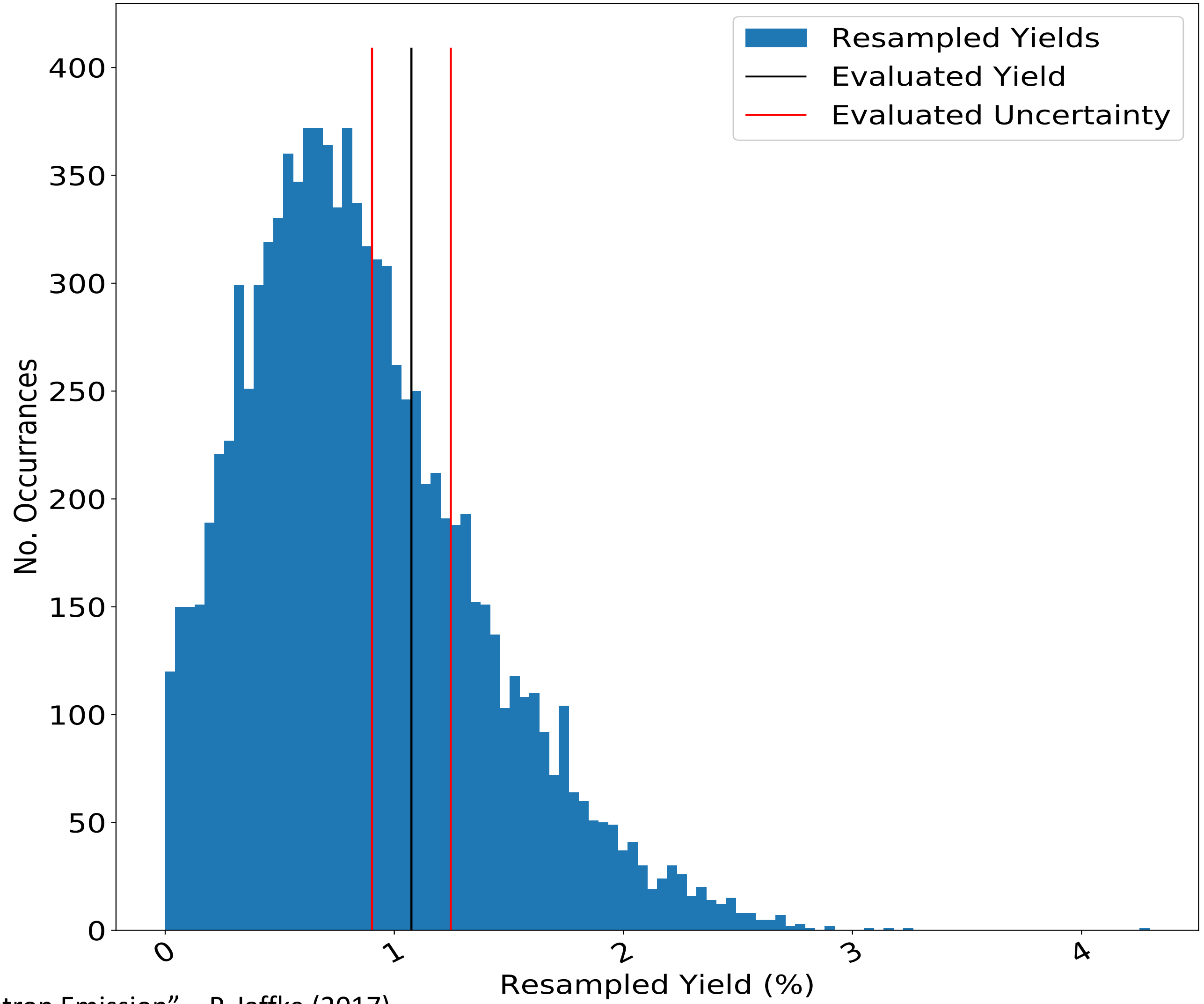
- The use of $P(\nu, A)$ data that was fitted to the England and Rider evaluation eliminates the bimodality in this example.
- The average of this distribution very closely matches the evaluated yield.



Issues and Challenges

- The use of $P(\nu, A)$ data that was fitted to the England and Rider evaluation eliminates the bimodality in this example.
- The average of this distribution very closely matches the evaluated yield.

- Inconsistency of $P(\nu)$ / $P(\nu, A)$ with the E&R evaluation is a known issue.
- Jaffke (2017) previously noted this issue [1].



[1] – "Identifying Inconsistencies in Fission Product Yield Evaluations with Prompt Neutron Emission" – P. Jaffke (2017)

Issues and Challenges

- Partial correlations between A chains on same side of the fission product distribution are uncharacterized.
- This is because yields along each A chain are sampled independently of each other.
- Methods to introduce correlations between A chains on the same side of the distribution while introducing minimal fission model dependence will be investigated.

Conclusions

- A model-agnostic method for independent fission yield covariance matrix generation is being developed.
- **This method has been successfully applied to all 61 compound systems in the England and Rider evaluation.**
- Initial results demonstrate expected behavior and trends.
- Final results will serve as an interim solution for independent fission yield covariance matrices until a new evaluation is completed.
  - Results will be made publicly available through publication appendices and will be accessible at nucleardata.berkeley.edu.

Future Work

- Perform validation checks and compare covariance matrices to those obtained by complementary generation methods.
- Obtain $P(\nu, A)$ distributions from FREYA and compare results to fitted $P(\nu, A)$ data.
    - Ramona Vogt and Jørgen Randup are working to provide this data.
    - This would introduce model dependence.
- Incorporate uncertainties on isomer-to-ground-state ratios from Madland and England (1977) [1].
    - While these ratios were used in the England and Rider evaluation the uncertainties from this publication were not explicitly mentioned.

[1] – "The Influence of Isomeric States on Independent Fission Product Yields" – Madland and England (1977)

Thank You!

Eric F. Matthews