Covariance work at LLNL

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LLNL/CNP Group

- Covariance data in XENDL
- Probability based uncertainty quantification

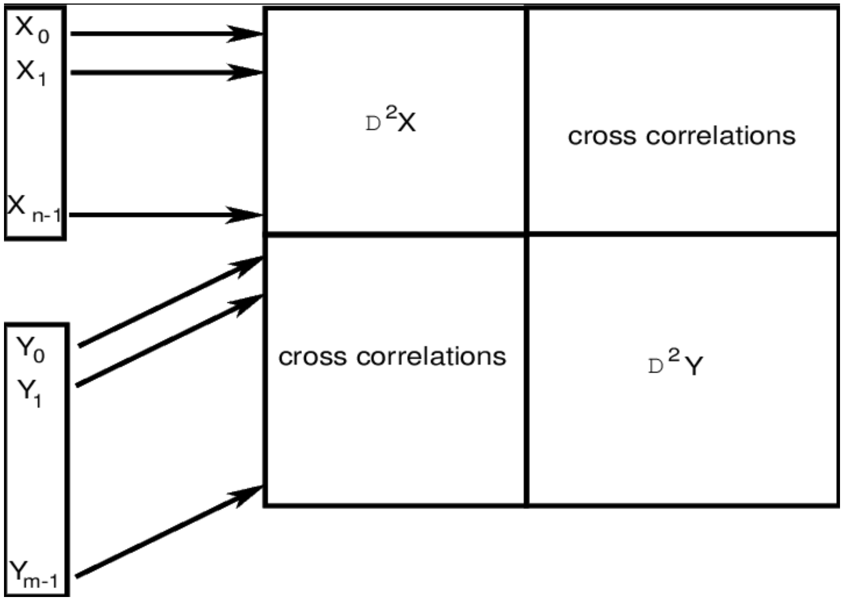
Covariance data in XEndl

- Covariance matrices can be large
  - Want a compact representation.
- Disparate data sets can be coupled
  - e.g., the ^{239}Pu(n,f) cross section is often measured relative to the ^{235}U(n,f) cross section
- Discovering which other data co-varies with a given datum is not straight forward.

We have developed data structures that address these issues

XEndl ideal tool to store complex data

- Have representation of matrices, vectors
- Linear algebra can be used to compress matrices
- Hyperlinks connect data to subspace of covariance matrix
- Can discover if two sets co-vary by comparing hyperlink URLs



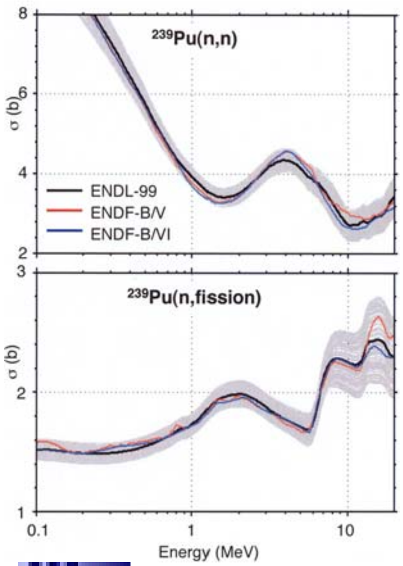
Variance of data may not obey Gaussian statistics and correlations may be non-linear

Target:

Probability distributions for metrics based on knowledge of the **nuclear data**

1.
Sample the nuclear data.

$L_i =$
$(\sigma_{i0}, \ldots, \sigma_{ik}, \ldots)$



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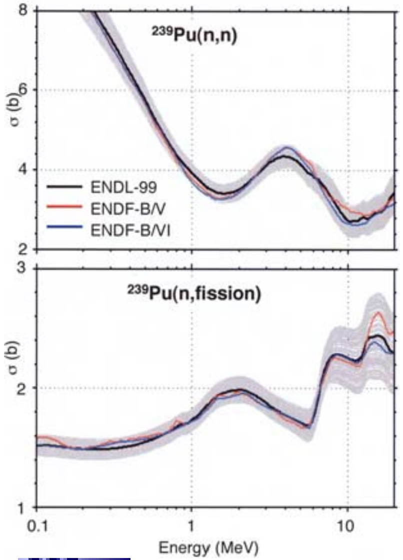
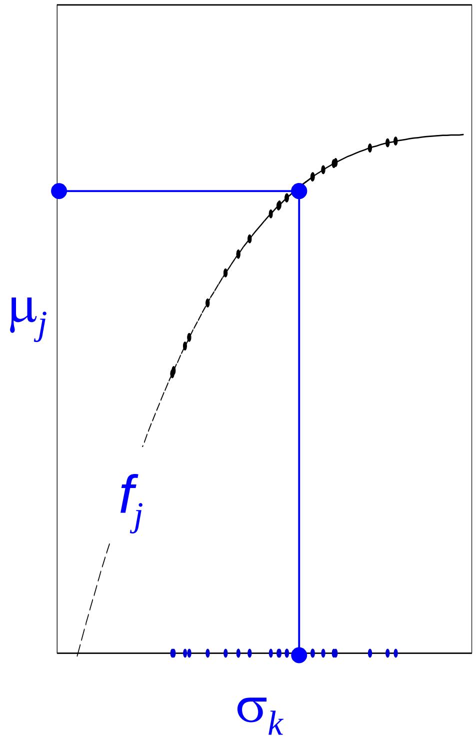
2.
Calculate metrics for each library.

$\mu_{ij} = f_j(L_i)$





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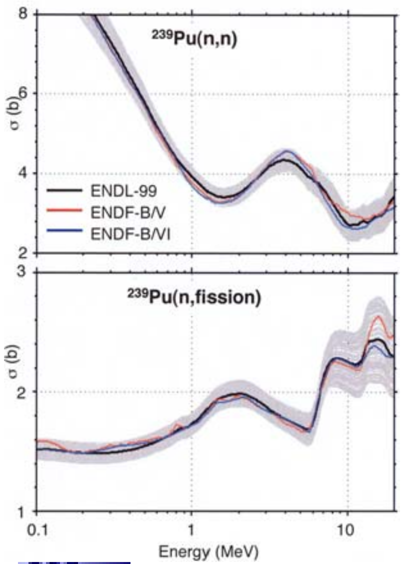
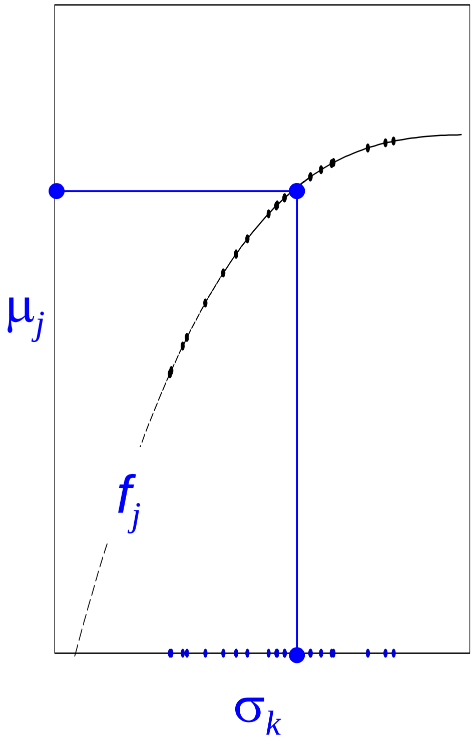
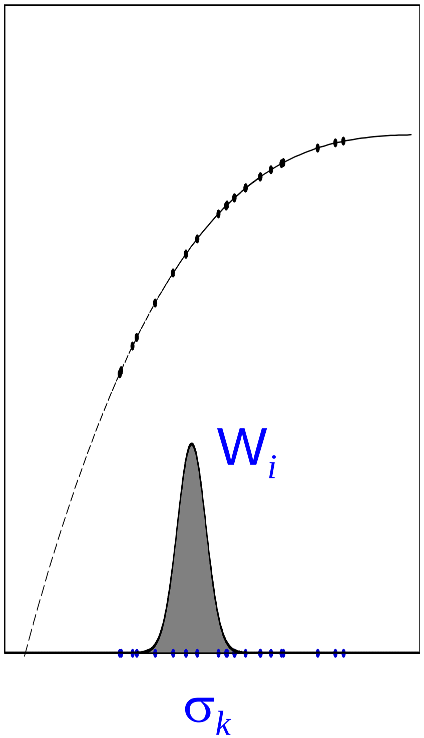
3.
Weight the libraries.

$W(L_i)$

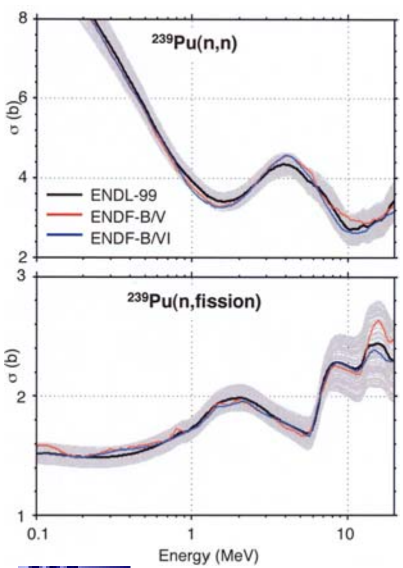


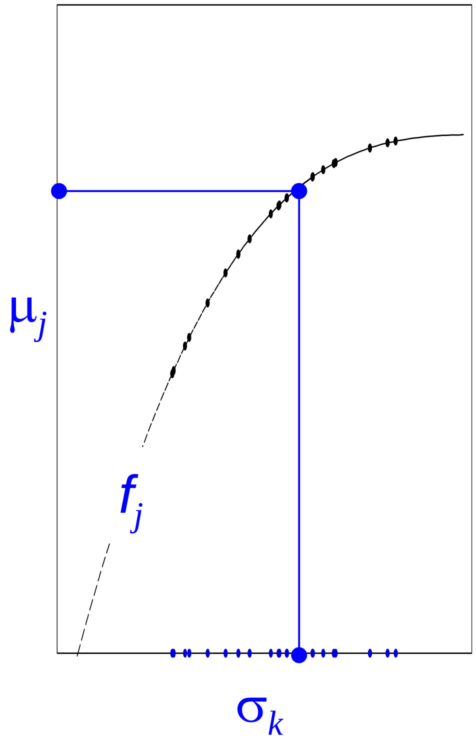


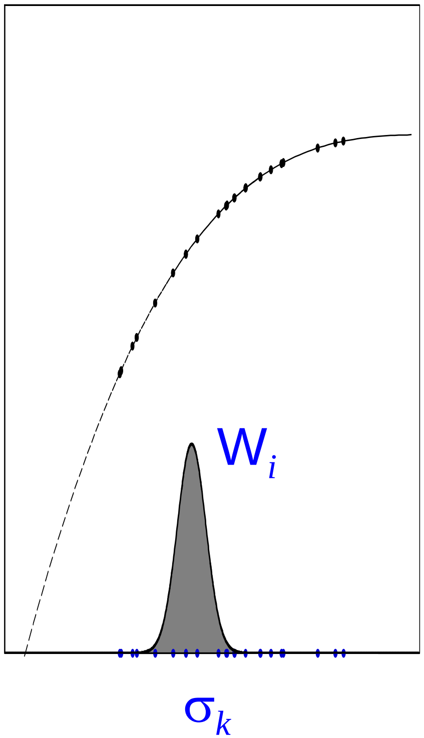


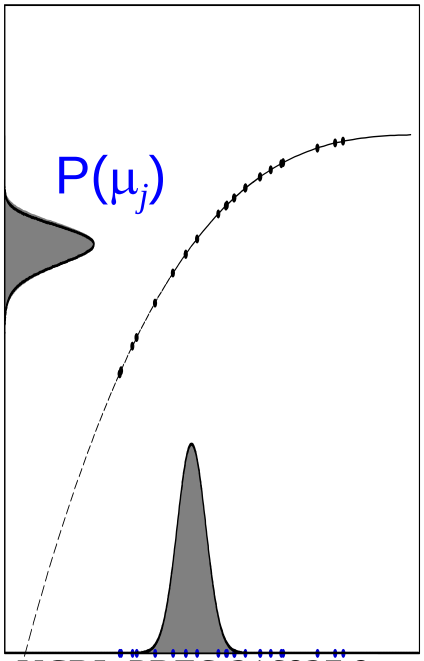
Target: **Probability distributions** for metrics based on knowledge of the nuclear data

1. Sample the nuclear data.	2. Calculate metrics for each library.	3. Weight the libraries.	4. Histogram the metrics.
$L_i = (\sigma_{i0}, \ldots, \sigma_{ik}, \ldots)$	$\mu_{ij} = f_j(L_i)$	$W(L_i)$	$P(\mu_j)$



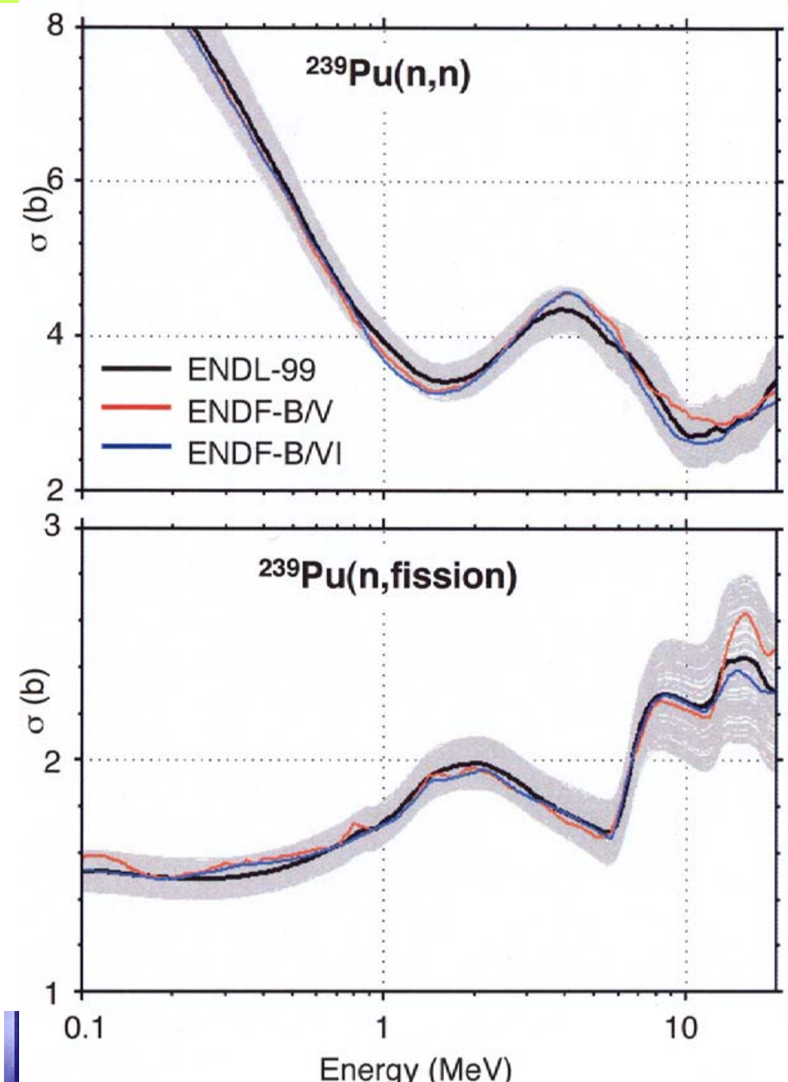






1. Sample the nuclear data.

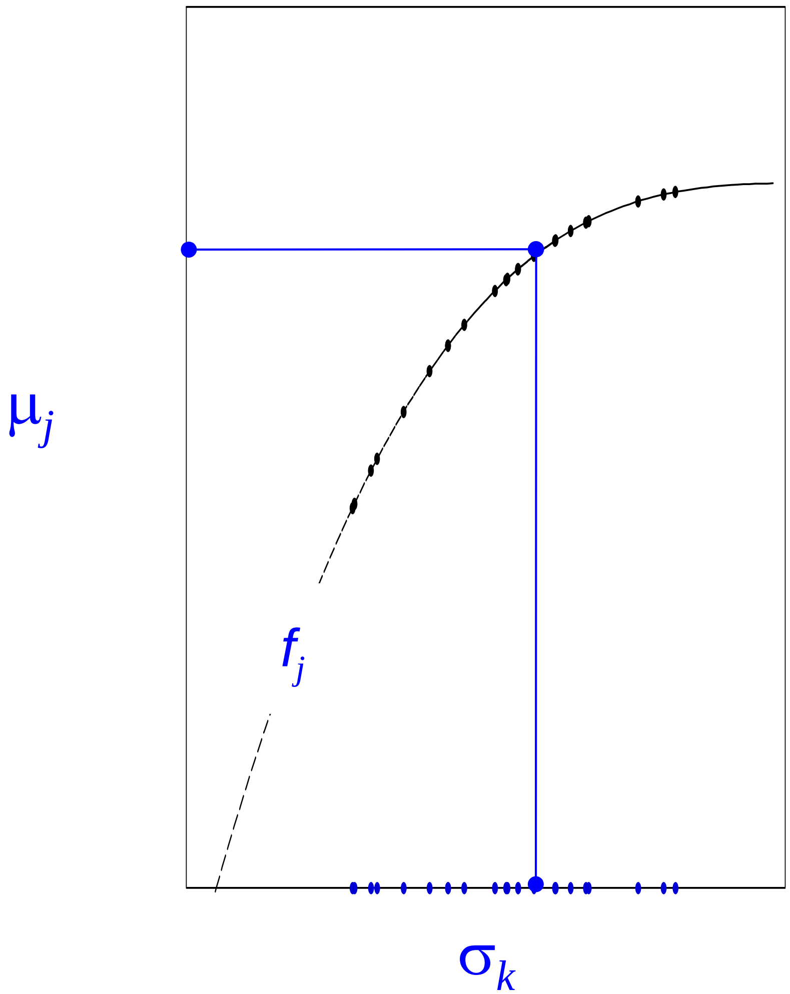
$$L_i = (\sigma_{i0}, \dots, \sigma_{ik}, \dots)$$



- Reactions:
  - ^{239}Pu(n,n)
  - ^{239}Pu(n,n')
  - ^{239}Pu(n,f)
- Energy dependent variations
- Data types
  - Cross section
  - Angular Distribution
  - Outgoing Neutron Energy
  - Fission Neutron Multiplicity

2. Calculate metrics for each library.

$$\mu_{ij} = f_j(\mathrm{L}_i)$$



- Run simulation
  - to each system studied
  - for each sampled library, L_i

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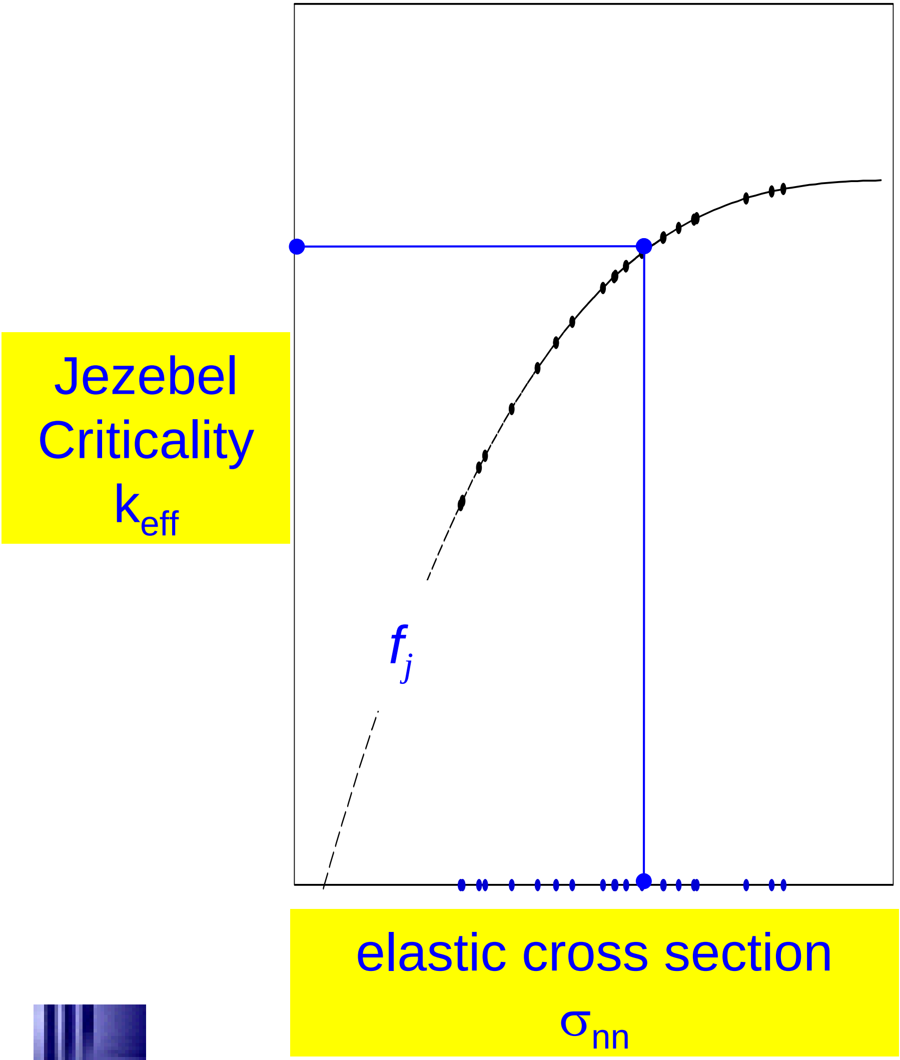

- Run simulation
  - to each system studied
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- Models
  - Jezebel
- Metrics
  - Jezebel criticality, k_{eff}

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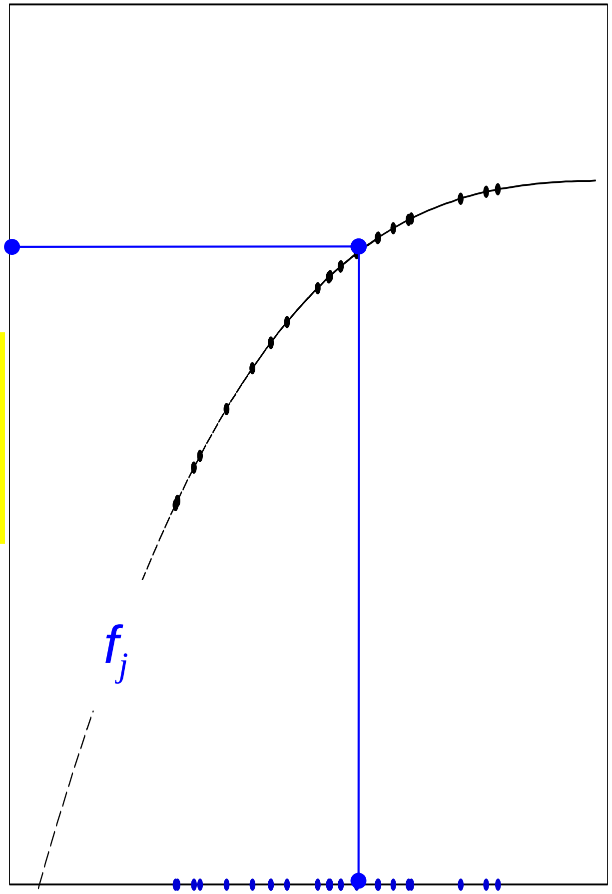
System 1 m_1



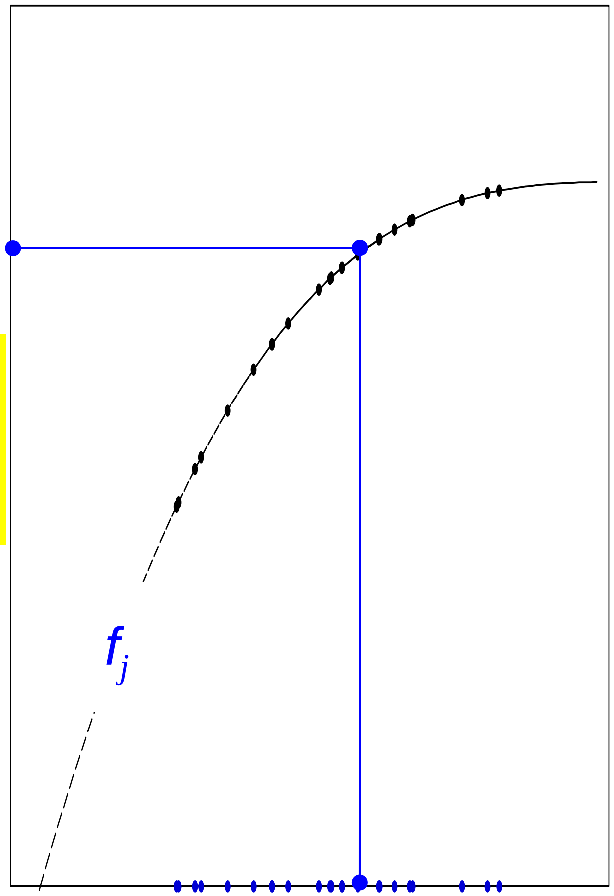
Outgoing neutron energy E'

- Run simulation
  - to each system studied
  - for each sampled library, L_i
- Models
  - Jezebel
  - System 1
- Metrics
  - Jezebel criticality, k_{eff}
  - Metric, m1

2. Calculate metrics for each library.

$$\mu_{ij} = f_j(L_i)$$

System 2 m_2



Fission neutron multiplicity $\bar{\nu}$

- Run simulation
  - to each system studied
  - for each sampled library, L_i
- Models
  - Jezebel
  - System 1
  - System 2
- Metrics
  - Jezebel criticality, k_{eff}
  - Metric, m1
  - Metric, m2

2. Calculate metrics for each library.

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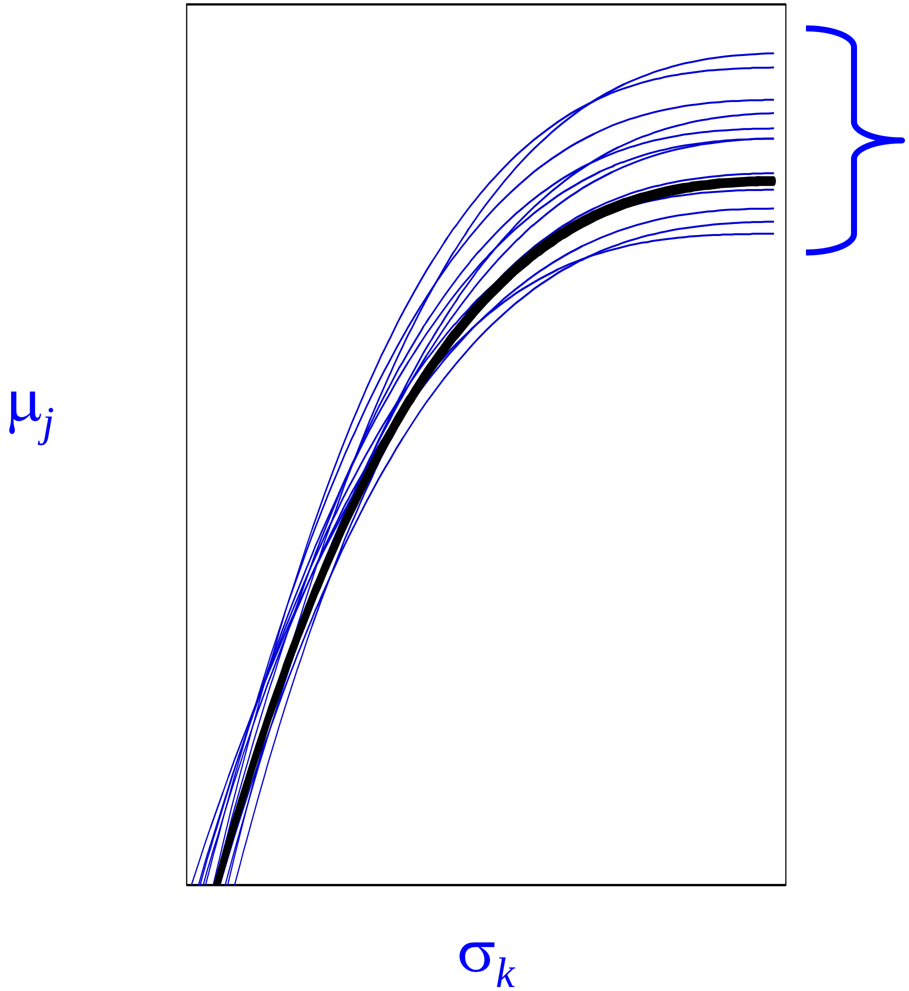

Effect of other nuclear data,

$\sigma_{m \neq k}$

or other physics,

e.g. …

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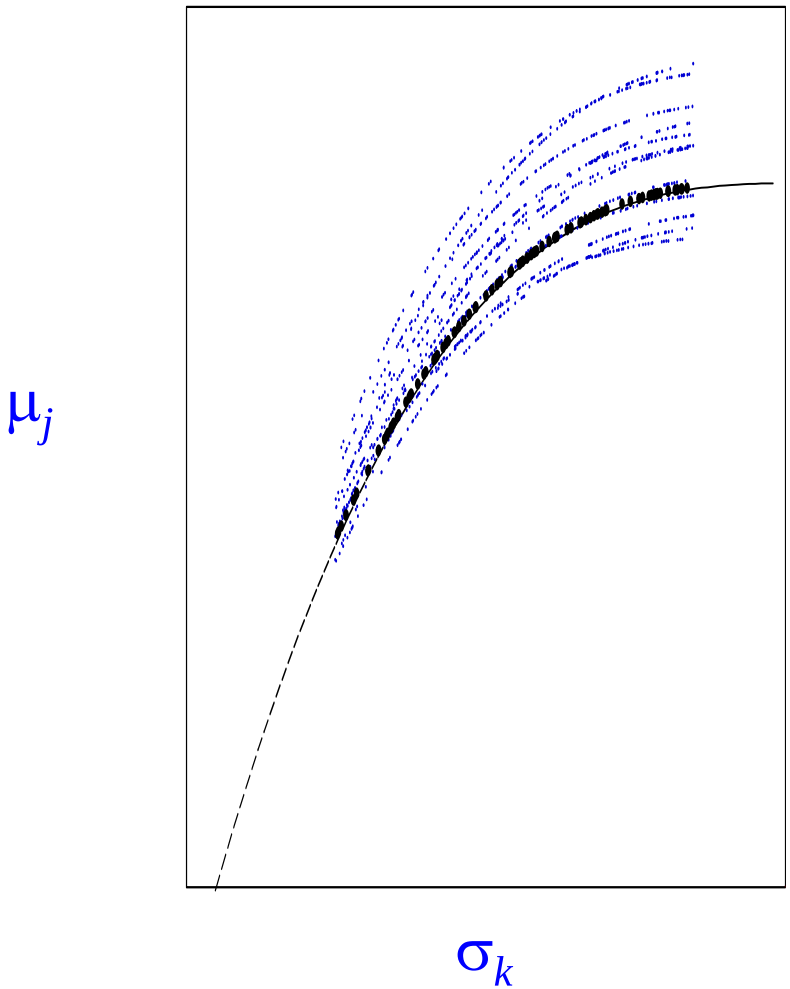


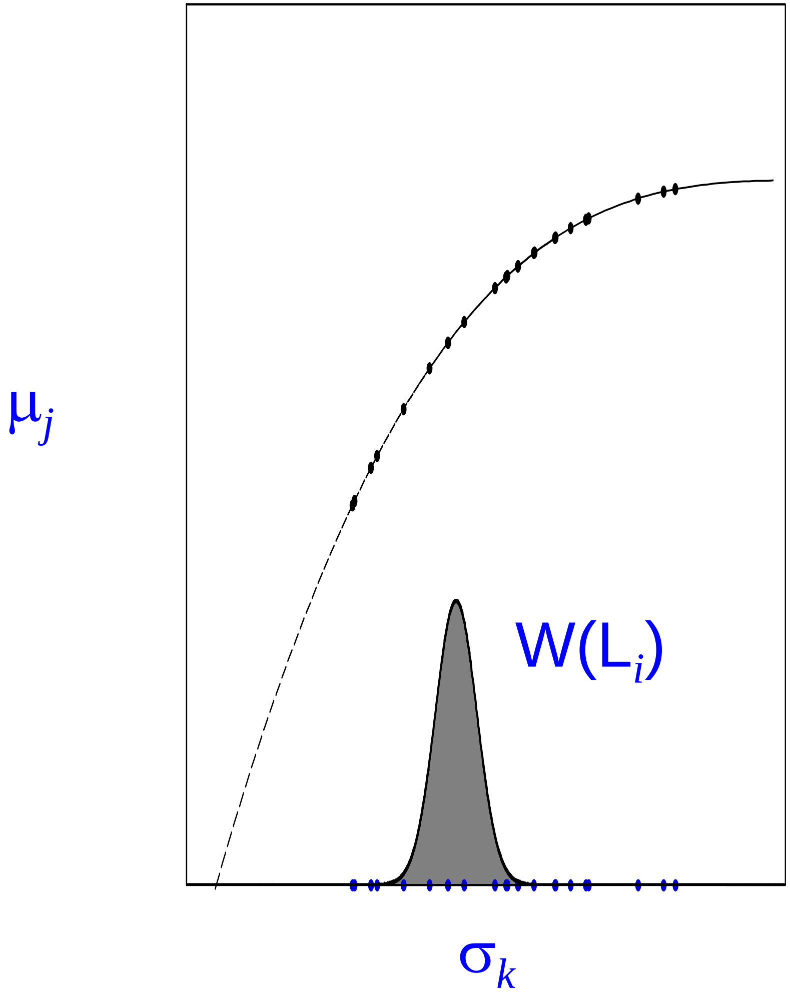
Effect of other nuclear data,
$\sigma_{m \neq k}$

or other physics,
e.g. …

So we vary all parameters simultaneously.

3. Weight the libraries.

$W(L_i)$



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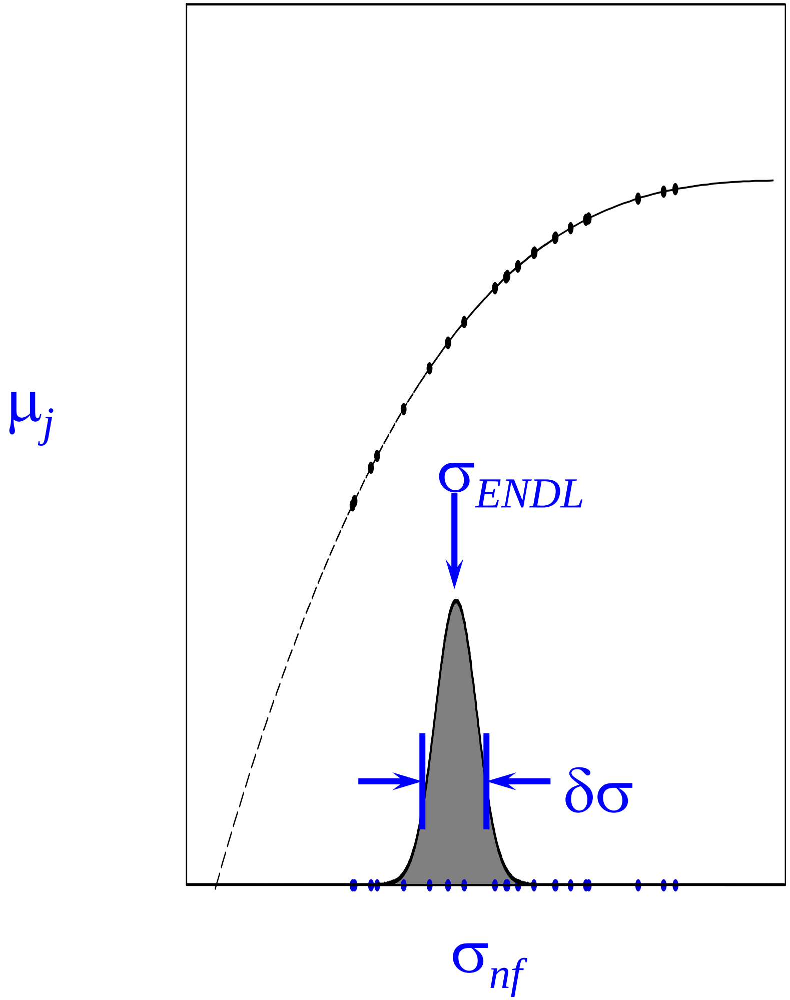


Weight by

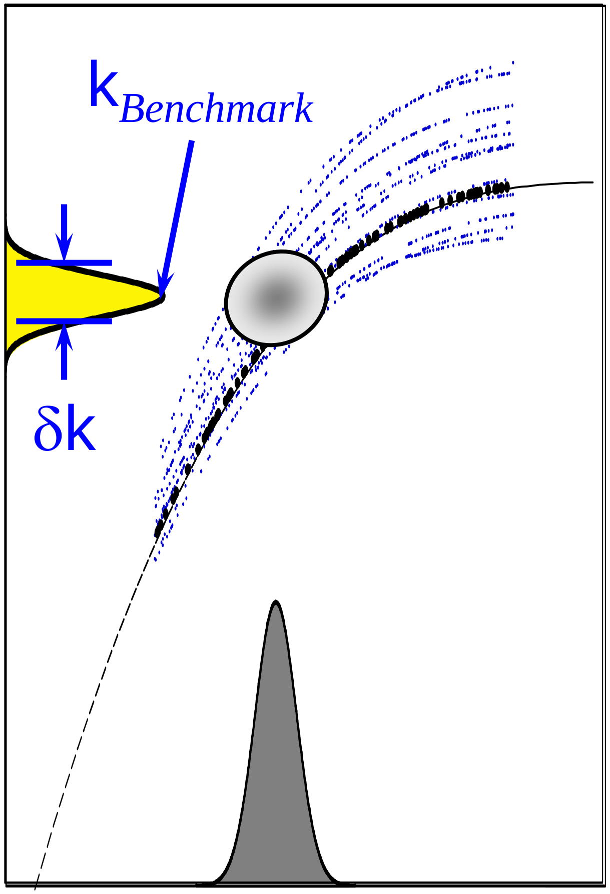
Direct fit to measured or evaluated nuclear data…

$$W(L_i) = W_0 \exp\left[\frac{1}{2}\left(\frac{\sigma_{nf,i} - \sigma_{nf,ENDL}}{\delta\sigma_{nf}}\right)^2\right]$$

3. Weight the libraries.

$W(L_i)$

Jezebel k_{eff}



$\sigma\bar{\nu}$

Weight by

Direct fit to measured or evaluated nuclear data…

$$W(L_i) = W_0 \exp\left[\frac{1}{2}\left(\frac{\sigma_{nf,i} - \sigma_{nf,ENDL}}{\delta\sigma_{nf}}\right)^2\right]$$

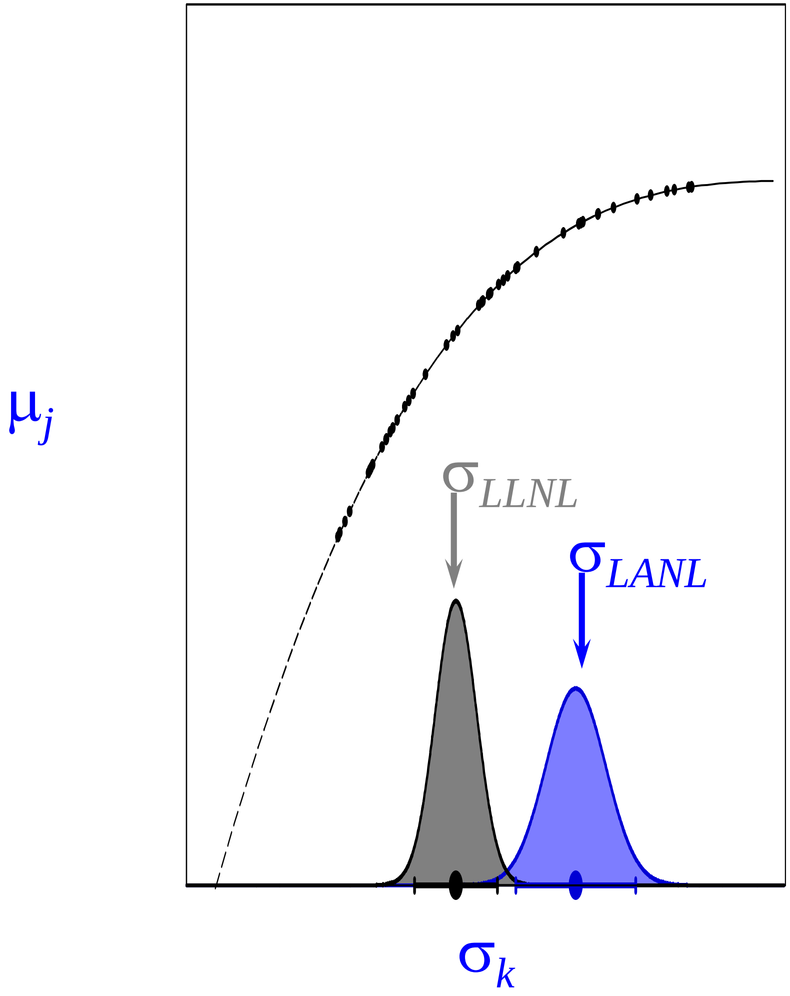
Or by,

fit of calculated metric to a measured values…

$$W(L_i) = W_0 \exp\left[\frac{1}{2}\left(\frac{k_i - k_{Jezebel}}{\delta k}\right)^2\right]$$

3. Weight the libraries.

$W(L_i)$



Flexible enough to handle…

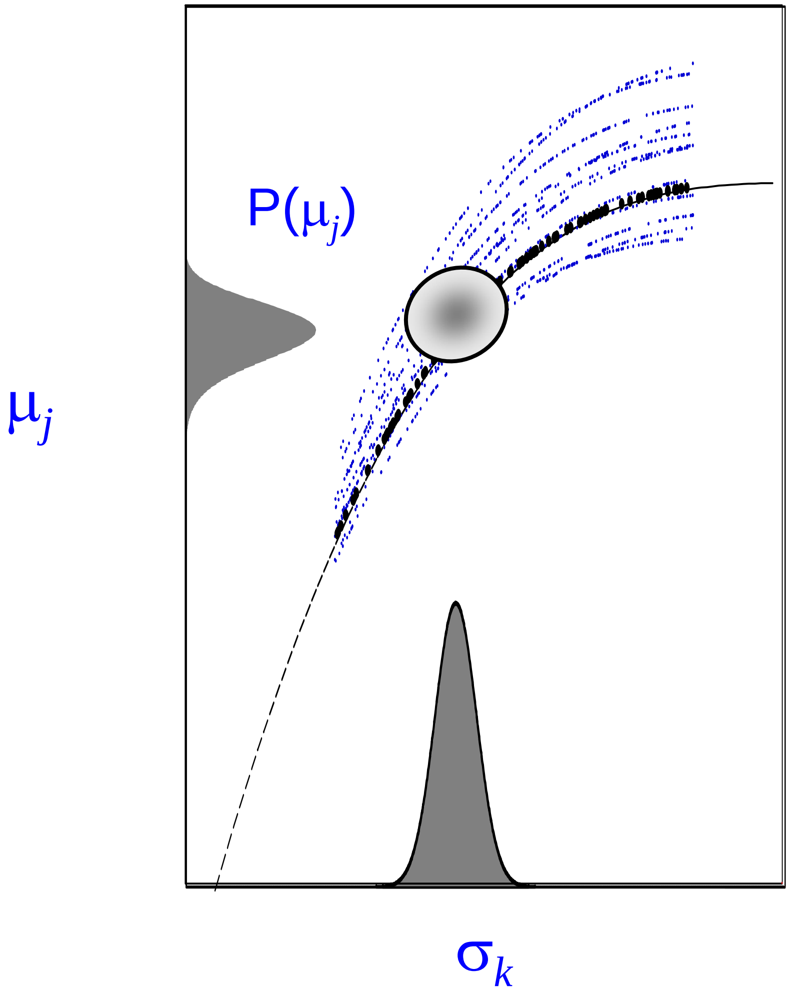
non-Gaussian distributions

Or…

inconsistent evaluations.

4. Histogram the metrics.

$P(\mu_j)$



The weighted histogram

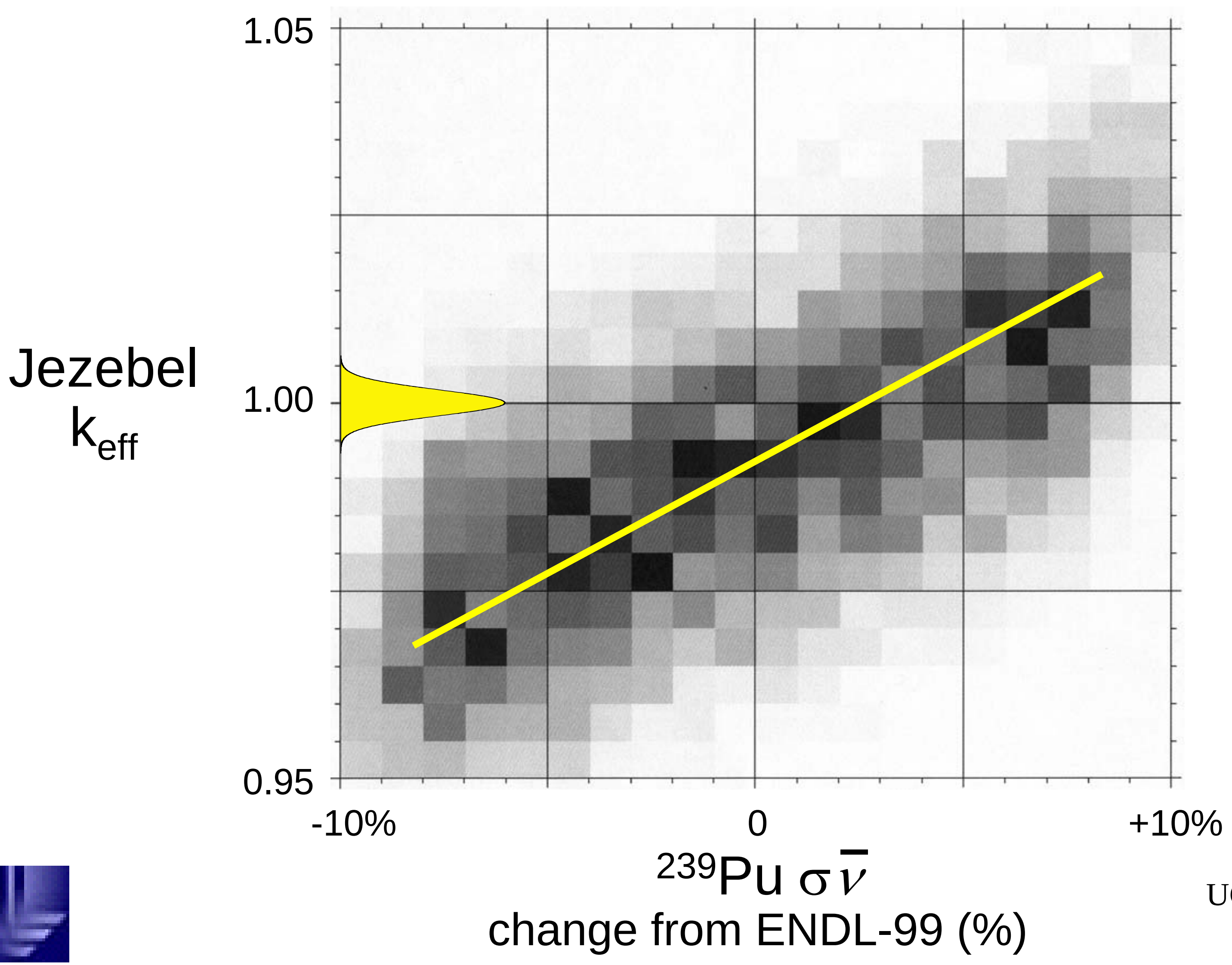
$P(\mu_j)$

represents the state of

knowledge of the metric

μ_j

Jezebel criticality, k_{eff}, versus $^{239}Pu\ \sigma\bar{\nu}$ at 2 MeV



New Uncertainty Quantification scheme

- Instead of data and covariance, store:
  - Ensemble of data realizations
  - Post and prior weights
- Proof of concept shown
- Code being integrated into our nuclear data infrastructure