Covariance work at LLNL

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11/2/2010

Nuclear data covariance matrices can be huge and unwieldy

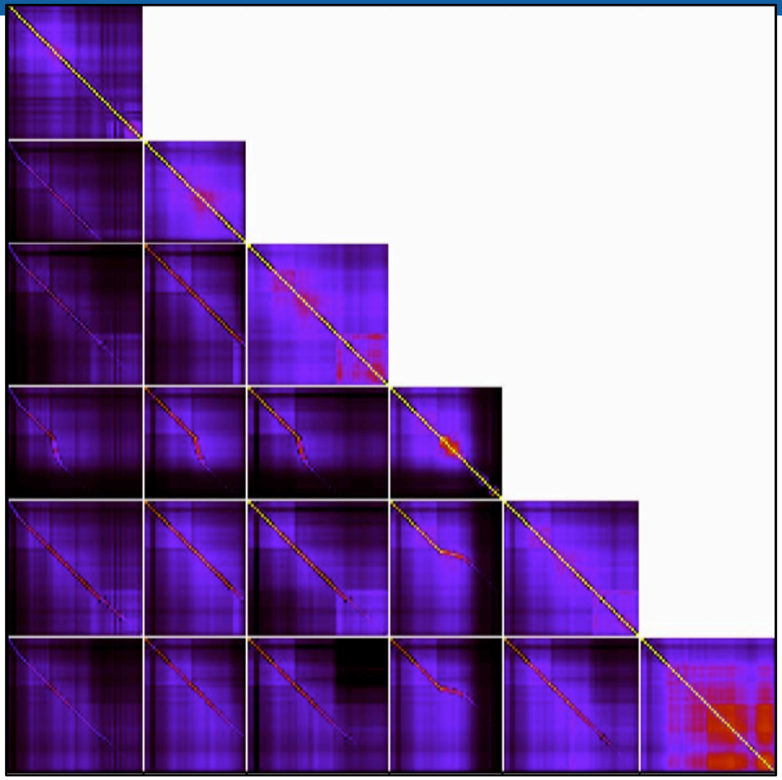
- **The FULL covariance matrix of an evaluation is way too big to be used:**

3 big σ's: (n,tot), (n,el), (n,γ)	5000 pts. ea.
~ 10 discrete level excitation σ's: (n,n')	100 pts. ea.
~ 5 threshold σ's: (n,2n), (n,p), (n,3n), etc.	100 pts. ea.
If fissions, have fission σ too	5000 pts. ea.

- **Most channels have ~2 outgoing particles (usu. γ & n)**
  - Assume isotropic, but each has ~ 10 outgoing E' points
  - So has 10 x (number of points in σ)
- **This comes out to ~ 1.5 x 10^5 points/evaluation (neglecting fission)!**
- **Note, this neglects cross-isotope correlations:**
  - Reaction model, common parameters in modeling
  - Ratio experimental data (e.g. ^{239}Pu(n,f)/^{235}U(n,f))

The FULL covariance matrix (for just one evaluation) would require ~ 10^{10} entries: it would be impractical to use the entire thing

Practical (partial) solutions to dimensionality problem; all of these have already been tried by the nuclear data community



Option:UCRL#

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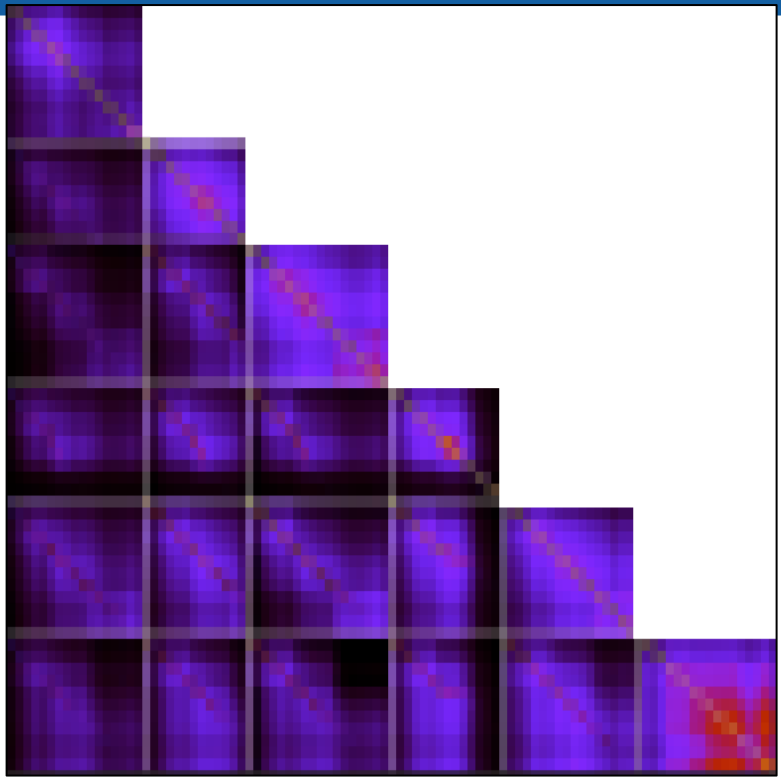
- **Group the covariance**

  Lowers resolution



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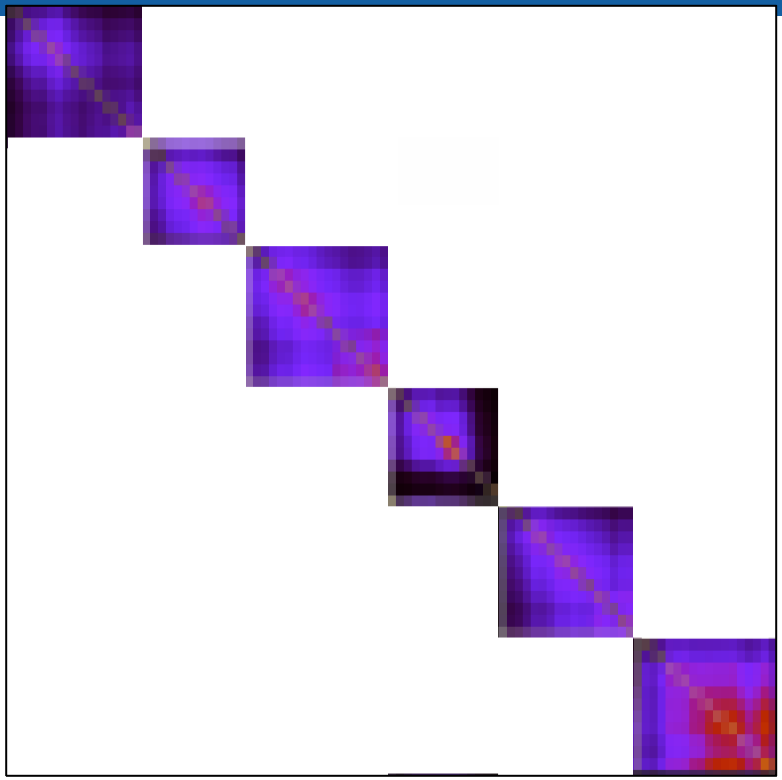
- **Throw out cross correlations**
  - What if my project is sensitive to those correlations?



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- **Guess which subspaces users need, throw out rest**
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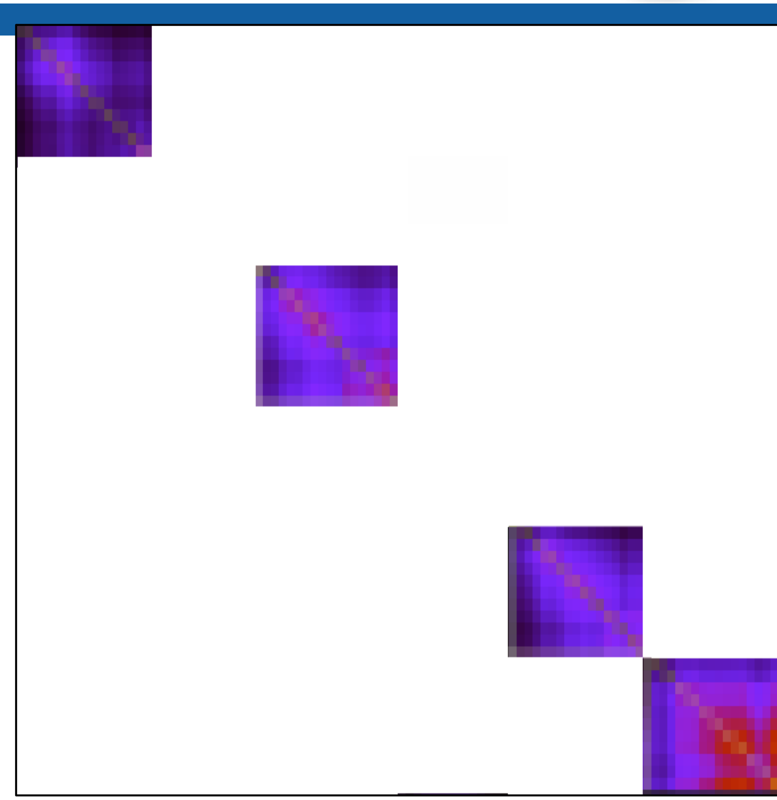
  - What if my project is not sensitive to something you kept?



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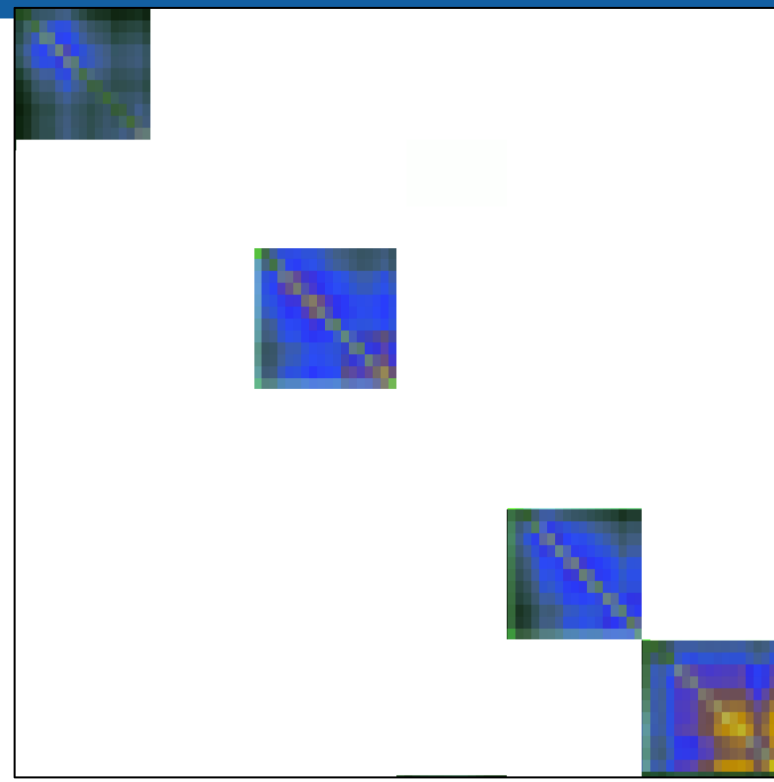

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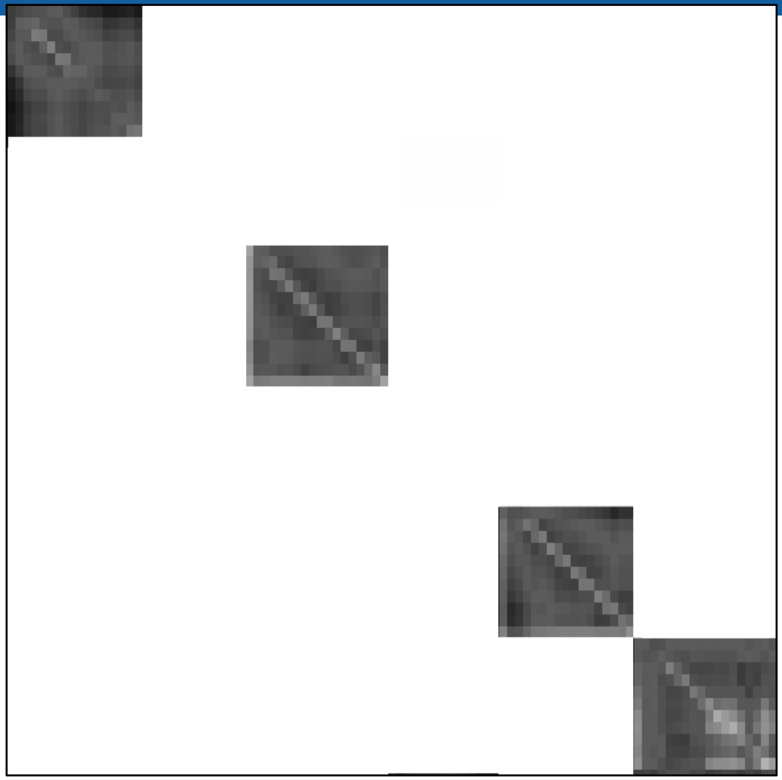

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- **Double precision -> single precision**
  - Lowers precision of entries, for sure leads to numerical artifacts (e.g. non-positive eigenvalues)

- What do I propose to do about it?

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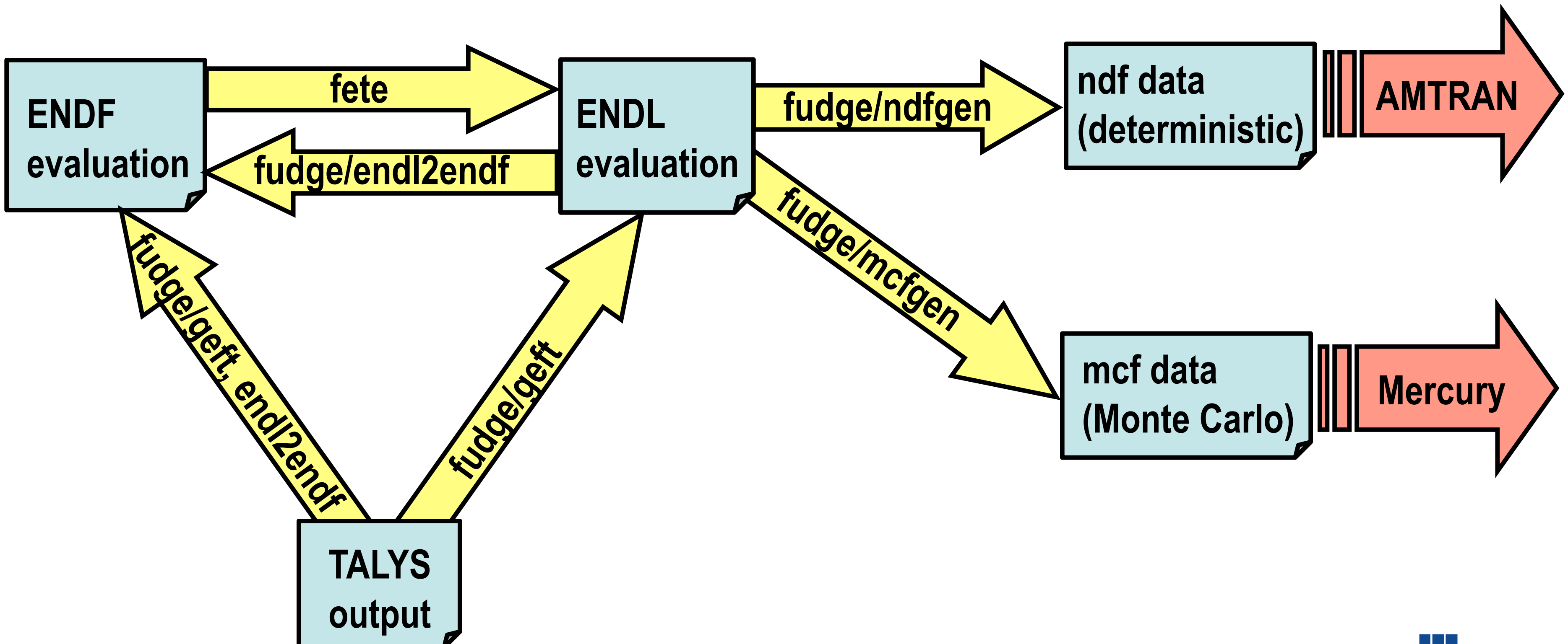
  - … nothing
- I will use the existing covariance data however

LLNL nuclear data processing system supplies Monte Carlo and deterministic transport codes



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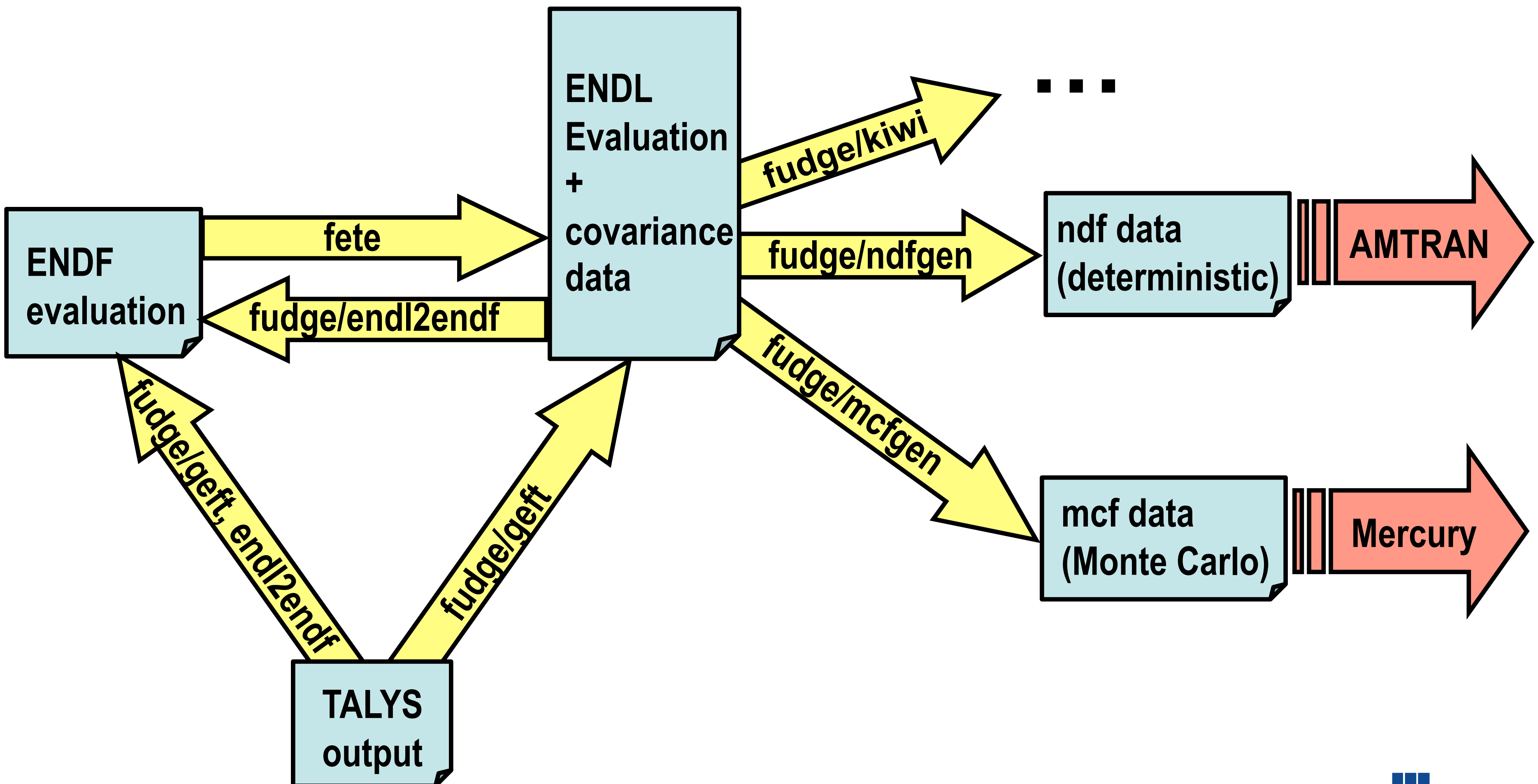
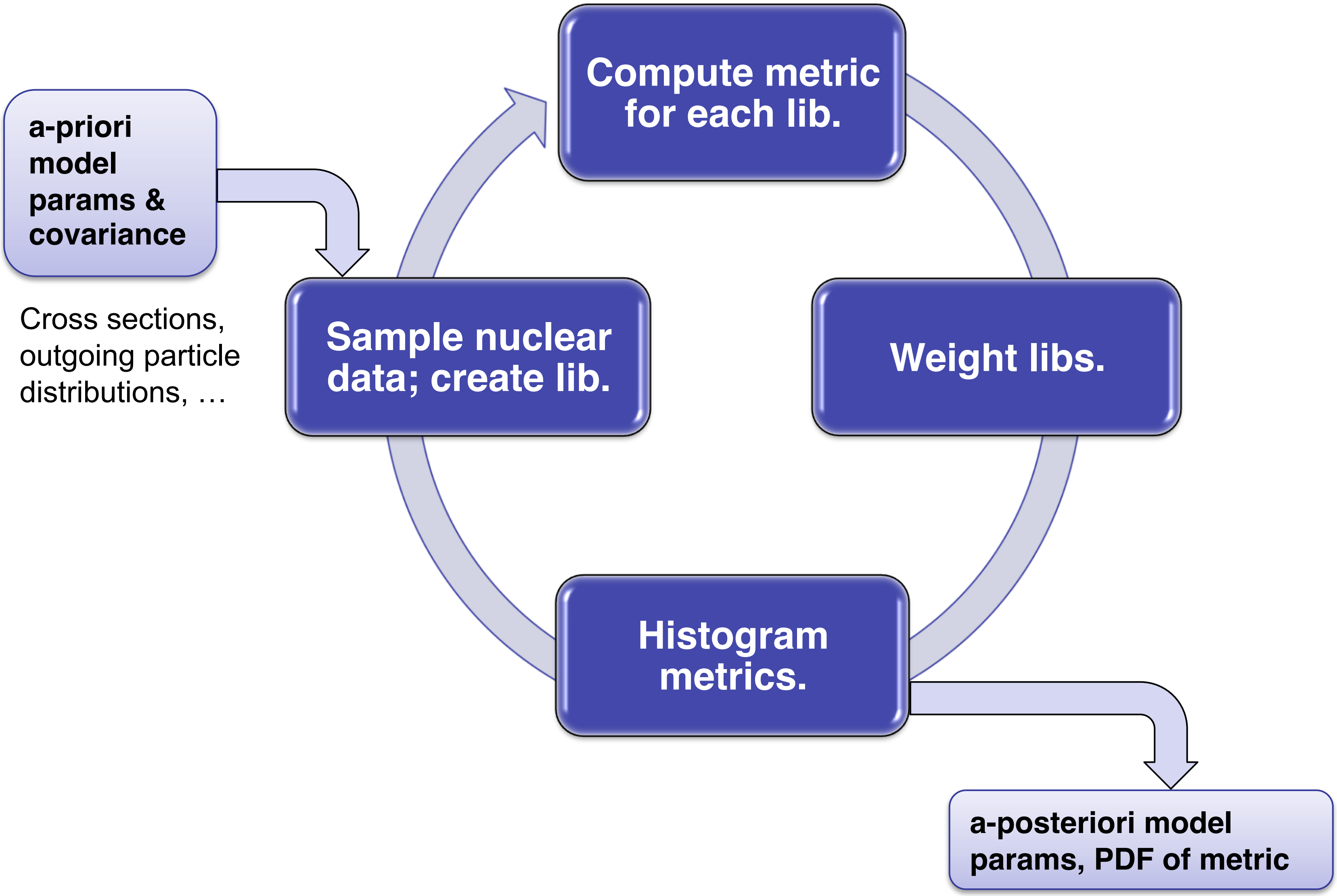


Want probability distributions for metrics based on knowledge of the nuclear data



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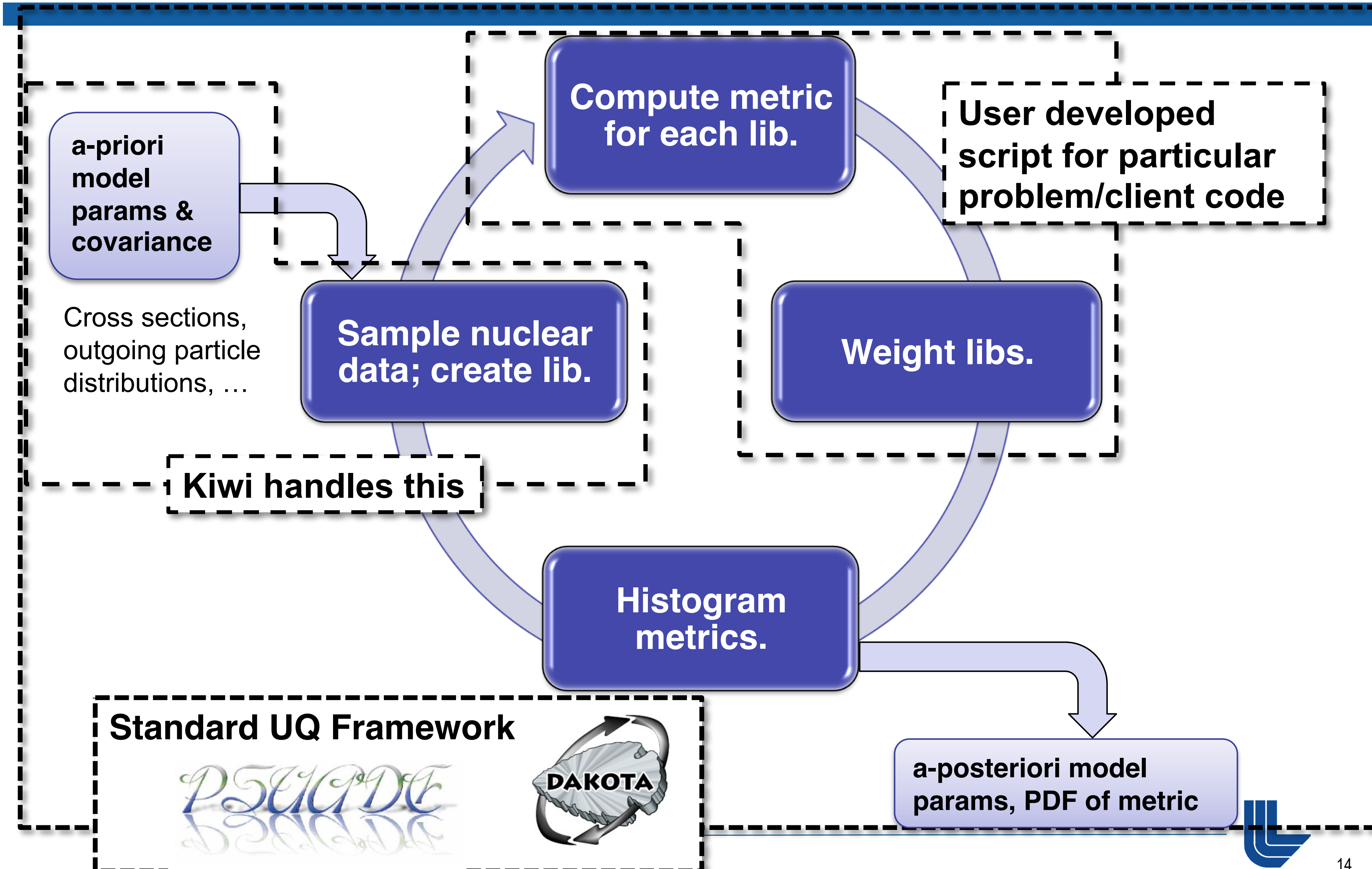
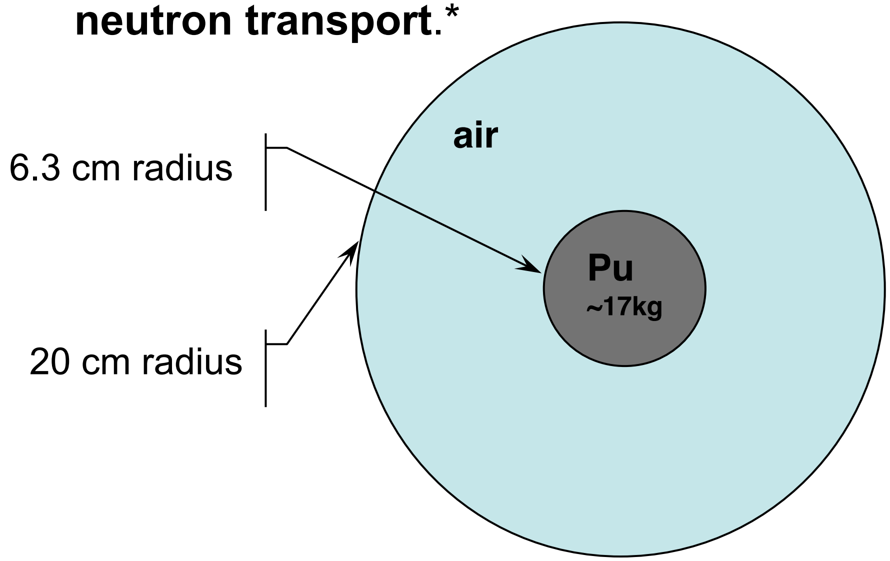


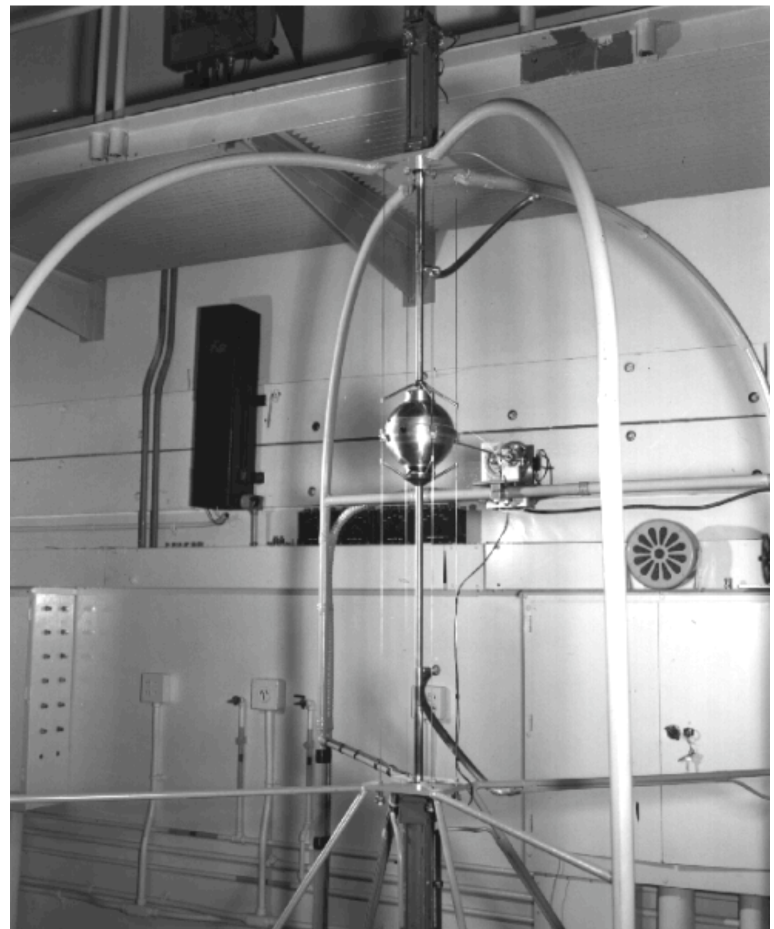
Status of kiwi rewrite vs. requirements

- ☑ **Drive using PSUADE or Dakota or stand-alone**
- ☐ **Documented** (in progress)
- ☐ **Not so easy to use** (can't be helped it seems)
- ☑ **Generated libraries:**
  - ☑ Make either Monte-Carlo (mcf), deterministic (ndf), or tdf libraries
  - ☑ User defined isotope lists so files not humongous
- ☑ **How data varies:**
  - ☑ Use data covariance (e.g. from ENDF/B-VII)
  - ☑ Use data uncertainties
  - ☑ Use user-imposed uncertainties
  - ☑ Simple interface for all kinds of variation (esp. for cov.)

A sample UQ study on the Jezebel critical assembly

- **ICSBEP Handbook case # PU-MET-FAST-001** (NEA/NSC/DOC(95)03, ed. B. Biggs (2009))
- **Ball of mostly Pu** (%'s by atomic fraction):
  - 92% ^{239}Pu
  - 3% Ga
  - 5% other Pu
- **1D model using AMTRAN deterministic neutron transport.***

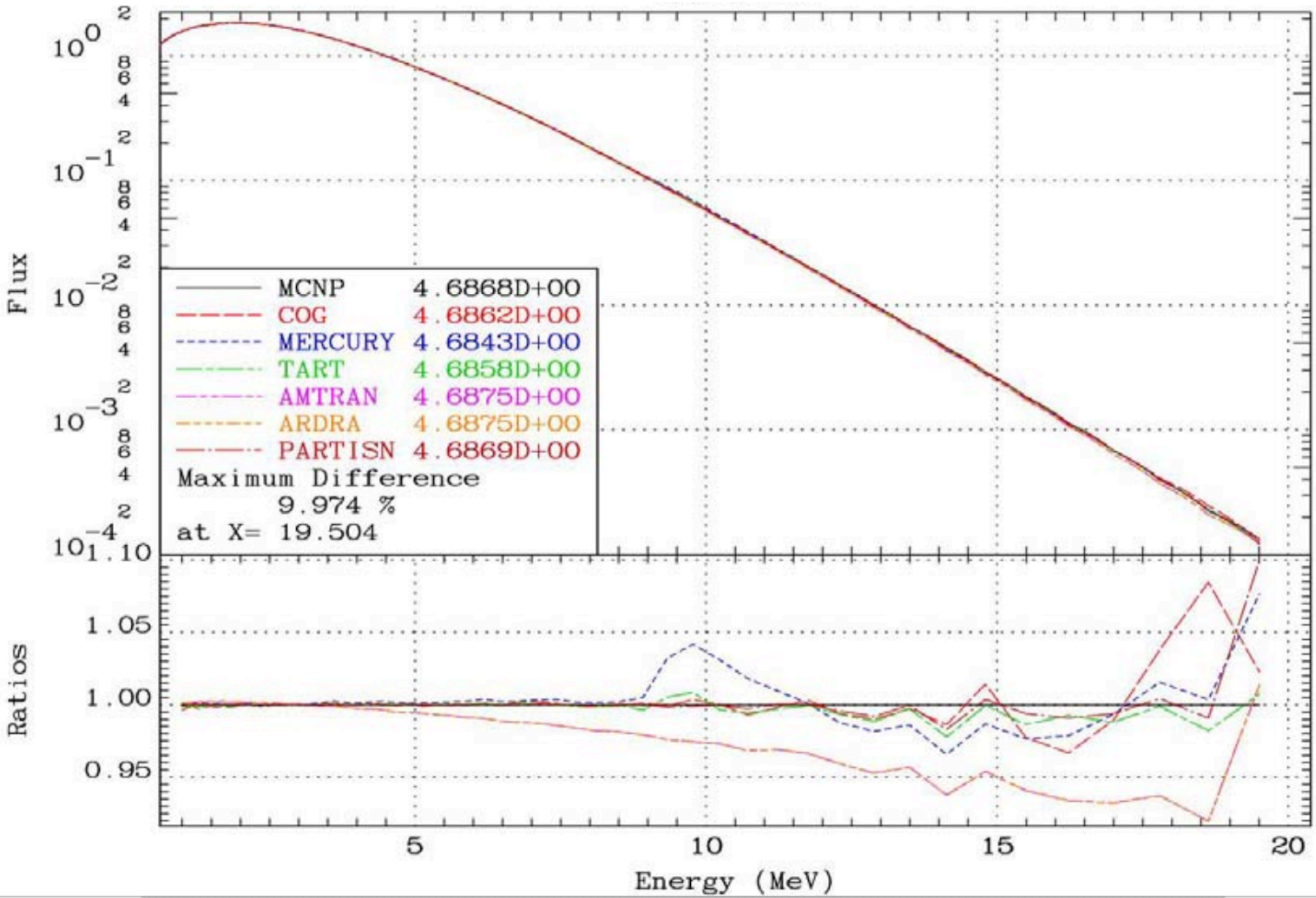




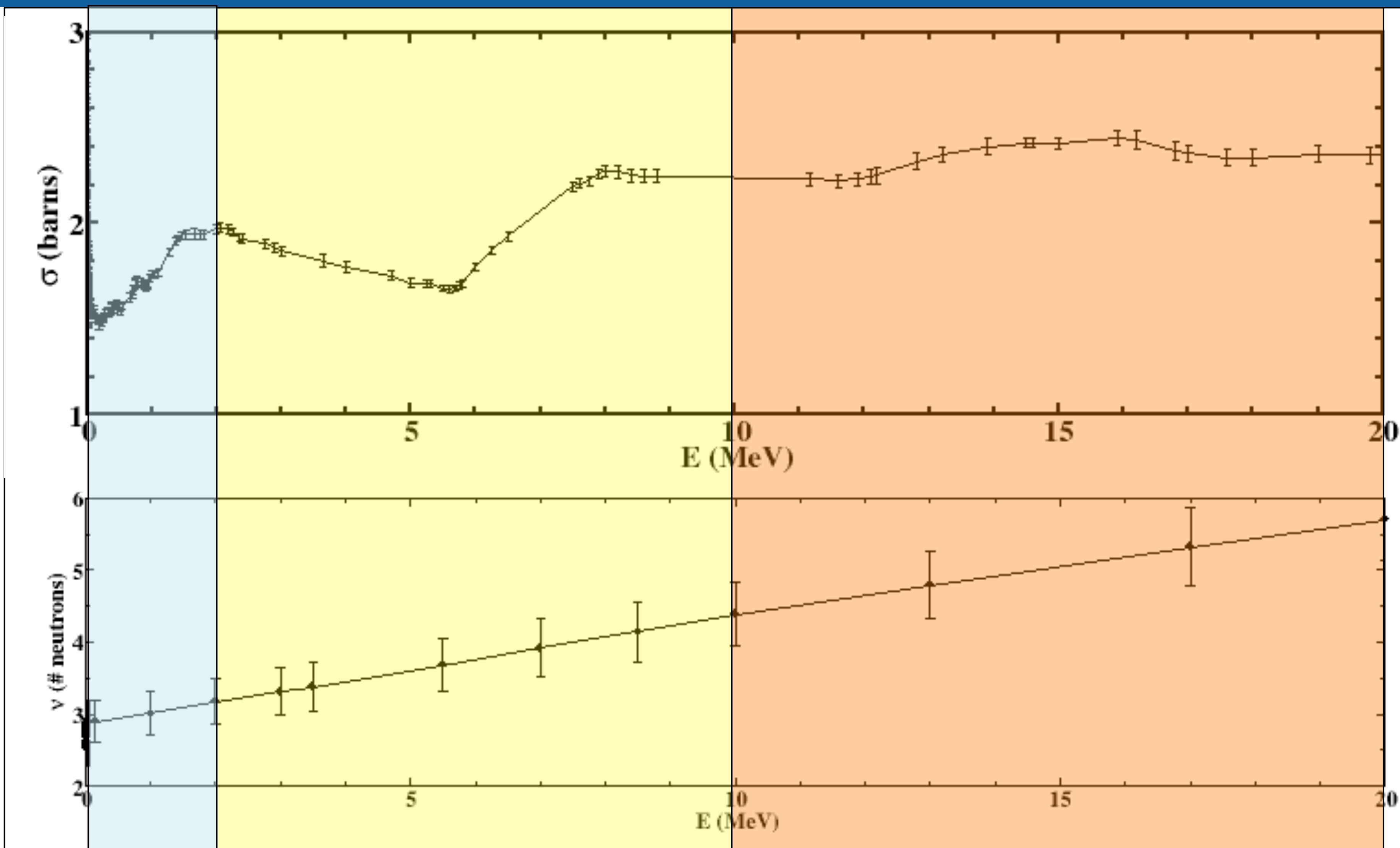
Jezebel ^{239}Pu critical assembly (1960)

* Clouse, C. J., *Parallel Deterministic Neutron Transport with AMR, in Computational Methods in Transport, edited by Graziani, F.R., Springer-Verlag, Pages 499 - 512 (2006).*

Jezebel has a “hard” neutron flux, peaking around 3 MeV



What we varied: $^{239}Pu(n,f)$ cross section and prompt neutron multiplicity (prompt nubar) in three energy groups



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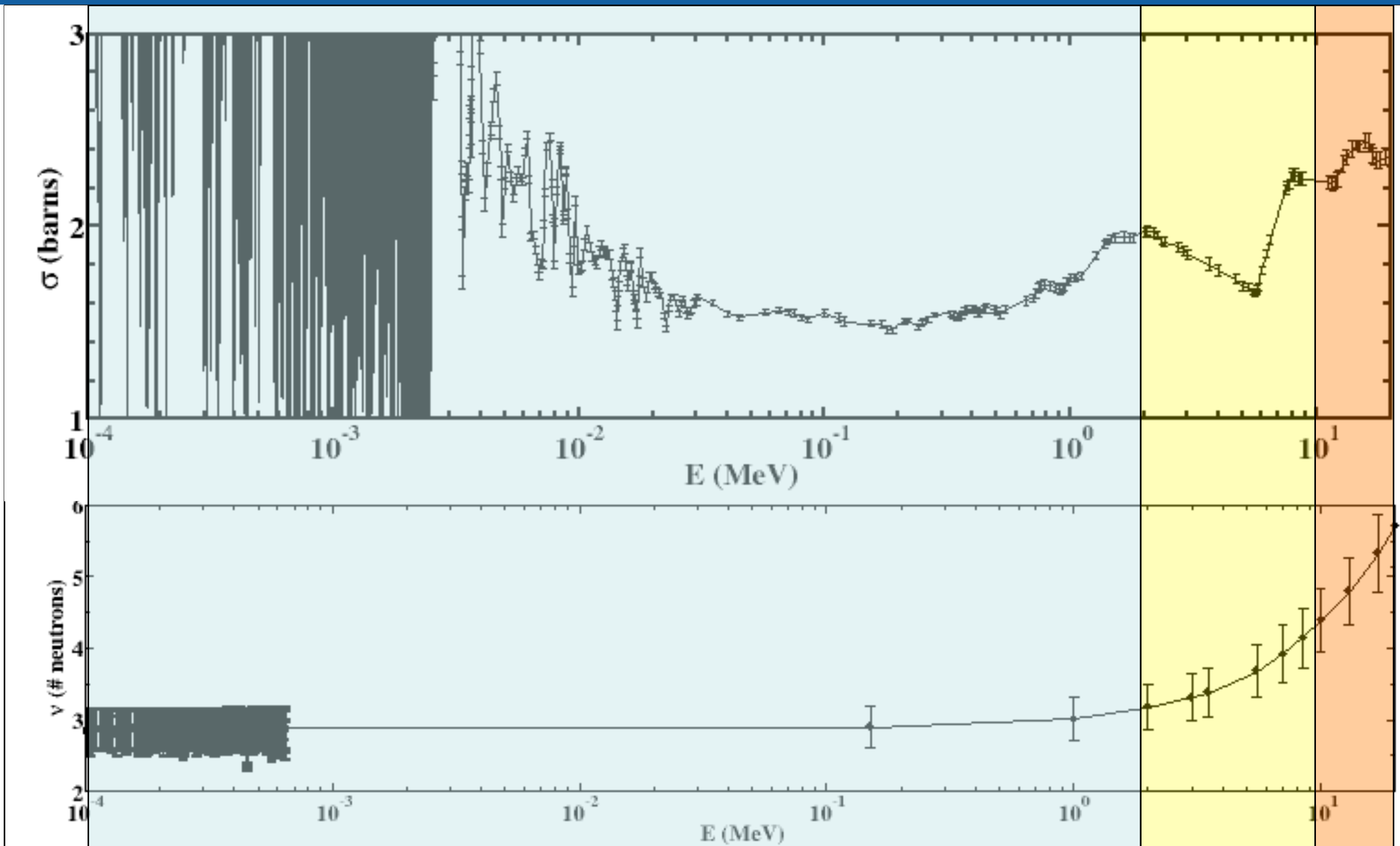

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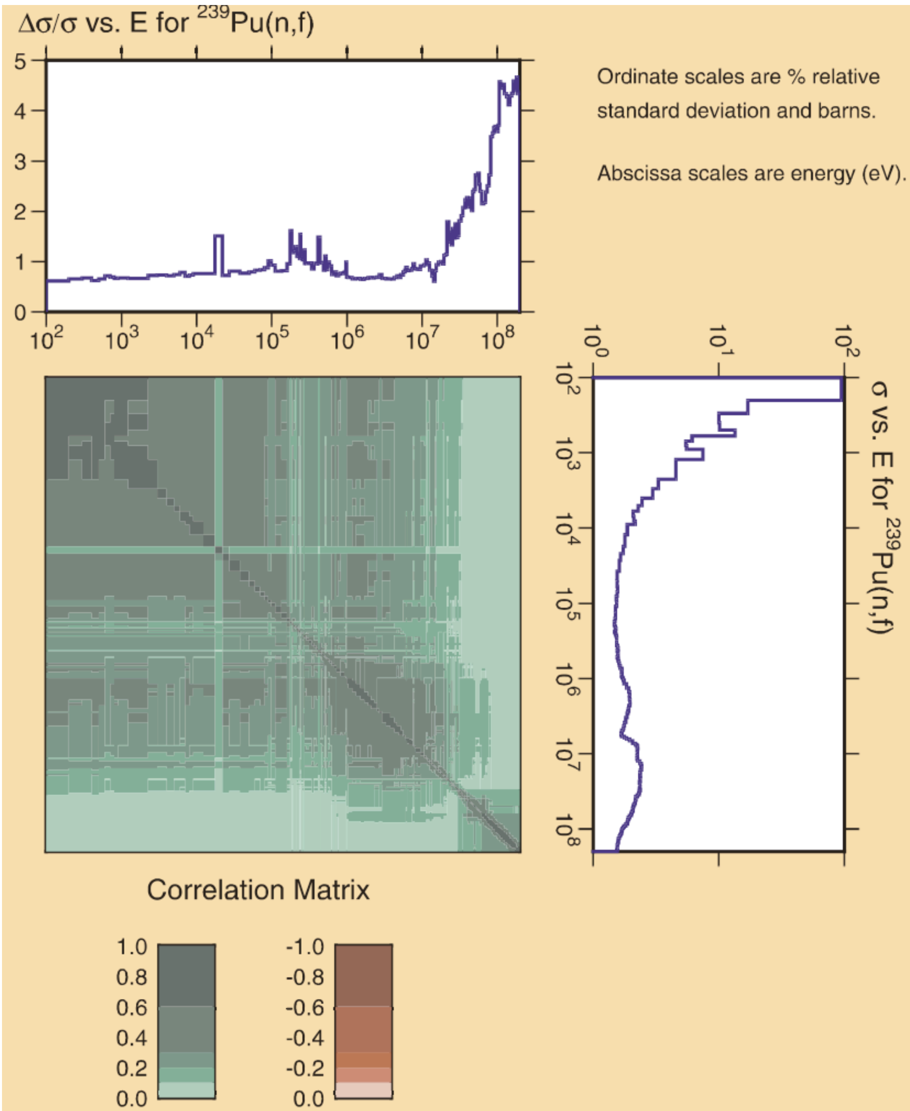
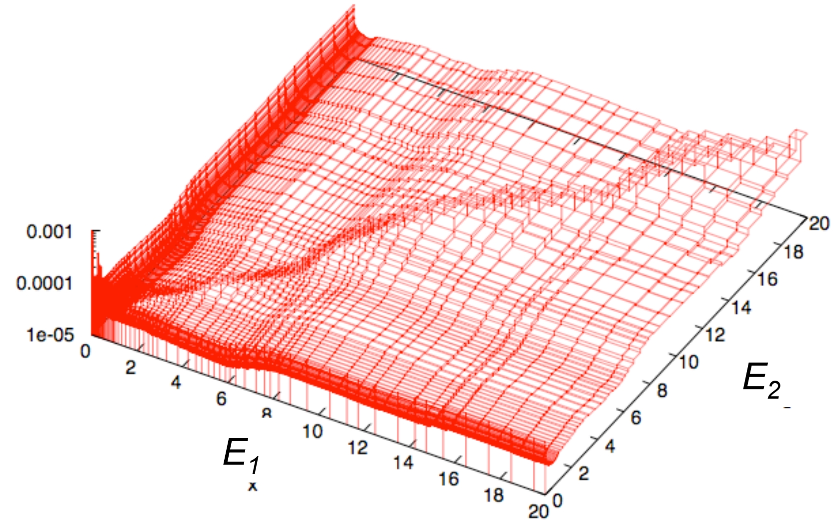
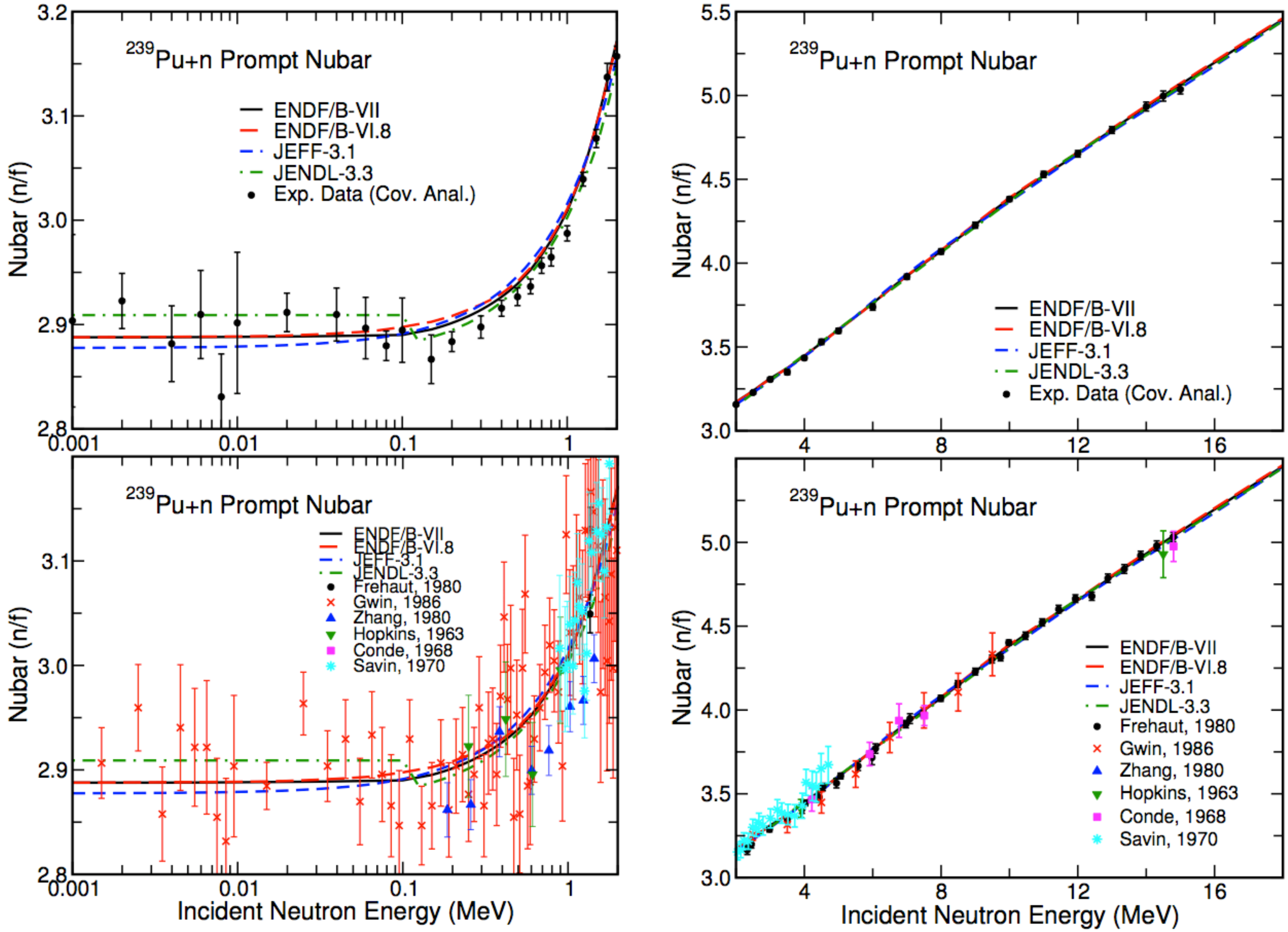
We used the (n,f) cross section and its covariance from the ENDF/B-VII.0 nuclear data library





- **Matrix taken from ENDF/B-VII.0 evaluation**
- **Given in two energy ranges:**
  - Resonance region (E < 100 keV)
  - High energy (E > 100 keV)
- **Matrix was not positive definite:**
  - Perform eigenvalue decomp.
  - Remove small & negative eigenspaces
- **Significant off-diag. correlations**

The ENDF/B-VII.0 ^{239}Pu(n,f) evaluation (used in ENDL2009.0) included beautiful fit to prompt nubar



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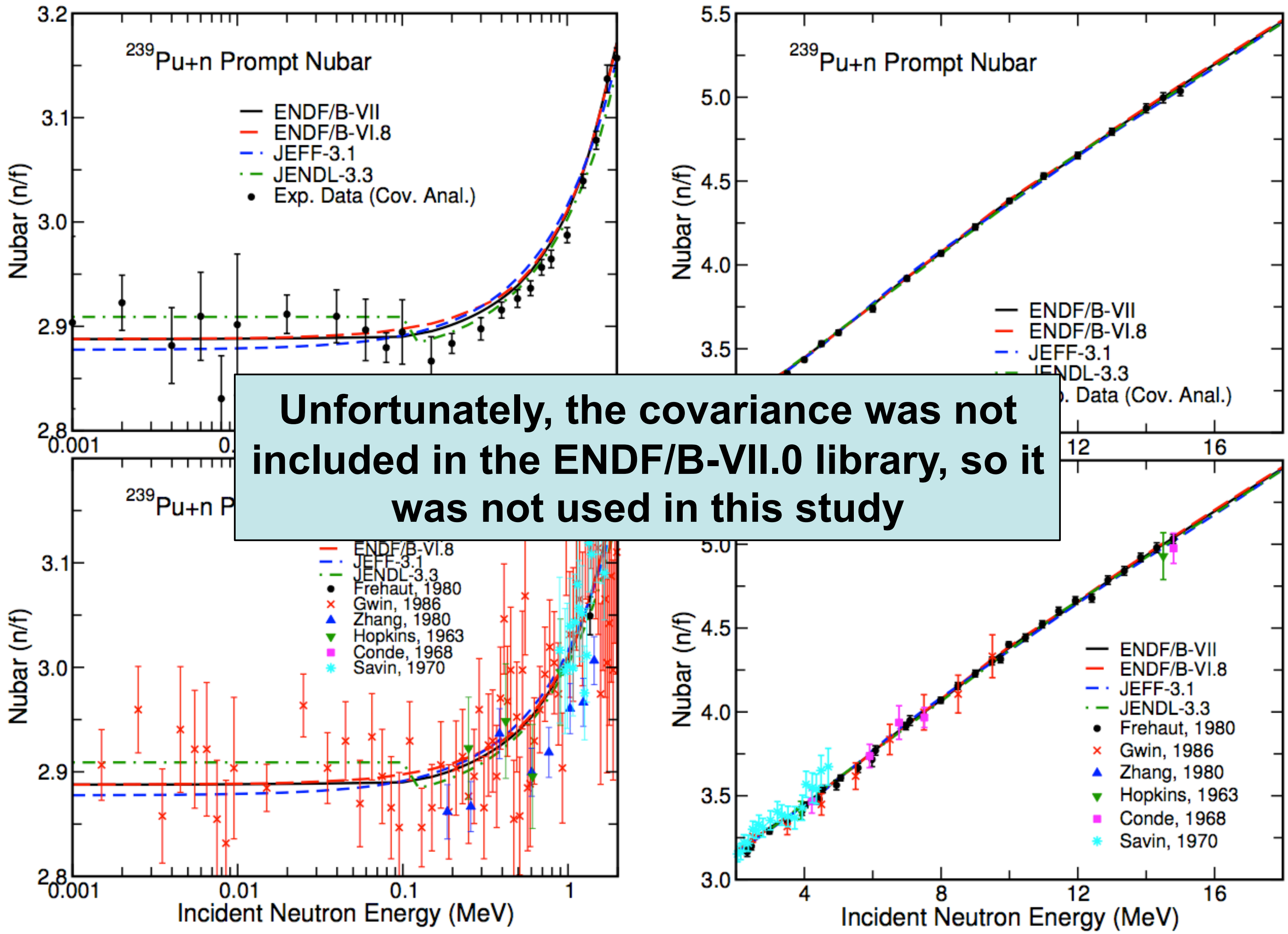
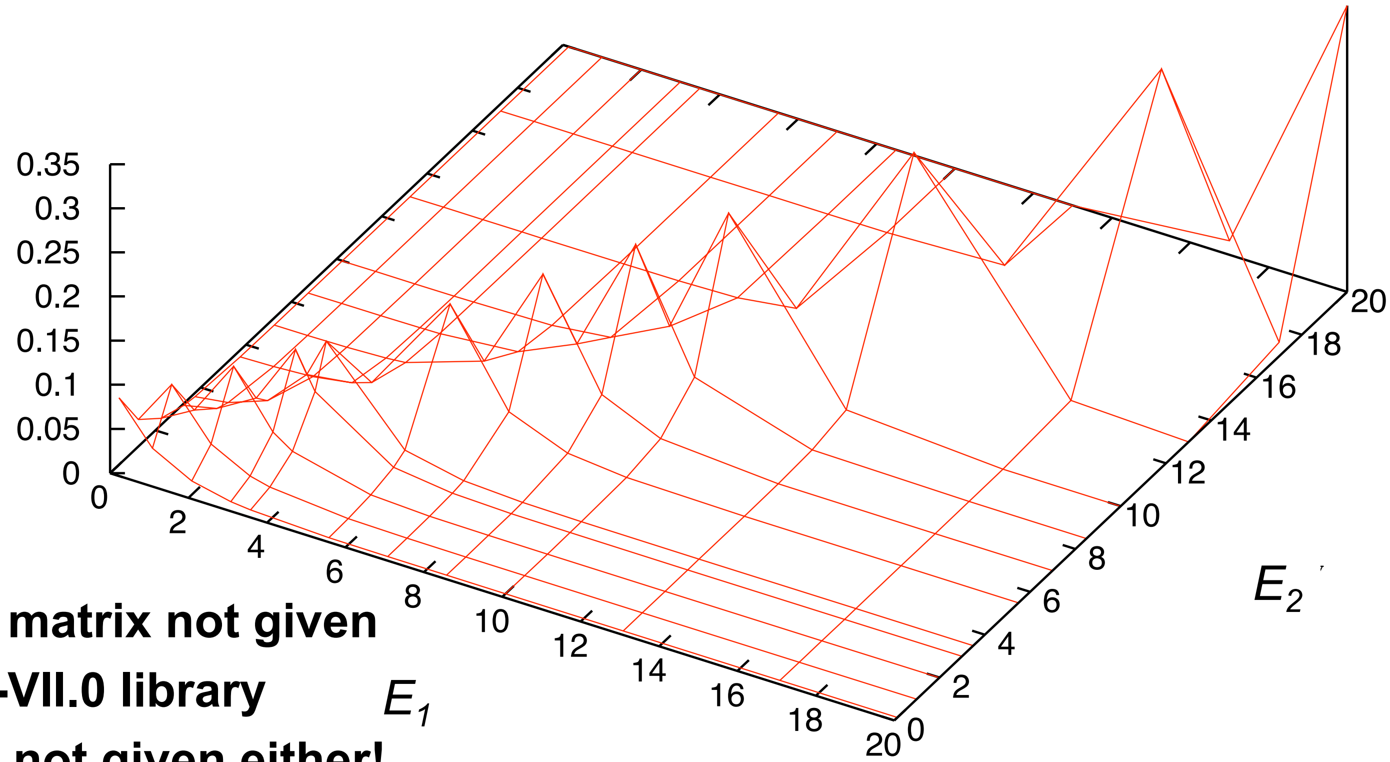


Unfortunately, the covariance was not included in the ENDF/B-VII.0 library, so it was not used in this study

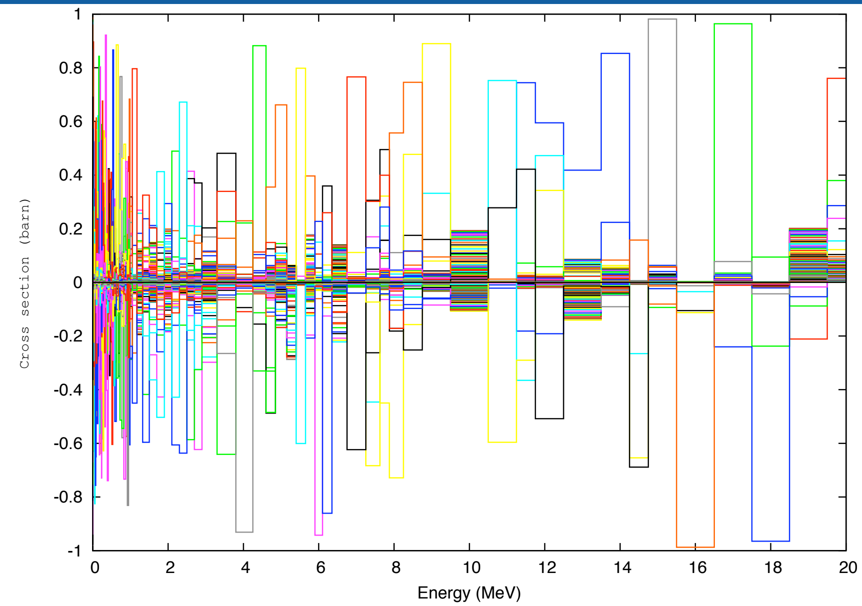
We were forced to manufacture our own nubar covariance



- **Covariance matrix not given in ENDF/B-VII.0 library**
- **Uncertainty not given either!**
  - Assume 10% rel. uncertainty: way too big by factor of 5
  - Actual uncertainty undoubtedly much smaller, but not given in any modern data library (this is despite efforts of several groups of evaluators)
- **Manufactured by**
  - Assume off-diagonal correlation shape: $\exp\left(-\frac{|E_1 - E_2|}{\Delta E}\right), \text{ with } \Delta E = 1\ MeV$

How we varied

- Principal Component Analysis (PCA) of covariance matrix is do-able, but not very user friendly
  - Eigenvalues, λ_i, and eigenvectors, u_i, may be easy to convert into samples
  - Explaining shape of sample to users is not



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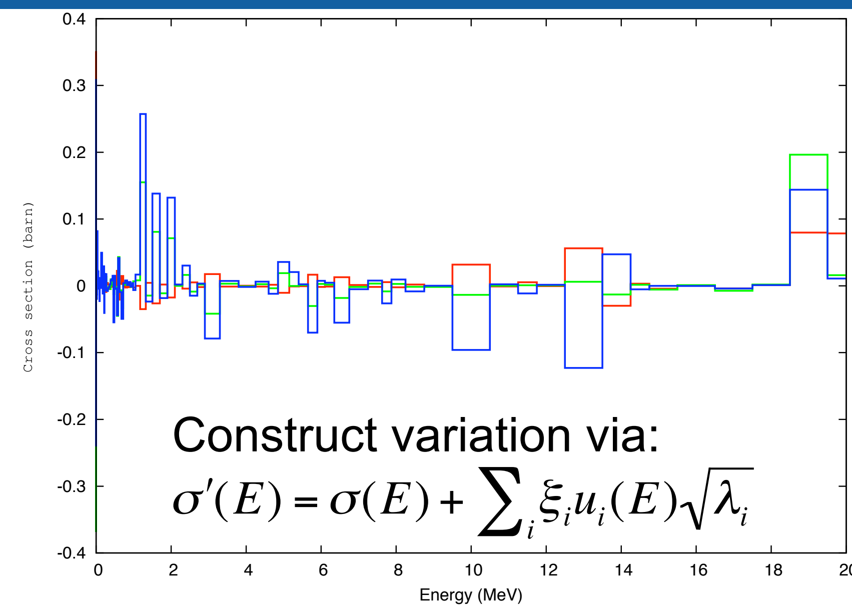
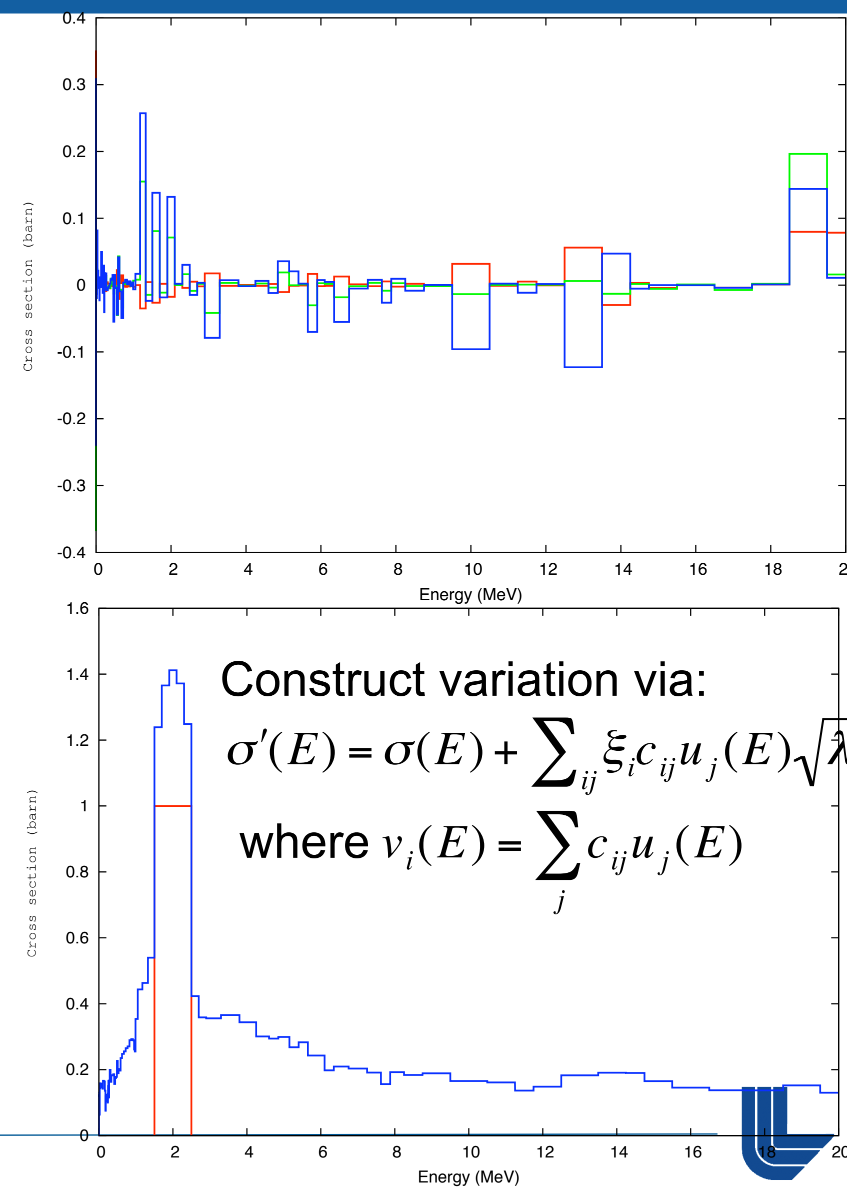


How we varied

- Principal Component Analysis (PCA) of covariance matrix is do-able, but not very user friendly
  - Eigenvalues, λ_i, and eigenvectors, u_i, may be easy to convert into samples
  - Explaining shape of sample to users is not
- Instead, user requests a variation shape, v_i, then we give them the closest thing in the eigenbasis of the covariance
- Using new variations, perform standard sampling & variation as in PCA

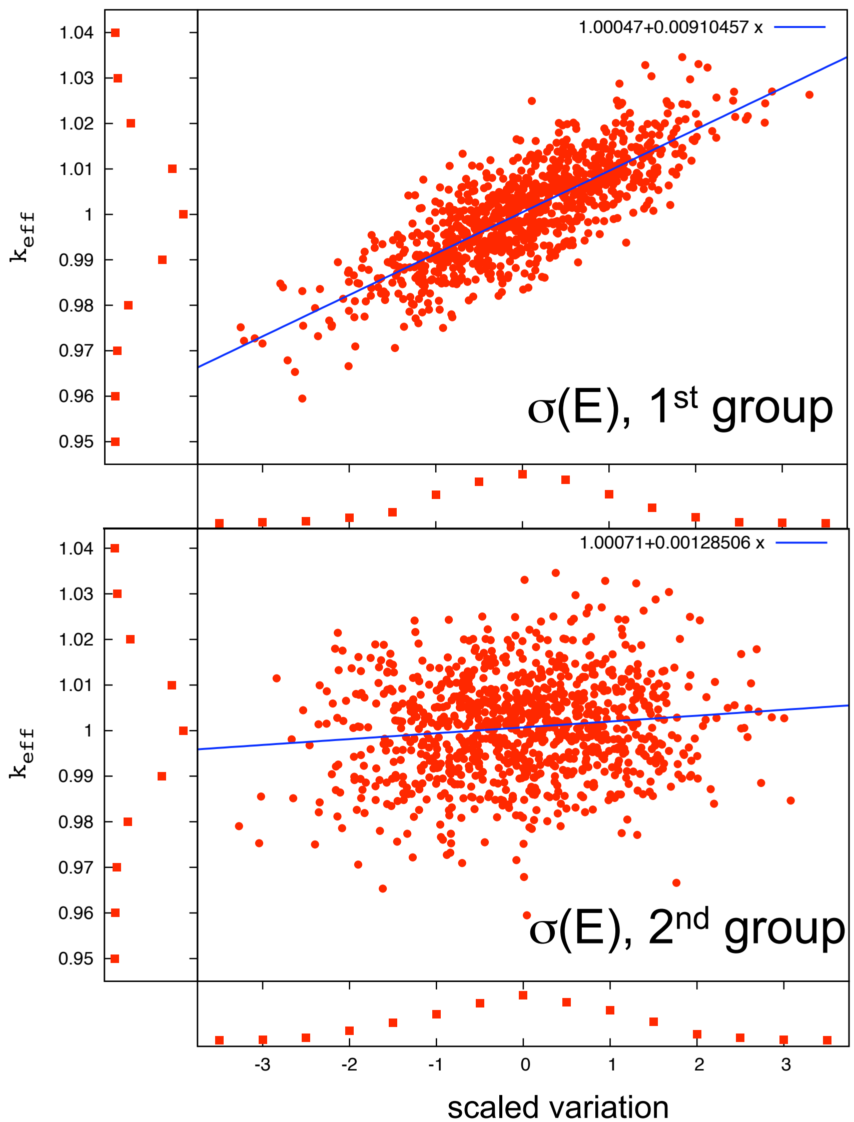


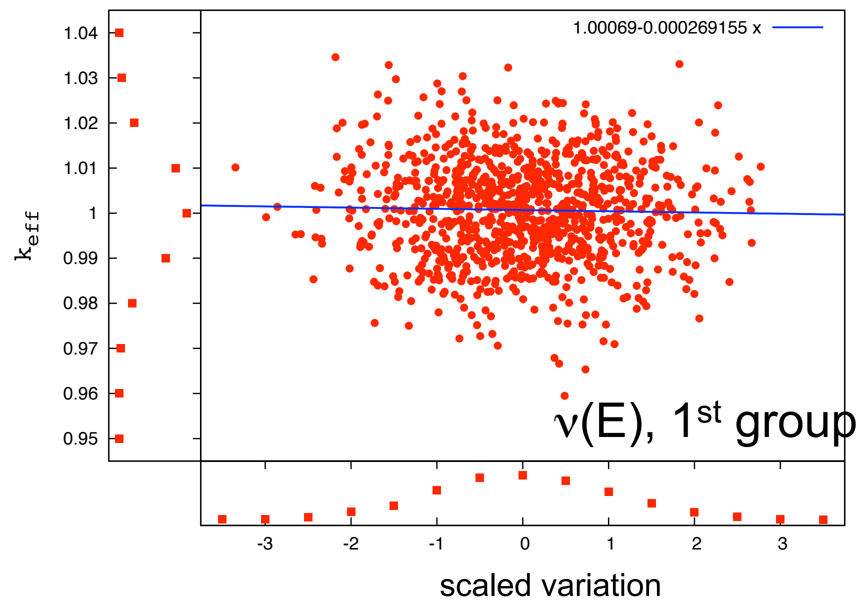
Construct variation via:

$$\sigma'(E) = \sigma(E) + \sum_{ij} \xi_i c_{ij} u_j(E) \sqrt{\lambda_j}$$

where $v_i(E) = \sum_j c_{ij} u_j(E)$

What we found





985 realizations

Strong sensitivity to cross section apparent, especially in lower 2 energy groups.

Weak sensitivity to multiplicity probably due to gross over estimate of uncertainties

Option:UCRL#

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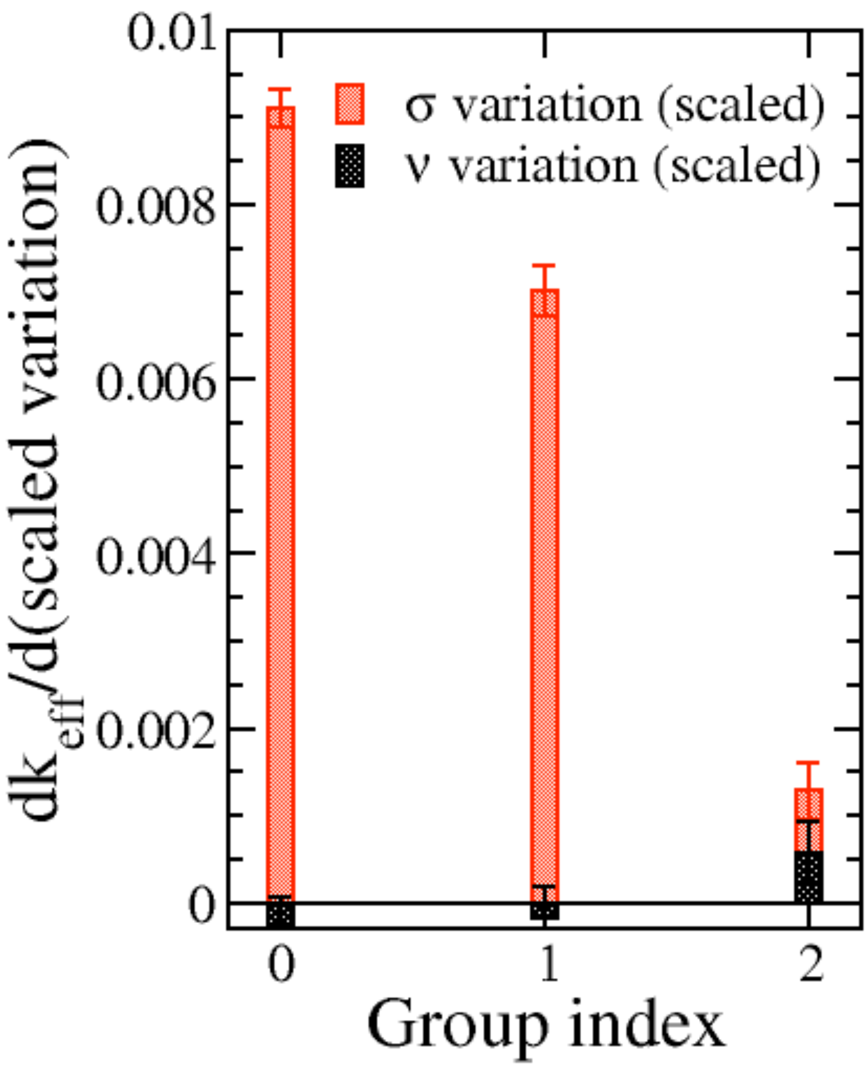
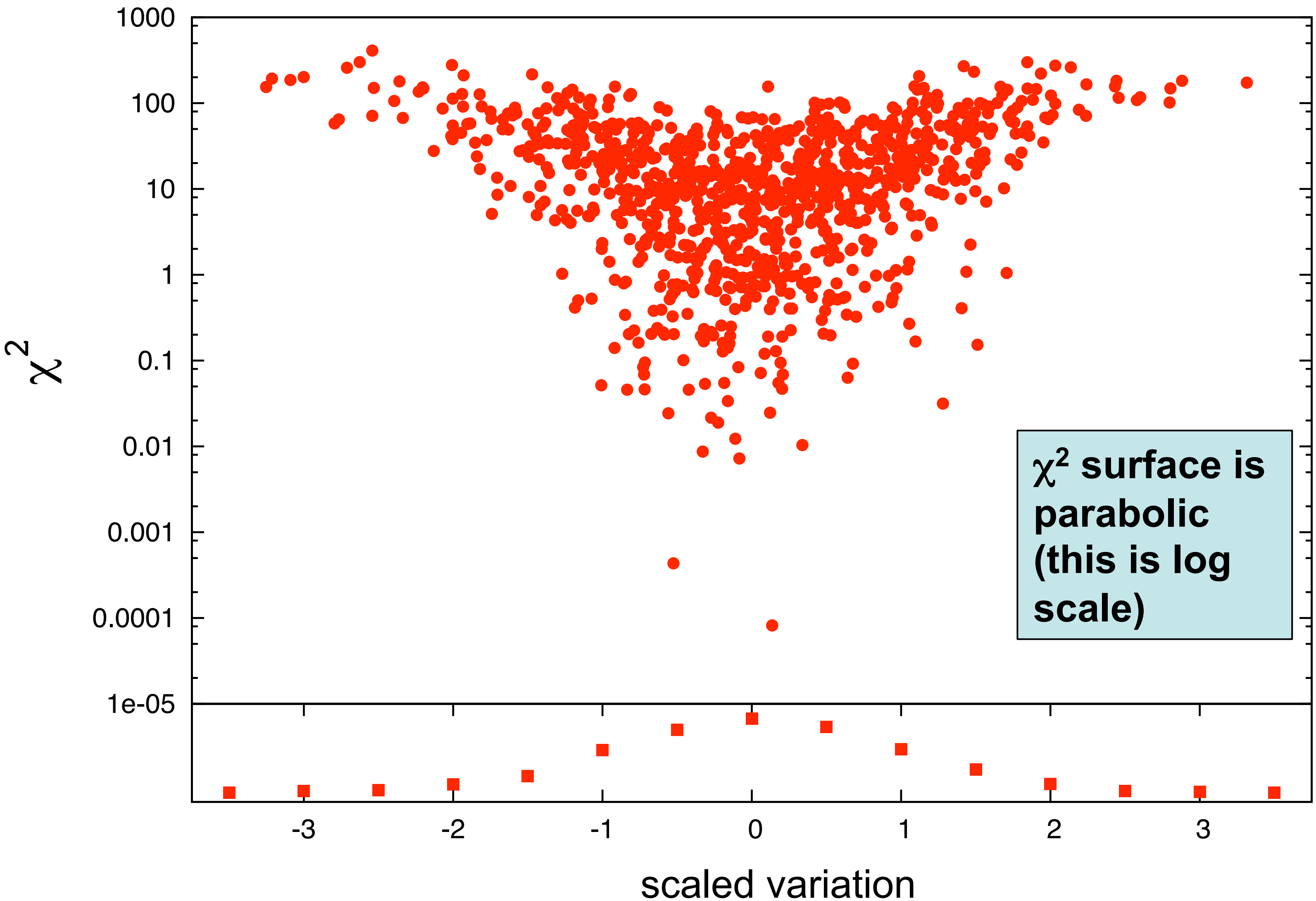


Surprisingly, response of k_{eff} to variations in nubar (which were far overstated) are negligible and consistent with zero.

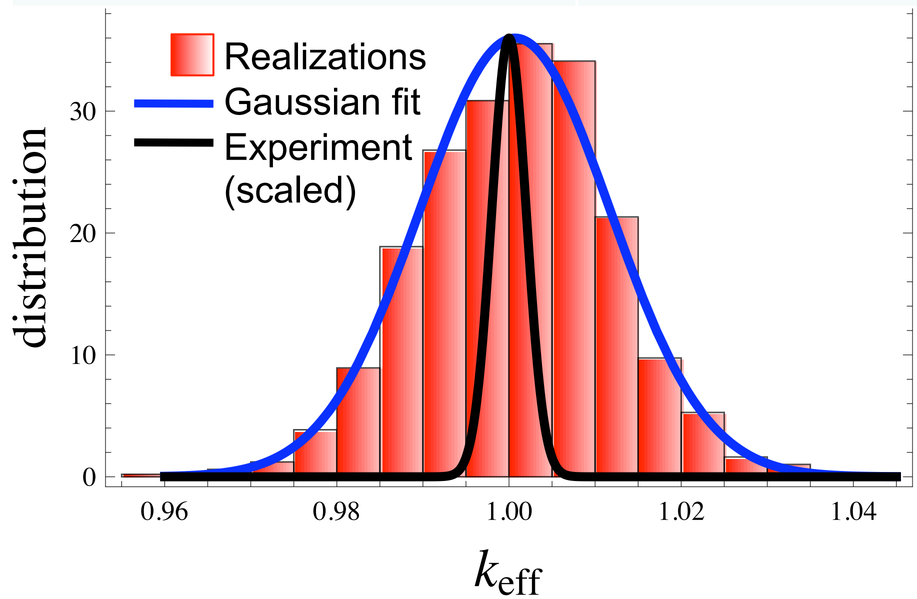
Response to k_{eff} to variations in cross section are sizeable in first two groups, negligible from 10 MeV onwards (in the last energy group).

What we found



Summary of k_{eff} for Jezebel

	k_{eff}
Experiment	1.000 ± 0.002
Using mean values	1.0006609
Sensitivity matrix approach*	0.9953 ± 0.00024
Monte Carlo approach	1.00069 ± 0.0111



Not a fair comparison: Gila & Leal used ENDF/B-VI library for mean values, took covariance from JENDL-3.3 library. They also varied (n,el) and (n,γ) cross sections.
They used the TSUNAMI and SCALE system.

* From Choong-Sup Gila and L.C. Leal, “A Sensitivity and Uncertainty Analysis of keff Values on Fast and Thermal Benchmarks with the Covariance Data,” International Conference on Reactor Physics, Nuclear Power: A Sustainable Resource Casino-Kursaal Conference Center, Interlaken, Switzerland, September 14-19, 2008.