PFNS: Consistent Evaluations, UQ, and Propagation of Uncertainties

[1,2]M. E. Rising, [1]P. Talou, [2]A. K. Prinja,

[1]T. Kawano, and [3]M. White

[1]T-2 Theoretical Division
Los Alamos National Laboratory

[2]Department of Chemical and Nuclear Engineering
University of New Mexico

[3]XCP-5 Applied Physics Division
Los Alamos National Laboratory

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Motivation

- **Uncertainty Quantification:**
  - Nuclear application community in need of nuclear data uncertainties
  - Nuclear data: cross sections, angular distributions, prompt fission neutron spectra, etc.
  - Importance: cross section uncertainties ~ PFNS uncertainties
  - Update/include PFNS evaluations in ENDF/B-VII library
    - Theoretical model changes
    - New experimental results

- **Uncertainty Propagation:**
  - Nuclear data uncertainties are meaningless unless impact on applications is quantified
  - Feedback to nuclear data community: theoretical physics, experimental measurements, correlations in older experiments, etc.

Systematic Evaluation and UQ of Prompt Fission Neutron Spectra (PFNS)

- "Systematic Uncertainty Quantification of Prompt Fission Neutron Spectra," M.E.Rising, P.Talou, T.Kawano and A.K.Prinja, submitted to Nucl. Sci. & Eng. (LA-UR-12-21035).
- **Los Alamos model for PFNS, extended with anisotropy parameter**
  D.G. Madland and J.R. Nix, *Nucl. Sci. Eng.*, **81**, 213 (1982).
- **Input *prior* model parameters**
  A. Tudora, *Ann. Nucl. Energy*, **36**, 72 (2009).
- **Experimental database from EXFOR / IAEA CRP**
  + UQ following Standards Evaluation Methodology (GMA)
- **Bayesian Kalman filter**

Systematic Uncertainty Quantification of Prompt Fission Neutron Spectra

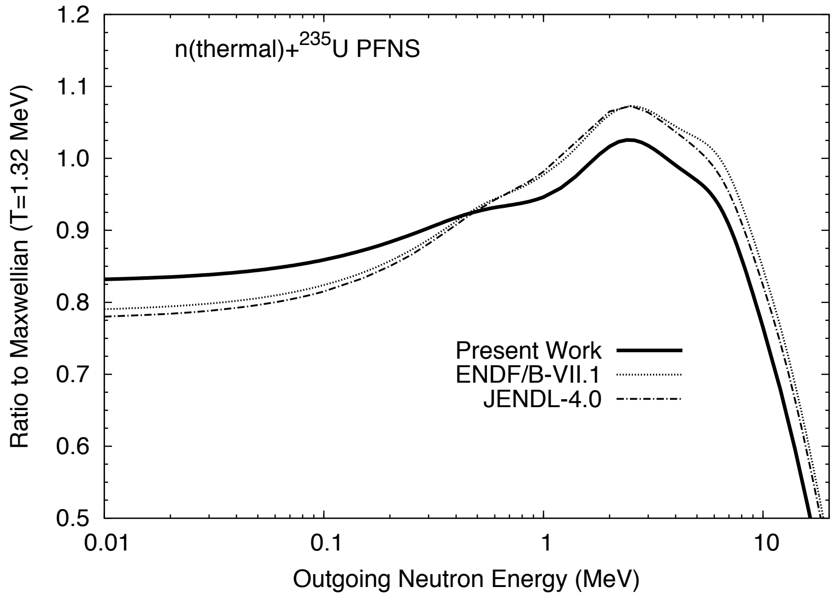
M.E.Rising*,†, P.Talou*, T.Kawano* and A.K.Prinja†

**T-2, Nuclear and Particle Physics, Astrophysics and Cosmology Theoretical Division, Los Alamos National Laboratory, USA*

†Chemical and Nuclear Engineering Department, University of New Mexico, USA

Los Alamos Model (LAM) with Anisotropy Parameter

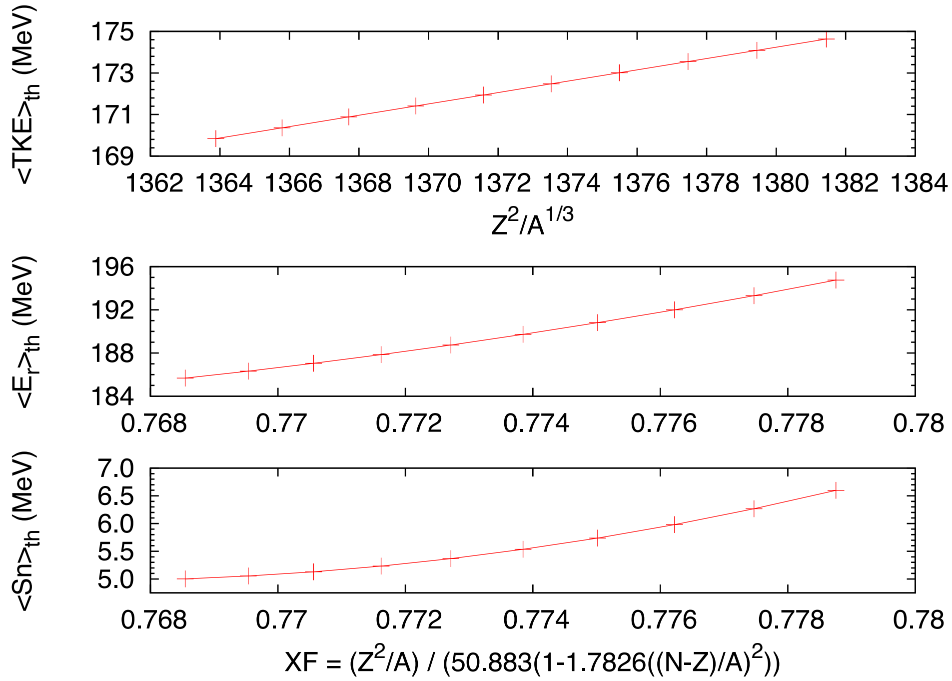
- **LAM based on nuclear evaporation theory and averaging over fission fragment distribution**
- **Few tunable parameters**
- **Recent evaluation includes anisotropy parameter, b**
- **Original LAM / Extended LAM:**



$$N(E) = \frac{1}{2\sqrt{E_f T_m^2}} \frac{1}{1+b/3} \int_{(\sqrt{E}-\sqrt{E_f})^2}^{(\sqrt{E}+\sqrt{E_f})^2} d\epsilon \sigma_c(\epsilon)\sqrt{\epsilon} \left(1 + b\frac{(E-\epsilon-E_f)^2}{4\epsilon E_f}\right) \int_0^{T_m} dT k(T) T \exp(-\epsilon/T)$$

LAM parameters

- **Study a suite of isotopes**
- **Advantages:**
  - Cross-isotope correlations!
  - Consistent evaluation procedure
  - Reasonable evaluations and UQ where no data exist
- **Limitations:**
  - Incident energy dependence not yet considered
  - Experimental database is limited with discrepant data
- Prior parameters: A.Tudora, *Ann. Nucl. Energy*, **36**, 72 (2009).



$$\langle \mathrm{TKE} \rangle_{th} = \alpha_1 + \alpha_2 \frac{Z^2}{A^{1/3}} \, ,$$
$$\langle E_r \rangle_{th} = \alpha_3 + \alpha_4 x + \alpha_5 x^2 \, ,$$
$$\langle a \rangle = A/\alpha_6 \, ,$$
$$b = \alpha_7 \, .$$

$$x = \left(\frac{Z^2}{A}\right) / \left(50.883\left(1 - 1.7826\left(\frac{N-Z}{A}\right)^2\right)\right)$$

Evaluation Methodology: Experimental Data

- **Differential data in EXFOR database**
- **Use GMA code methodology to calculate experimental covariance**
  W.P. Poenitz and S.E. Aumeier, ANL/NDM-139 (1997).
- **IAEA CRP on Prompt Fission Neutron Spectra for Actinides (R. Capote)**
  - Some modifications to experimental datasets
  - Computed experimental covariance matrices

Uranium PFNS Differential Measurements

Mass # (A)	First Author	Date	E_{inc} (MeV)	E_{out} (MeV)	EXFOR Entry
233	Miura	2002	0.55	0.7-12.1	22688-002
233	Lajtai	1985	thermal	0.03-3.855	30704-002
233	Starostov	1985	thermal	0.83-9.3	40930-004
233	Boytsov	1983	thermal	0.025-4.6	40873-002
235	Kornilov	2010	thermal	0.68-11.8	31692-002
235	Vorobyev	2010	thermal	0.21-10.8	41516-017
			. . . .		

Evaluation Methodology: Kalman Filter

- **Assumes a normal distribution shape for posterior PDF**
- **For linear Kalman filter, LAM is taken to be a linear, first-order approximation**

$$f(\vec{x}) \cong f(\vec{x}_0) + \mathbf{C}(\vec{x} - \vec{x}_0)$$

- **Combining experimental data and theoretical model**
  - Posterior parameters:

$$\vec{x}_1 = \vec{x}_0 + \mathbf{P}\mathbf{C}^T\mathbf{V}^{-1}(\phi - f(\vec{x}_0))$$
$$= \vec{x}_0 + \mathbf{X}\mathbf{C}^T\left(\mathbf{C}\mathbf{X}\mathbf{C}^T + \mathbf{V}\right)^{-1}(\phi - f(\vec{x}_0))$$

  - Posterior parameter covariance matrix:

$$\mathbf{P} = (\mathbf{X}^{-1} + \mathbf{C}^T\mathbf{V}^{-1}\mathbf{C})^{-1}$$
$$= \mathbf{X} - \mathbf{X}\mathbf{C}^T\left(\mathbf{C}\mathbf{X}\mathbf{C}^T + \mathbf{V}\right)^{-1}\mathbf{C}\mathbf{X}$$

PFNS

$$\Phi = f(\vec{x}_1)\,,$$

$$\mathbf{F} = \mathbf{C}\mathbf{P}\mathbf{C}^T$$

Numerical Results: $^{229-238}U$

- **Parameter prior, posterior and uncertainties**

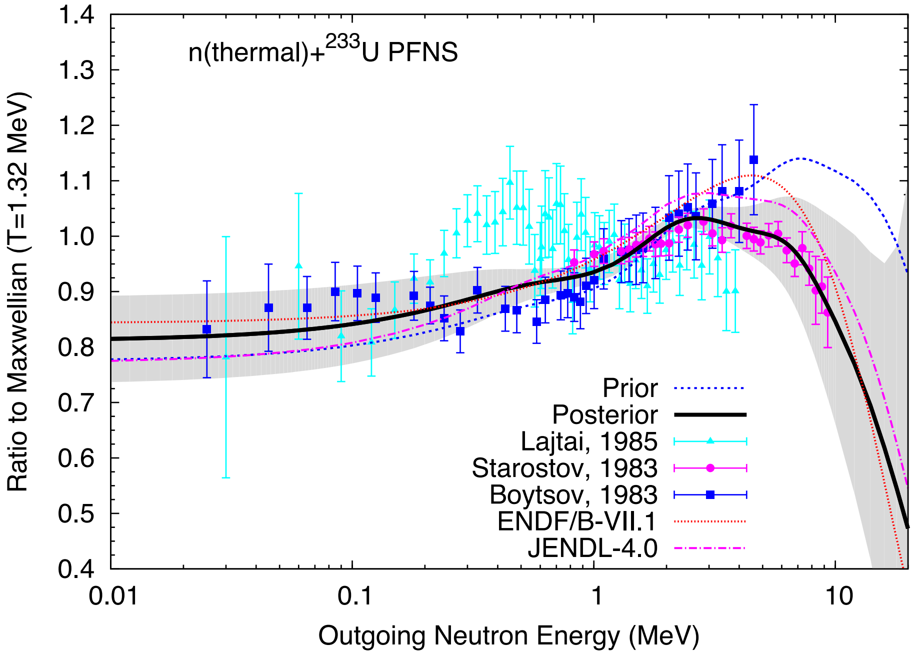
Parameter	Prior Value	Prior Uncertainty (%)	Posterior Value	Posterior Uncertainty (%)
α_1	171.412	2.0	168.567	0.52
α_2	0.273	100.0	0.228	78.29
α_3	187.850	6.0	185.125	0.37
α_4	784.342	50.0	442.208	63.56
α_5	25586.4	25.0	20783.4	30.04
α_6	11.000	4.0	10.094	3.78
α_7	0.100	50.0	0.098	16.04

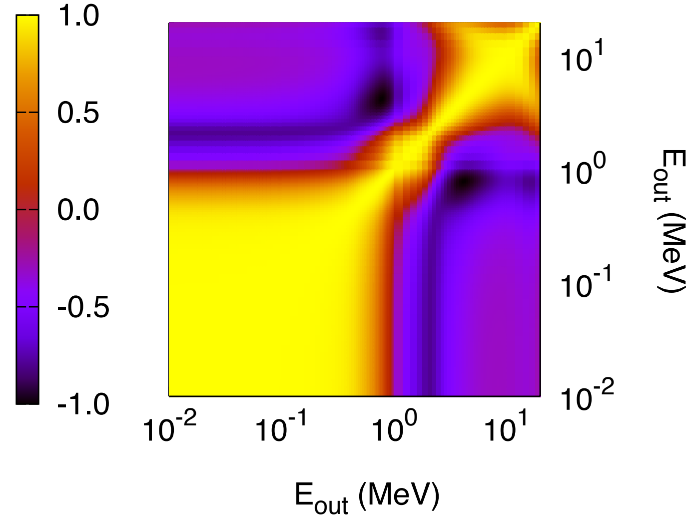
- **Parameter posterior correlations**

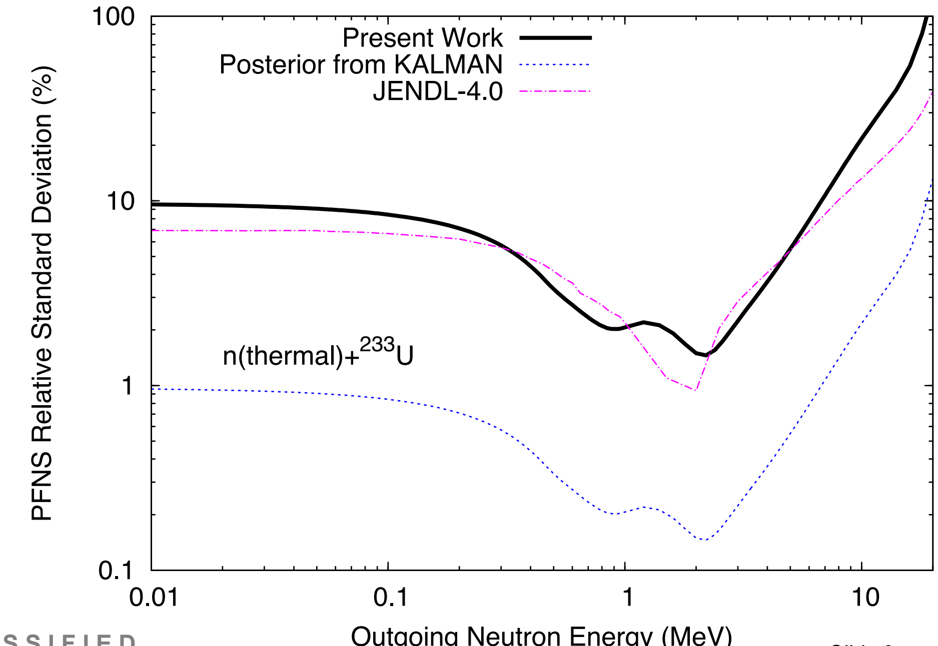
Parameter	α_1	α_2	α_3	α_4	α_5	α_6	α_7
α_1	100						
α_2	-1	100					
α_3	36	0	100				
α_4	-3	97	0	100			
α_5	-3	-4	0	-2	100		
α_6	61	-1	-50	-2	-3	100	
α_7	25	0	7	-2	-1	11	100

Numerical Results: ^{233}U

- **ENDF/B-VII.1 missing covariance matrix for n+^{233}U PFNS**



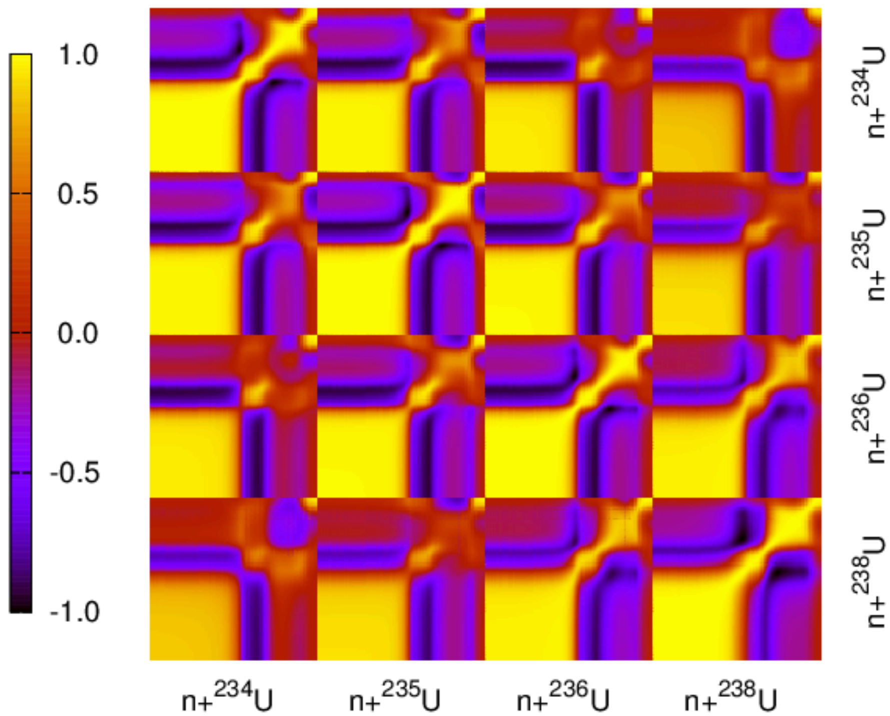




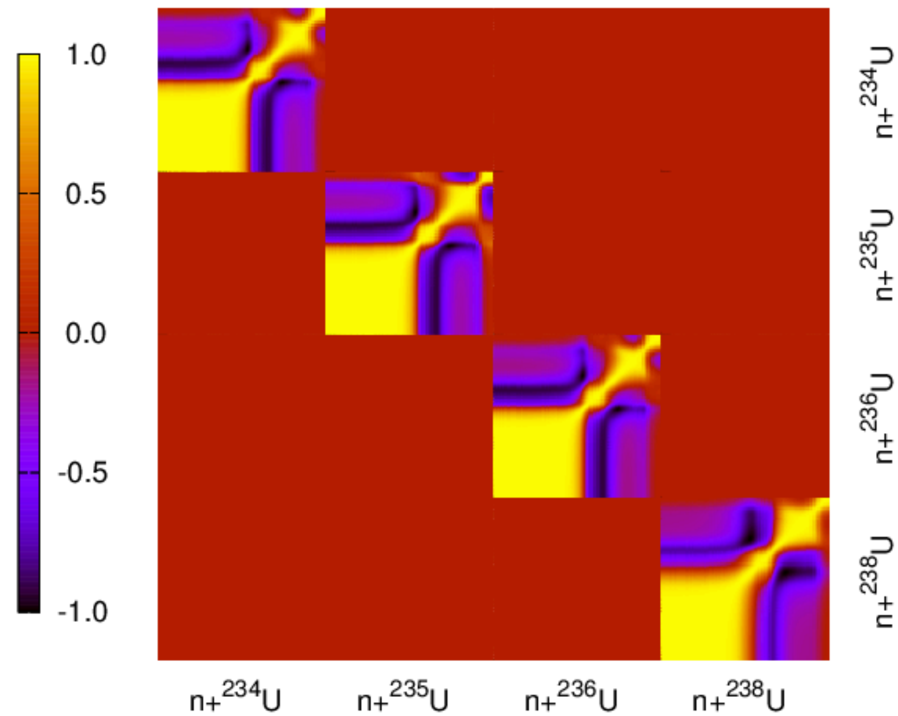
Numerical Results: Cross-Isotope PFNS Correlations

- **Big Ten assembly contains: ^{234}U, ^{235}U, ^{236}U, and ^{238}U**

Correlated PFNS



Uncorrelated PFNS



Numerical Results: Cross-Isotope PFNS Correlations

- **Big Ten assembly:**
  - Contains 10 metric tons of uranium metal
  - Average of 10% ^{235}U enrichment ➔ Intermediate enriched uranium
  - Fast critical assembly
  - MCNP5-1.60 two-zone homogenized cylindrical core model (IEU-MET-FAST-007)
- **Integral Quantities:**
  - Multiplication factor: k_{eff}
  - Spectral Indices: $I^{(238f)}$, $I^{(237f)}$, and $I^{(239f)}$
- **Comparison of U.S. nuclear data libraries**

Integral Parameter	Data Library		Present Work	Experimental Benchmark*
	ENDF/B-VII.0	ENDF/B-VII.1		
k_{eff}	0.99496(7)	0.99460(7)	0.99243(7)	0.9948(13)
$\mathcal{I}^{(238f)}$	0.0353(6)	0.0358(7)	0.0353(6)	0.03739(34)
$\mathcal{I}^{(237f)}$	0.312(2)	0.313(3)	0.311(2)	0.3223(30)
$\mathcal{I}^{(239f)}$	1.163(5)	1.162(5)	1.163(5)	1.1936(84)

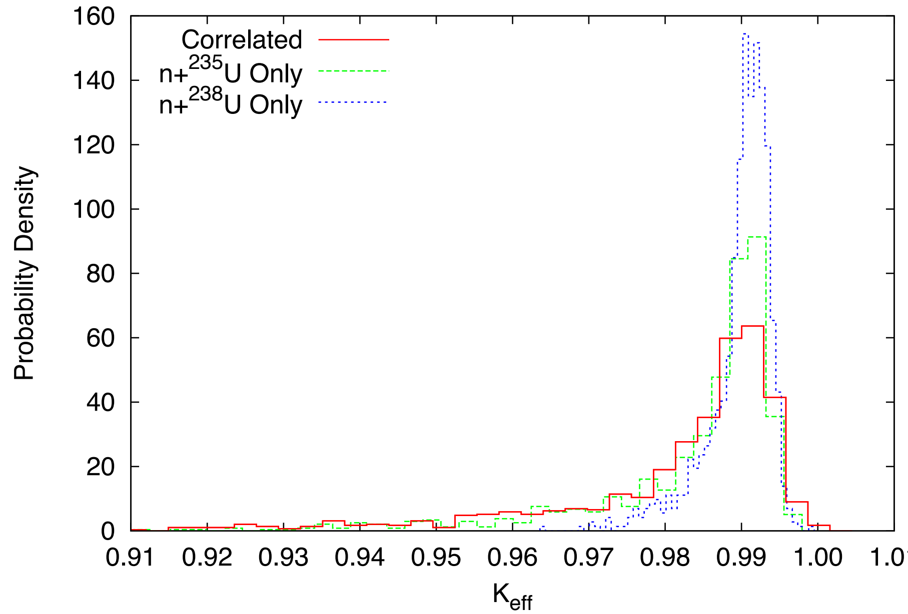
*Taken From ICSBEP Handbook

Numerical Results: Cross-Isotope PFNS Correlations

- **Uncertainty propagation:**
  - Principal Component Analysis (PCA) on model parameter covariance

$$\vec{x}_m = \langle \vec{x} \rangle + \sum_{k=1}^{K} \sqrt{\lambda_k} \vec{\varphi}_k \xi_{k,m}$$

  - Assume independent Gaussian distribution for principal components
  - "Brute force" Monte Carlo: 1,000 realizations



Integral Parameter	Monte Carlo Statistics (%)	Uncertainty (%)					
		Uncorrelated					Correlated
		^{234}U	^{235}U	^{236}U	^{238}U	Total	Total
k_{eff}	0.010	0.010	1.437	0.009	0.430	1.500	1.818
$\mathcal{I}^{(238f)}$	2.000	1.557	6.707	1.525	2.359	7.436	8.303
$\mathcal{I}^{(237f)}$	0.300	0.543	1.644	0.546	0.703	1.947	1.974
$\mathcal{I}^{(239f)}$	0.400	0.086	0.160	0.075	0.085	0.214	0.190

Conclusions

- **New evaluations of the PFNS and uncertainties for all uranium and plutonium actinides below second-chance fission**
  - Submitted to NSE journal in May 2012
- **Modified ENDF/B-VII.1 data files including the new evaluations and covariance matrices available for testing**
- **Correlations between major and minor actinides exist through model parameters**
  - Impact on integral quantities seen in Big Ten assembly
  - More work on uncertainty propagation in preparation for ND 2013 (poster)

Questions?

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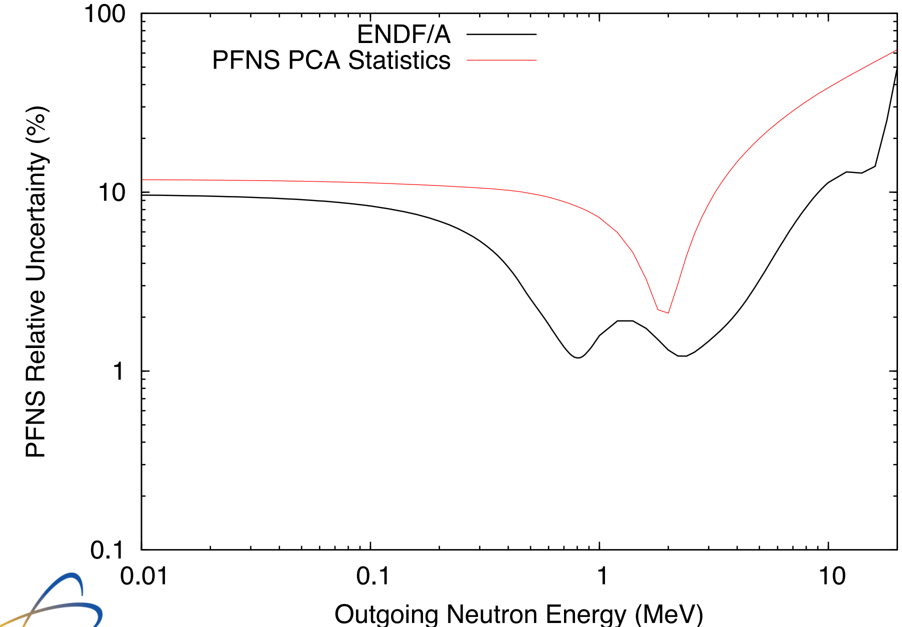
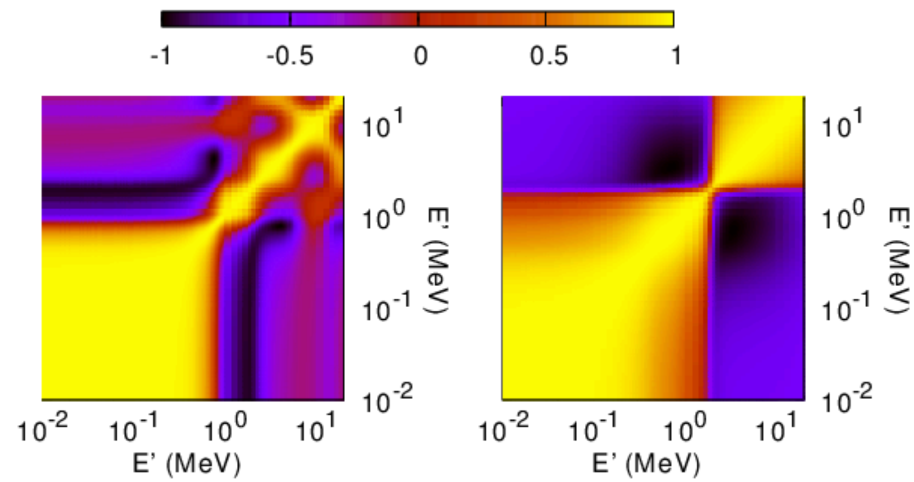
Additional Slides: Sampling Considerations

- **Systematic evaluation of PFNS**
  - New evaluation of uranium and plutonium
  - Cross-isotope correlations
  - Model parameter correlations (7x7 covariance matrix) vs. PFNS correlations
- **Sampling differences:**

$$\mathbf{F} = \mathbf{C}\mathbf{P}\mathbf{C}^T$$





(a) (b)

Abstract

This presentation consists of some recent work done on uncertainty quantification and propagation through fast critical assemblies of the prompt fission neutron spectra (PFNS) for many actinides. Specifically, we obtain cross-isotope correlations in the uranium and plutonium actinides and we study the impact of these correlations on the Big Ten fast critical assembly.