Reducing nuclear data uncertainties using differential and integral benchmark data

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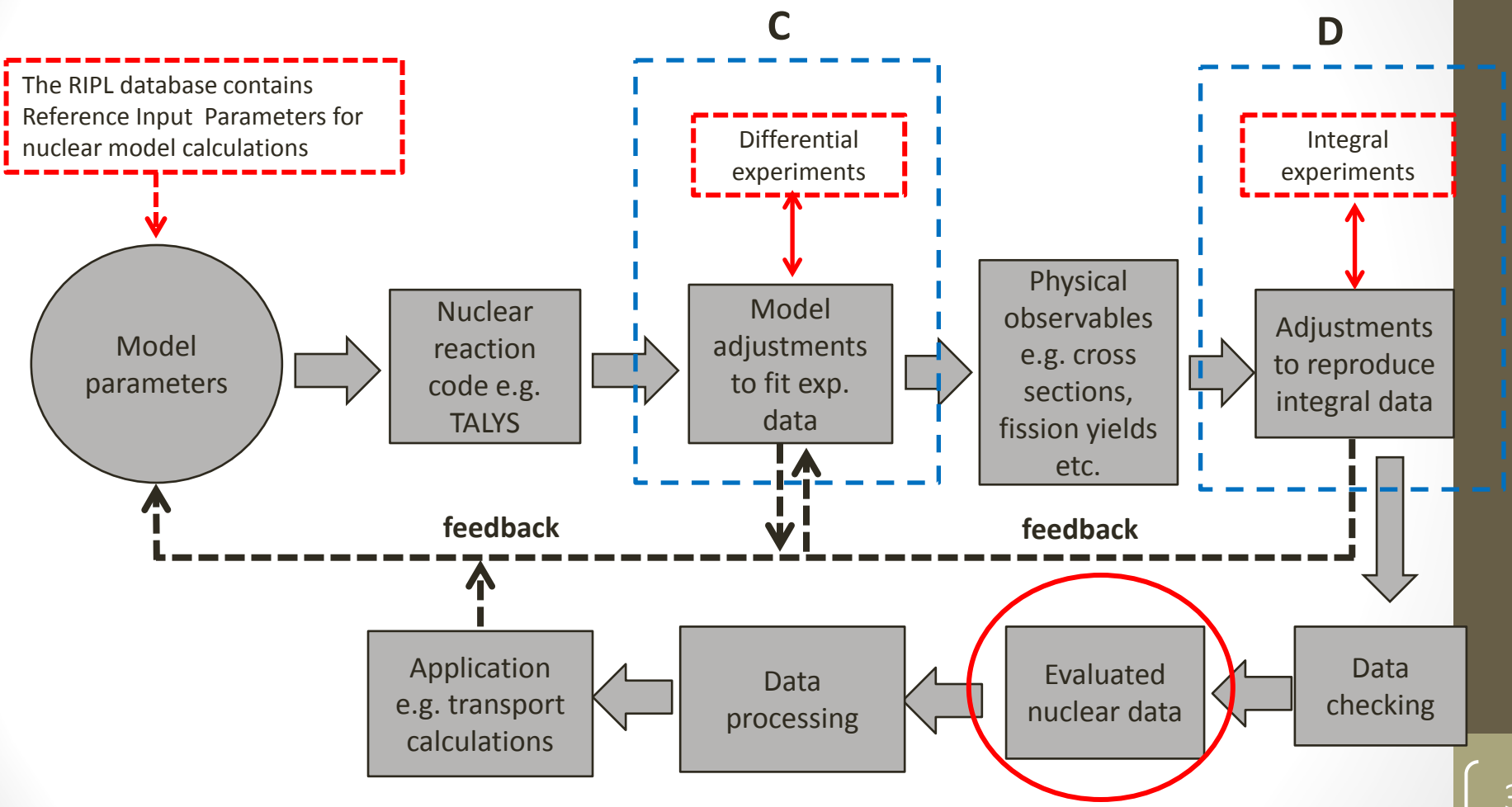
Outline

A. Modern nuclear data evaluation
B. Total Monte Carlo
C. Incorporating differential data
D. Incorporating integral data
E. Goal: Combine C and D (work on-going)
F. Some results
G. Conclusion

Modern nuclear data evaluation*



* A.J. Koning and D. Rochman (2012). Modern Nuclear data evaluation with the TALYS code system. Nuclear Data Sheets, 113 (12) 2841-2934

Uncertainty quantification

- Both differential data and integral data come with associated uncertainties

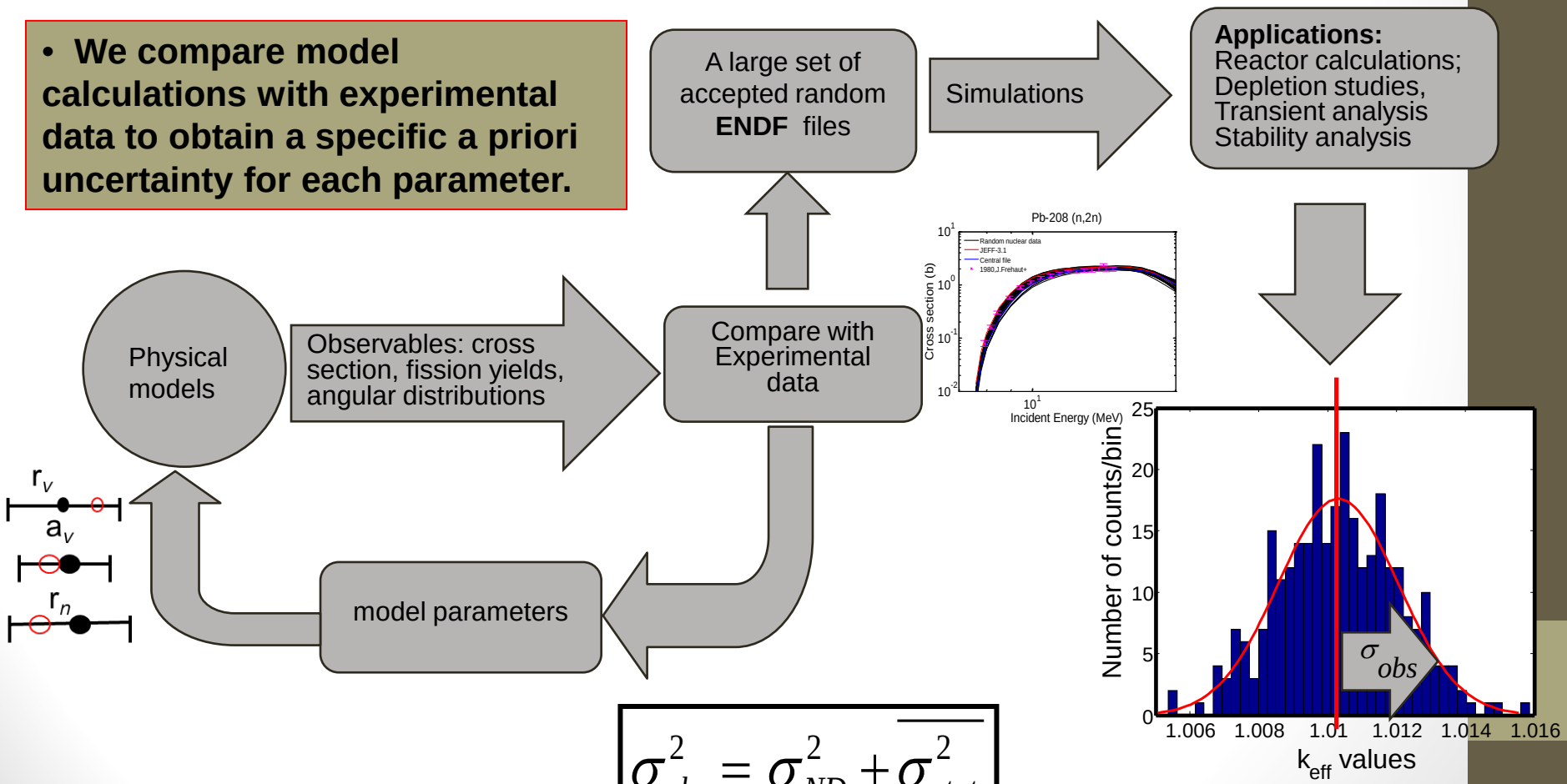
- ⇒ the end product – evaluated nuclear data files contains uncertainties as well

- A Monte Carlo based method called '**Total Monte Carlo (TMC)**' was developed in 2008 for nuclear data uncertainty quantification:
  - **Ref: A.J. Koning and D. Rochman, 2008. Annals of Nuclear Energy, 35 (11), 2024 – 20130.**

- Other methods exist

Total Monte Carlo (TMC)

- **We compare model calculations with experimental data to obtain a specific a priori uncertainty for each parameter.**



$$\sigma_{obs}^2 = \sigma_{ND}^2 + \overline{\sigma_{stat}^2}$$

Uncertainty reduction

Physical models parameters: TALYS based system (T6)

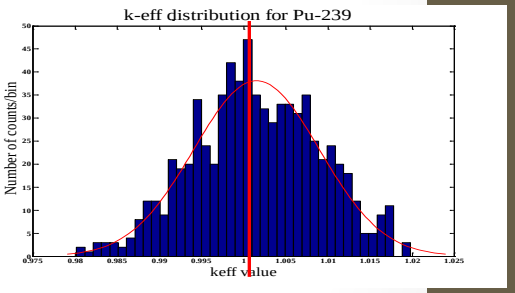
1st level of constraint: **Differential data**

A large set of acceptable ND libraries

Simulations: mcnp etc.

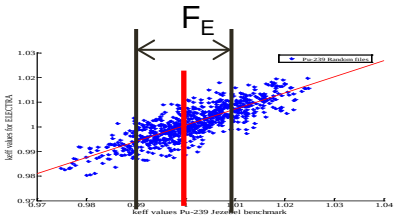
Applications: Criticality, burnup, Fuel cycle etc.

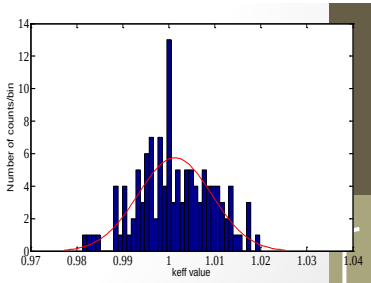
Prior k_{eff} distribution



Involves two steps:
Random nuclear data from the 1st step is used as the prior for the 2nd step.

2nd level of constraint: **Integral benchmarks**





Assign weights to random files

Weighted random files

Simulations: mcnp etc.

Applications: Criticality, burnup, Fuel cycle etc.

Posterior k_{eff} distribution

Incorporating differential data

- If $\mathbf{C_E}$ is our differential experimental covariance matrix;
- We can compute a generalized χ_k^2 :

$$\boxed{\chi_k^2 = \left(x - \tau(p^{(k)})\right)^T C_E^{-1}\left(x - \tau(p^{(k)})\right)} \qquad (*1)$$

- Where;
  - $\tau(p^{(k)})$ is a vector of calculated observables found in the ***k^th*** random file
  - $P^{(k)}$ is the parameter set of the ***k^th*** random file
  - x is a vector of experimental observables

- We then assign each random file a weight based on the likelihood function:

$$\boxed{w_{k(E)} = e^{-\frac{1}{2}\chi_k^2}} \qquad (*2)$$

Ref: P. Helgesson et. al., 2014. . Incorporating experimental information in the TMC methodology using file weights. Int. Workshop on Nuclear Data Covariances

2nd level of constraint - Incorporating integral data

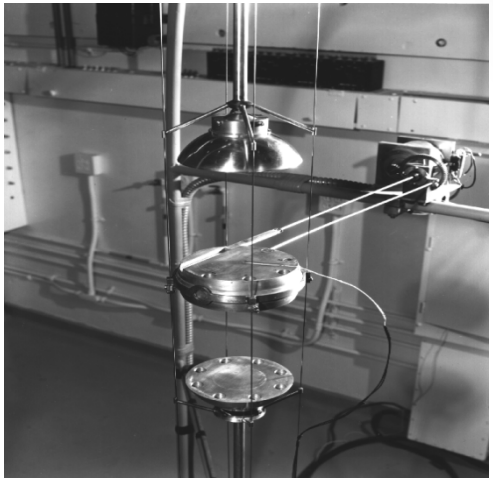
- Criticality benchmark cases
- Application case
- Incorporate integral data
  - Accept/reject method
  - Assign weights based on the likelihood function

Cases available

1. **Benchmark cases:**

- **International Criticality Safety Benchmark Evaluation Project (ICSBEP)**
  - Contains about 4708 critical and subcritical configurations etc.

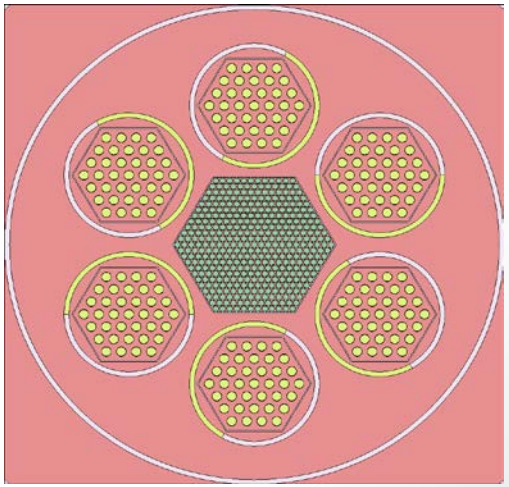
- **Experiments are Categorized into:**
  - fissile media (Pu, HEU, LEU etc.)
  - physical form of the fissile material
  - neutron energy range



Benchmark example – ^{239}Pu Jezebel.
Picture taking from the ICSBEP Handbook

2. **Application case:**

- European Lead-Cooled Training Reactor (ELECTRA)
- Part of GEN-IV research in Sweden
- Research and training



Wallenius et al., 2012. Nuclear Technology Vol. 177, p. 303-313.

Incorporating integral data

- Only relevant benchmarks for a particular application system must be used
  - **Ref: E. Alhassan et. al., 2014. Selecting benchmarks for reactor calculations. PHYSOR 2014 Int. Conference**

- We compute a similarity index using the Pearson correlation coefficient:

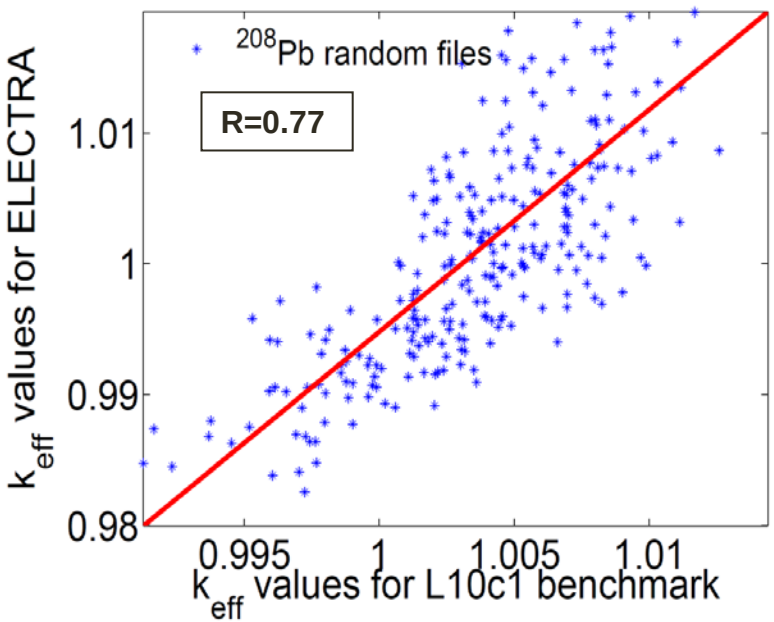
$$R = \frac{\mathrm{cov}(keff_{sys}, keff_{BM})}{\sigma_{keff_{sys}} \sigma_{keff_{BM}}}$$

- Simulations are performed with the same nuclear data for both application and benchmark cases

- Strong correlation → strong similarity
- Weak correlation → weak similarity

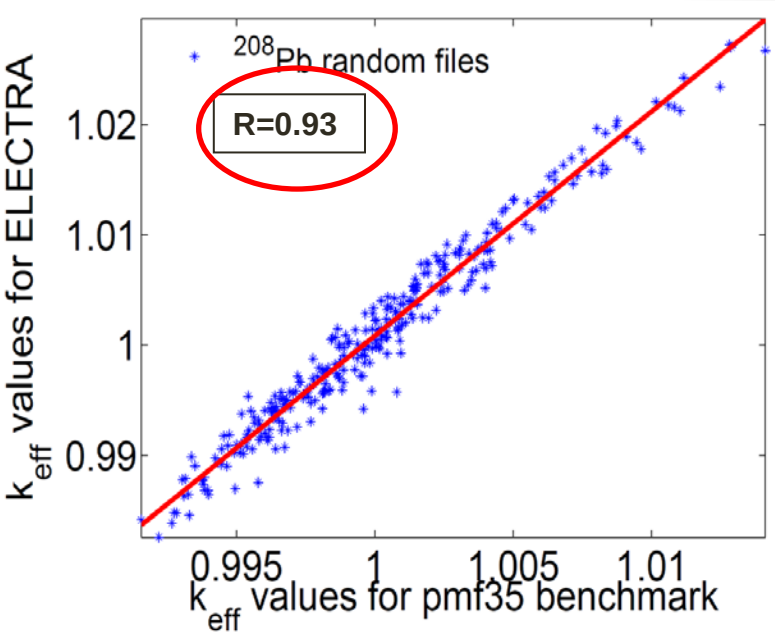
Similarity between benchmark and application case (ELECTRA)

ELECTRA against LCT17 case 2



LCT – LEU Compound Thermal

ELECTRA against pmf35

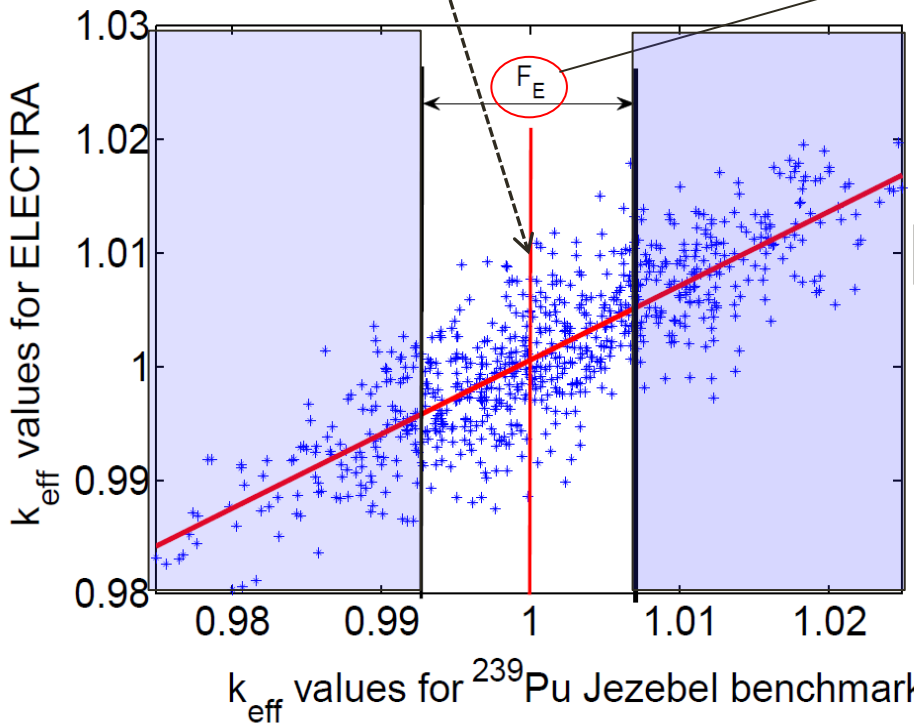


PMF– Plutonium Metallic Fast

Perturbed Pb-208 nuclear data were used

Accept/reject method

Evaluated Benchmark k_{eff} value = 1.000 ±0.002



R=0.83

F_E=238 pcm

- F_E is directly proportional to the evaluated benchmark uncertainty, σ_E:

$$F_E \propto \sigma_E \Rightarrow F_E = \kappa \sigma_E$$

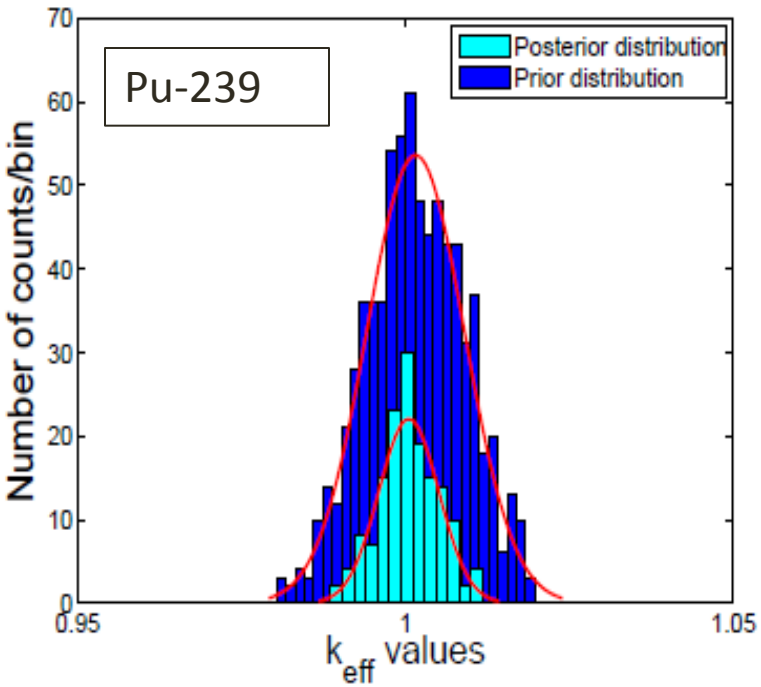
$$\kappa = \frac{1}{|R|}$$

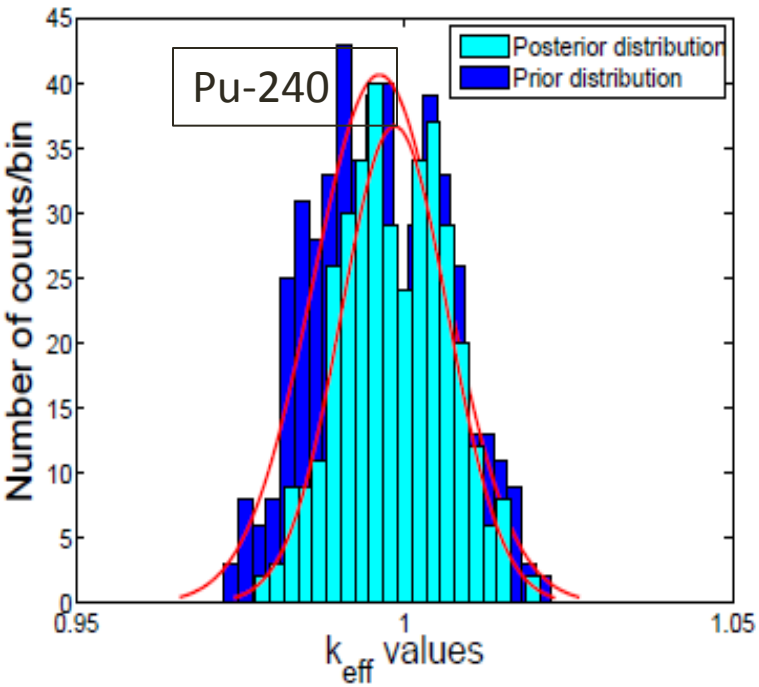
Where R is the Pearson correlation coefficient.

By setting $\kappa = \frac{1}{|R|}$ less weights are assigned to benchmarks with weak correlation to the application case while strongly correlated systems are assigned higher weights.

Prior – posterior k_{eff} distributions for Accept/reject method

Prior → Differential data only
Posterior → Differential and integral data





40% uncertainty reduction achieved for ELECTRA

20% uncertainty reduction achieved for ELECTRA

Using the likelihood function

- A more rigorous method is to base the uncertainty reduction on the maximum likelihood function
- Assign weights to random files using:

$$w_{i(B)} = \frac{e^{-\frac{1}{2}\chi_i^2 |R|}}{e^{-\frac{1}{2}\chi_{\min}^2 |R|}} \qquad (*3)$$

- ***R*** is the correlation between benchmark and the application case
- Chi-squared is given by:

$$\chi_i^2 = \frac{(k_{eff\,(i)}^E - k_{eff,\exp}^E)^2}{\sigma_E^2}$$

- ***R*** ensures that only relevant benchmarks for a particular application case are used.

Accept/reject vs. maximum likelihood

- **Results in brackets represent the percentage reduction achieved after implementing the two methods.**

Isotope	Benchmark	Prior [pcm]	Accept/reject [pcm]	Maximum Likelihood [pcm]
^{239}Pu	pmf1	723 ± 23	445 ± 15 (38%)	469 ± 32 (35%)
^{240}Pu	pmf1	1011 ± 32	809 ± 26 (20%)	869 ± 33 (14%)
^{241}Pu	pmf1	1191 ± 38	1191 ± 38 (0%)	1185 ± 41 (0.5%)

A significant reduction in uncertainty was achieved for Pu-239 and Pu-240 after adding benchmark information.

Our goal: Combine C and D

- **Thinking of two approaches:**

1. **Calculate a weighted total χ_T^2 (Similar to the Petten method):**

$$\chi_T^2 = \frac{w_B \chi_B^2 + w_E \chi_E^2}{w_B + w_E}$$

By plotting χ_T^2 as a function of random nuclear data, we can select a best file.

2. **Combine two weights; equation (*2) and (*3) (The Uppsala method):**

$$w_T = w_{k(E)} \times w_{i(B)}$$

For nuclear data uncertainty reduction

- Select the random file with the largest weight ***(best file for TENDL-2015?)***

- Post adjustment feedback to model calculations and experiments.

- **Method still under development (resonance region still a challenge).**

Conclusion

- We have proposed approaches for reducing ND uncertainties
- Method has been applied to:
  - A full LFR core at BOL
  - A set of criticality benchmarks from the ICSBEP handbook.
- A significant reduction in ND uncertainty was achieved.
- Methods can provide updated covariance matrix information and model parameter distributions for post adjustment feedback
- Apply these methods with multiple benchmarks is on-going
- Our goal: combine differential and integral data for nuclear data evaluation and uncertainty reduction (Improve TMC)

Thank you!

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