Influence of nuclear data parameters on integral experiment assimilation using cook’s distance

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Problem

What we have:

1. Nuclear data
2. Integral experiments
3. Adjustment method
4. Transposition: to interpolate the effect of ND uncertainties on ASTRID

Nuclear data and Covariances
CEA-COMAC files (prior)

+

Integral experiments
(JEZEBEL, FLATTOP…..)
[K_{eff} (C/E): uncertainty, sensitivity]

↓

Nuclear data and Covariances
CEA-COMAC files (posterior)

↓

ASTRID (Concept Reactor)
[K_{eff}: uncertainty, sensitivity]

Problem

What we are looking for:

- **Is the adjusted reliable?**
  - How good is the adjusted data ?
  - How many integral experiments are sufficient to adjust the nuclear data?
  - How many experiments are enough to represent a concept reactor?
  - How is an individual experiment (or ND) impacting the posterior?

- **Ways to convince:**
- Recipes to convince people about the methods:
  - Indicators for robustness of the method.
  - Validation domain and demonstrations to show that we are mastering the impact of inputs.

Background

- In the final stages of a nuclear reactor design work:
  - Requires a vast amount of computer simulations.
  - Must be made with well-defined datasets and codes
  - Well-validated versions of these datasets and codes.
  - Estimation for all sources of uncertainties.
  - Uncertainty quantification

VVUQ

- **Verification:**
  - Calculation scheme has no programming error.
  - Sequence of different modules is performed correctly.
- **Numerical Validation**: Comparing results with a standard calculation.
- **Experimental validation:** Comparing computation values with experiments.
- **Uncertainty quantification:** Uncertainties associated with nuclear data and system.

Transposition

- Transposition: interpolate the ability of a numerical ***scheme*** to predict the values (output) for a given application in terms of *uncertainty*.

- For a neutron parameter p (ex: k_{eff})

If the estimation of uncertainties obtained for a set of integral experiments {E} are: $\Delta(E)^{p}_{DN}$

Transposition is to estimate uncertainties on neutron parameter p for the concept R: $\Delta(R)^{p}_{DN}$

- Representativeness is often used to explain transposition:

Sensitivity of p wrt ND for R
Covariance of ND
Sensitivity of p wrt ND for E

$$r_{ER} = \frac{S_R \times M_\sigma . S_E^T}{\sqrt{S_R \times M_\sigma . S_R^T}\sqrt{S_E \times M_\sigma . S_E^T}}$$

Nuclear data adjustment

- **Nuclear data evaluation**: neutron induced reactions, theoretical models.
- Model *parameters* are predicted theoretically and are **uncertain** ➔ Uncertainty in ND
- Best set of *parameters*: comparing theory to experiments.

➔ Adjusted set of parameters

➔ Improved nuclear data

➔ Adjusted (reduced) nuclear data uncertainties

➔ Improved covariance matrices

How?

Bayesian inference

Approach: Bayesian inference

- $y = \{y_1, y_2, \ldots\ldots y_N\}$: experimentally measured values
- x: parameters defining a model (M) to simulate y
- t: calculated values using model to compare with y
- Conditional probability for the analysis of a new data set y

From theory

PDF of observed data set knowing x

$$p(\mathbf{x}|M,\mathbf{y},U) = \frac{p(\mathbf{x}|M,U).p(\mathbf{y}|\mathbf{x},M,U)}{\int d\mathbf{x}.p(\mathbf{x}|M,U).p(\mathbf{y}|\mathbf{x},M,U)}$$

$$posterior\,[p(\mathbf{x}|\mathbf{y},U)] = prior\,[p(\mathbf{x}|U)]\,.likelihood\,[p(\mathbf{y}|\mathbf{x},U)]$$

Bayesian inference

- Assimilate measurements information to adjust, update or reduce uncertainties

$$posterior\,[p(\mathbf{x}|\mathbf{y},U)] \propto e^{-(1/2)((\mathbf{x}-\mathbf{x_m})^T M_x^{-1}(\mathbf{x}-\mathbf{x_m})+(\mathbf{y}-\mathbf{t})^T M_y^{-1}(\mathbf{y}-\mathbf{t}))}$$

M_x: Cov. for x, M_y: Cov. for y, X_m: Prior information

Only if:
Prior, posterior and likelihood
All are ***Gaussian***

- The minimization of the following cost function:

$$\chi^2_{GLS} = (\mathbf{x}-\mathbf{x_m})^T M_x^{-1}(\mathbf{x}-\mathbf{x_m}) + (\mathbf{y}-\mathbf{t})^T M_y^{-1}(\mathbf{y}-\mathbf{t})$$

- **Alternatively, BMC method can be also used.**

C. De Saint Jean et al., Evaluation of Neutron-induced Cross Sections and their Related Covariances with Physical Constraints, Nuclear Data Sheets, 2018.

Use of Integral experiments

State update $$\boldsymbol{\sigma} - \boldsymbol{\sigma}_0 = M_\sigma.S^T(M_E + S.M_\sigma.S^T)^{-1}.(\mathbf{E} - \mathbf{C}(\boldsymbol{\sigma_0}))$$

Cov. update $$\widetilde{M}_\sigma = M_\sigma - M_\sigma.S^T(M_E + S.M_\sigma.S^T)^{-1}.S.M_\sigma$$

σ=Vector of nuclear data (cross sections, spectra…)
$N\sigma$= #isotopes X # reactions X #energy groups

$M\boldsymbol{\sigma}$: Cov. For ND
M_E: Cov. for E
$\boldsymbol{\sigma}_0$: Prior information
S: sensitivity of int exp {E} for p wrt ND

Transposition of uncertainties

Correction due to nuclear data

$$Co(R)_{DN} = C_R(\boldsymbol{\sigma}) - C_R(\boldsymbol{\sigma}_0) \approx S_R \times (\boldsymbol{\sigma} - \boldsymbol{\sigma}_0)$$

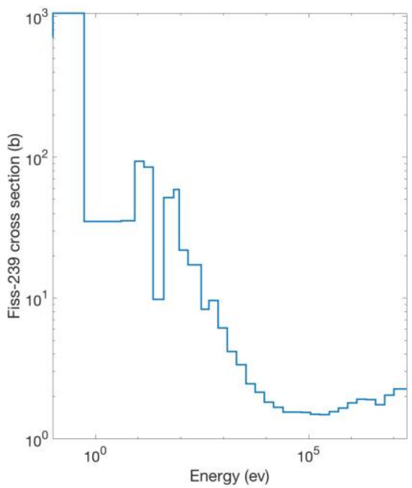
Uncertainty for the reactor concept

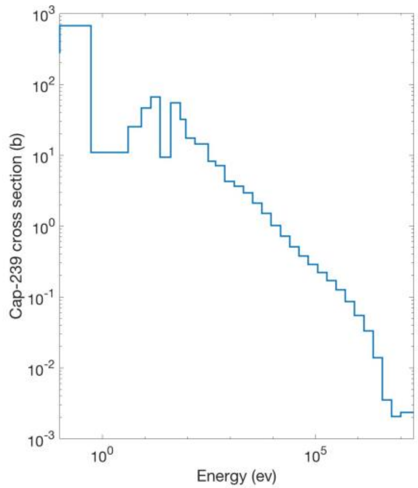
$$M_R = S_R \tilde{M}_\sigma S_R^T = S_R (M_\sigma - M_\sigma . S^T (M_E + S.M_\sigma . S^T)^{-1} . S.M_\sigma) \times S_R^T$$

Where S_R is the sensitivity of the reactor concept for parameter p wrt ND

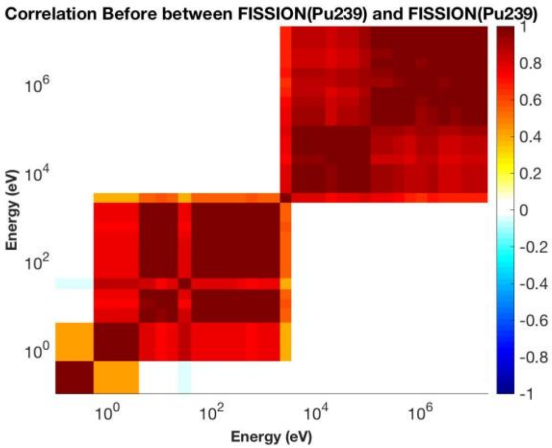
Test case:

Prior nuclear data: CEA-COMAC-V1 file (Corr. matrix)

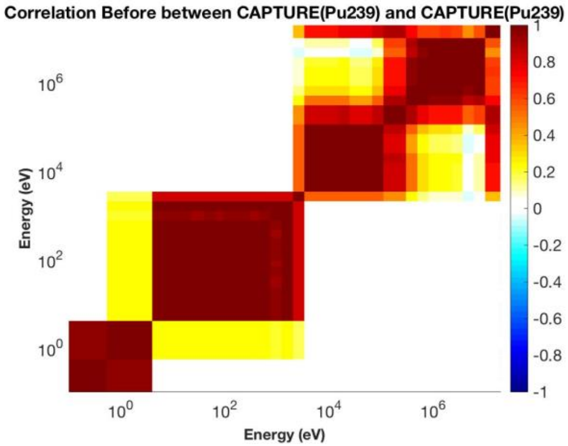




Pu239 Fission and Capture in 33 energy groups



Pu239 Fission correlation

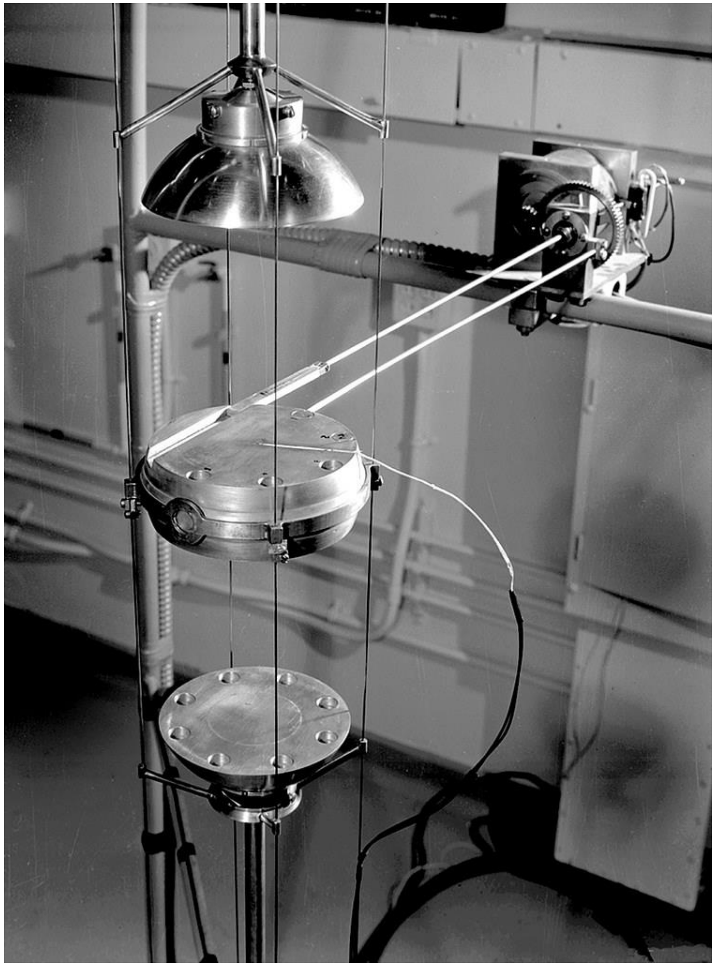


Pu239 Capture correlation

Integral experiment: JEZEBEL
Fitted parameters:
Case1. Pu239, Pu240, Pu241
Case2. Pu239 (Cap, Dis, Elas, Fiss, Inel, Nu, NXN)

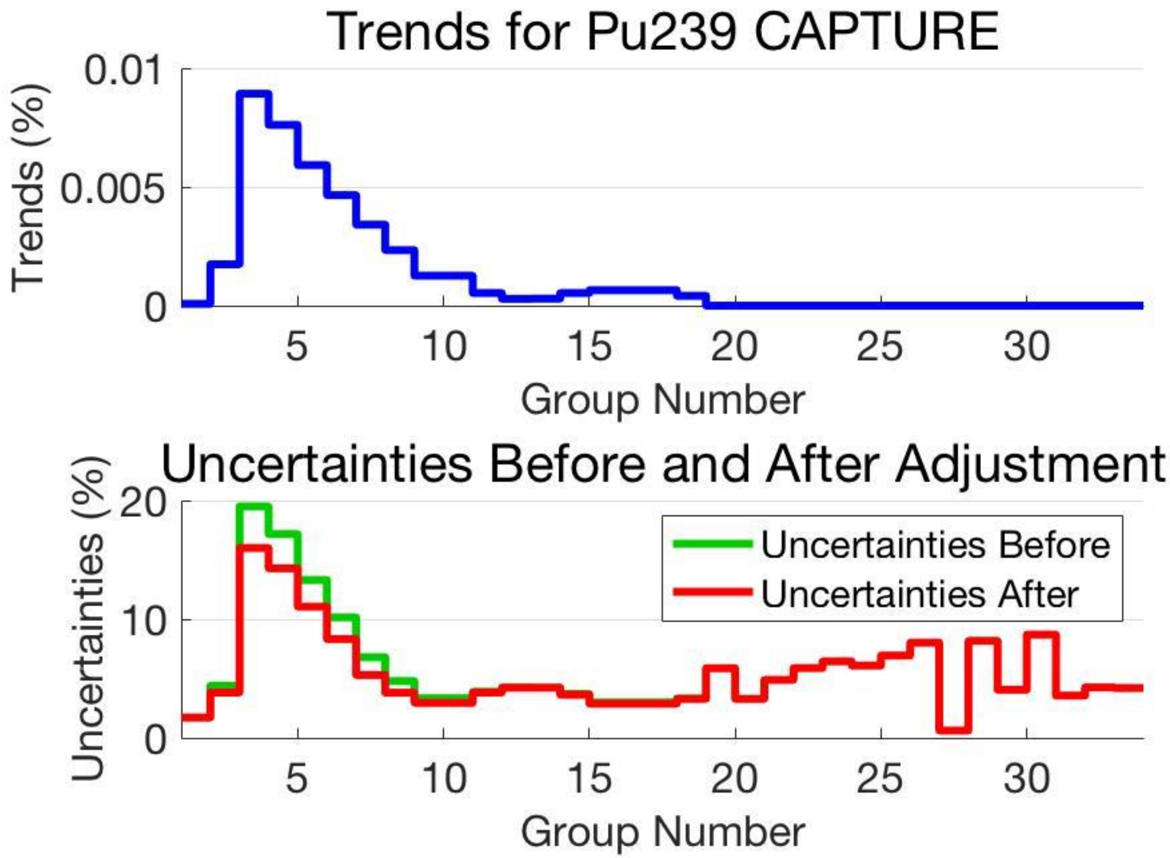
JEZEBEL experiment

- The Jezebel experiment was a very small spherical assembly of plutonium alloyed with gallium.
- Experiment was used to determine the critical mass of spherical and homogeneous Pu-alloy.
- Pu239 is a major component of the core.



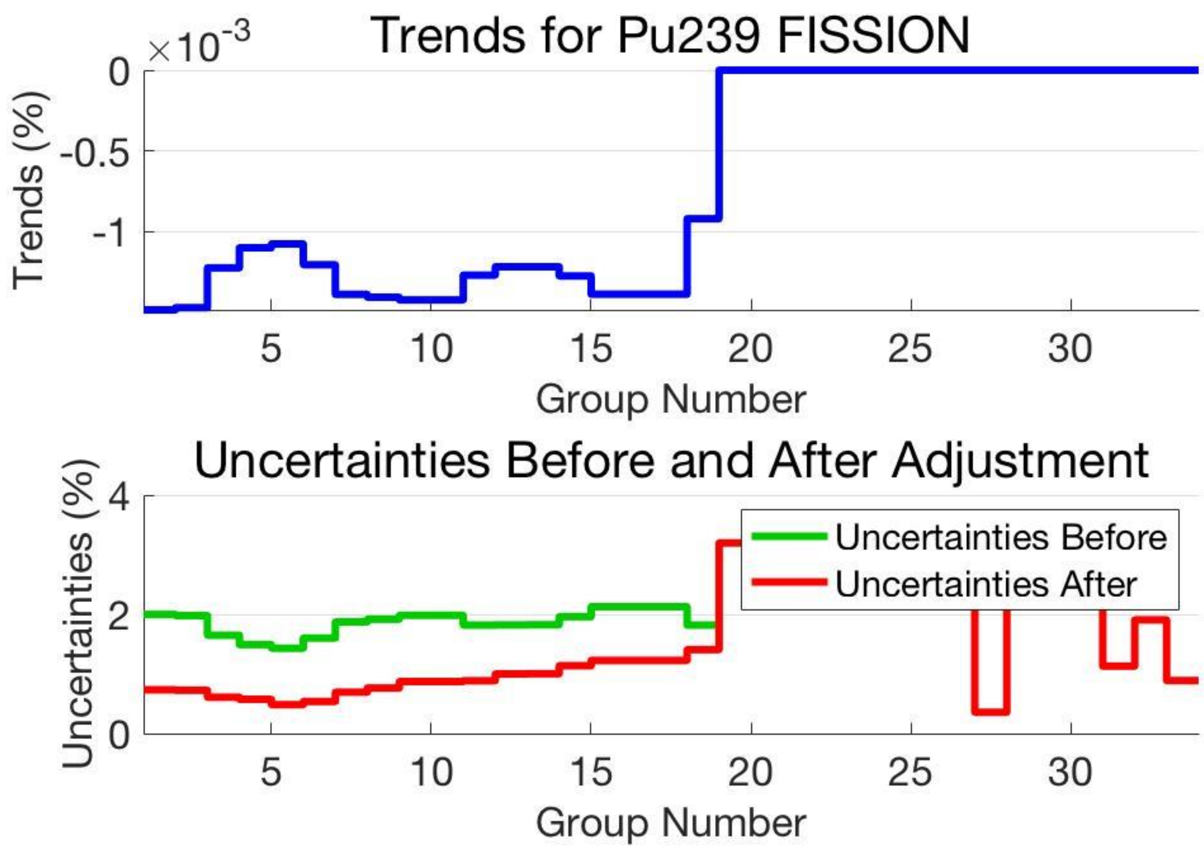
Benchmark example – ^{239}Pu Jezebel.
Picture taken from the ICSBEP Handbook

Uncertainty reduction in Pu239_Cap



Standard deviation [%] for Pu239 Capture: before and after adjustment
Adjusted parameters: Pu239, Pu240, Pu241

Uncertainty reduction in Pu239_Fiss



Standard deviation [%] for Pu239 Fission: before and after adjustment

Adjusted parameters: Pu239, Pu240, Pu241

More information: *C. De Saint Jean et al., Evaluation of Neutron-induced Cross Sections and their Related Covariances with Physical Constraints, Nuclear Data Sheets, 2018.*

Results: Adjustment, K_{eff} (C/E-1)

Before adjustment			
Fitting Parameters	**Pu(239, 40, 41), U238, Fe56, Na23, U235**	**Pu(239, Pu240, Pu241)**	**Pu239 only**
Initial value	0.001	0.001	0.001
Exp. unc.	0.25%	0.25 %	0.25 %
Initial unc.	1.4448%	1.4448%	1.4332%
After adjustment (with JEZEBEL)			
Final value	2.9068e-05	2.9069e-05	2.9531e-05
Final unc.	0.24611%	0.24611%	0.24627%
Transposition (to ASTRID)			
Initial value	0.001	0.001	0.001
Initial unc.	1.3639%	1.3639%	1.3639%
Final value	4.7753e-04	4.7753e-04	5.2137e-04
Final unc.	1.12848%	1.12848%	1.17286%

Transposition

Transposition (to ASTRID)	
Initial unc.	**1.3639**
Final Unc (fit: Pu239)	**1.1728**
Individual fit effect:	
PU239_Capture	1.363688
PU239_Distribution	1.35939
PU239_Elastic	1.36395
PU239_Fission	**1.19518**
PU239_InElastic	1.36374
PU_239_Nu	**1.34499**
PU_239_NXN	1.36392

- Most of the contribution in uncertainty reduction can be seen from Pu239_Fission and Pu239_NU data??

Issues:

- How good is the fit?
- Fitting test
  - Chi square test
    - Effective degree of freedom
  - Cook's distance: which ingredient is affecting the fit.
    - Nuclear data (isotope, reactions….)
    - Experiment

Cook's distance

Shows the influence of a data point in least square regression analysis

- In a regression fit, if the square error is:

$$e'e = (Y-X\boldsymbol{\beta})'(Y-X\boldsymbol{\beta})$$

- The mean square error: $s^2 = e'e/(n-p)$

Where
n: number of observation,
P: number of fitted parameters

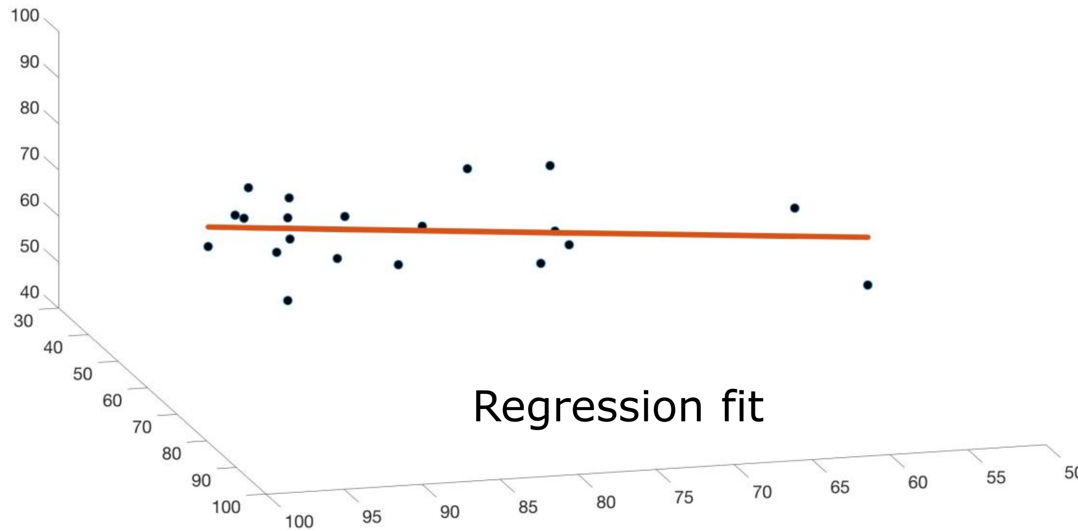
- The Cook's distance for the observation i

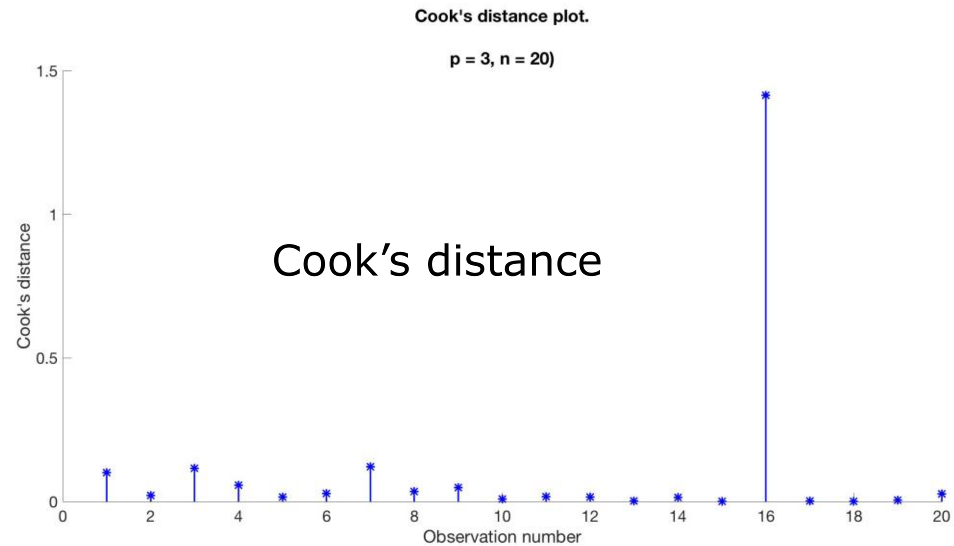
$$D_i = \sum_{j=1}^{N} \frac{(f(x_j) - f(x_j)_i)^2}{ps^2}$$

Where $f(x_j)_i$ is the fitted response when the i^{th} observation is excluded.

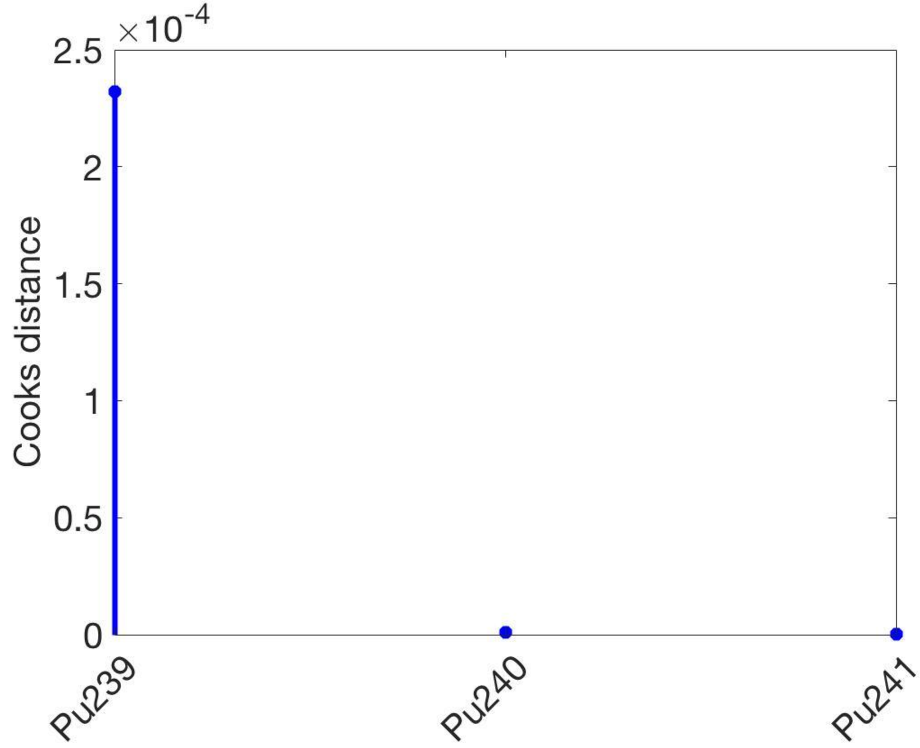
Example

X1	X2	Y
68	60	75
49	94	63
60	91	57
68	81	88
97	80	88
82	92	79
59	74	82
50	89	73
73	96	90
39	87	62
71	86	70
95	94	96
61	94	76
72	94	75
87	79	85
40	50	40
66	92	74
58	82	70
58	94	75
77	78	72



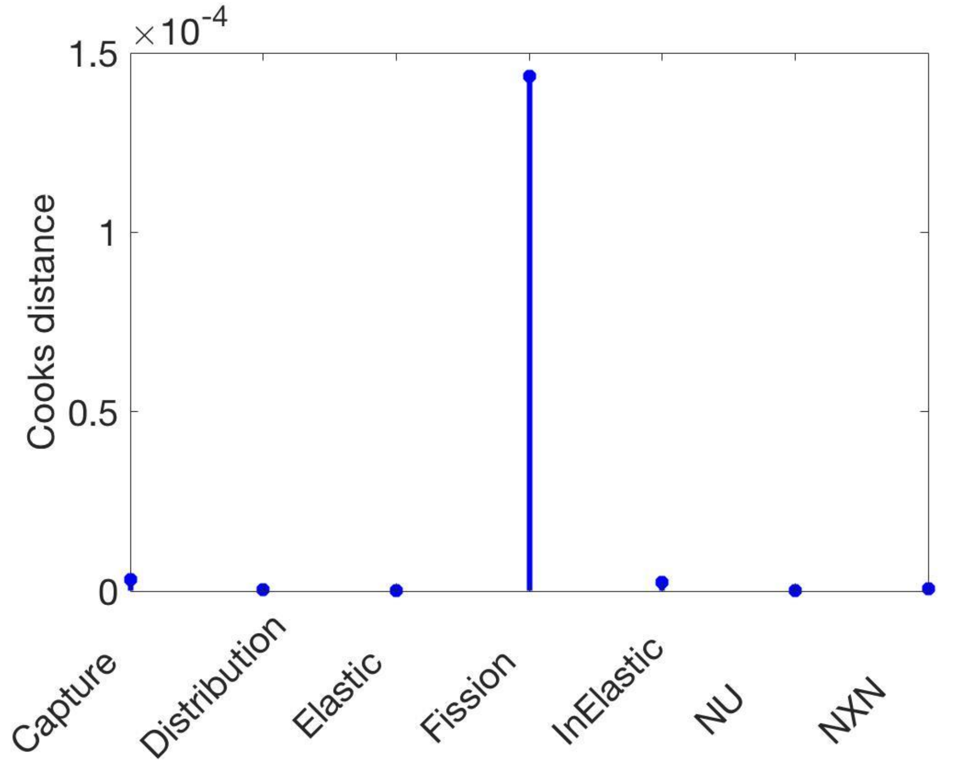


Test case 1: Influence of Pu isotopes on fit using Cook’s distance:



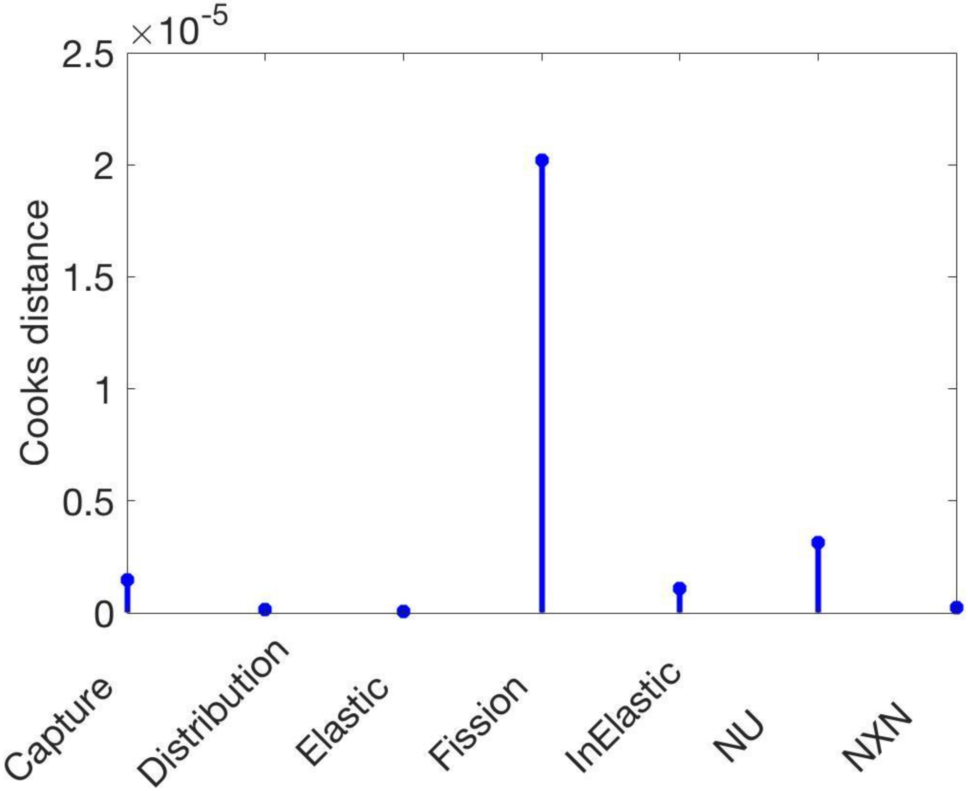
- Pu239 ND is the most influential isotope for the adjustment

Test case 2: Influence of Pu239 nuclear reaction using Cook's distance



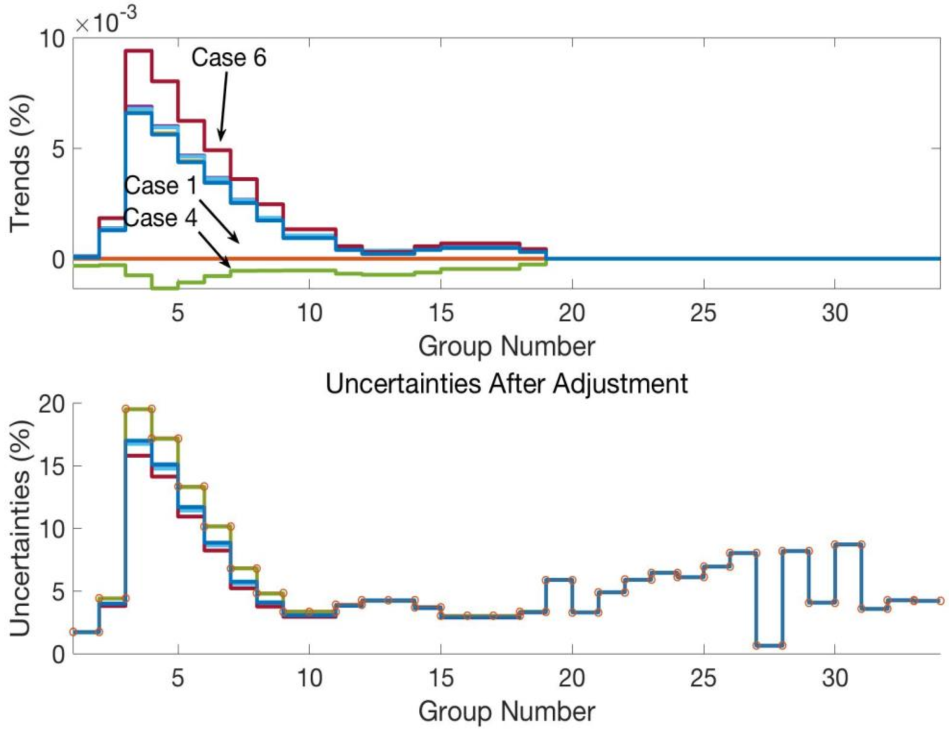
- For Pu239 data adjustment, Fission reaction is the most influential reaction.

Test case 2 (**Nu unc. in COMAC file is increased by 1%):** Influence of Pu239 nuclear reaction using Cook's distance



In Pu239 fit, Fission and nu reactions are influential reactions.

Case with large Cook's distance

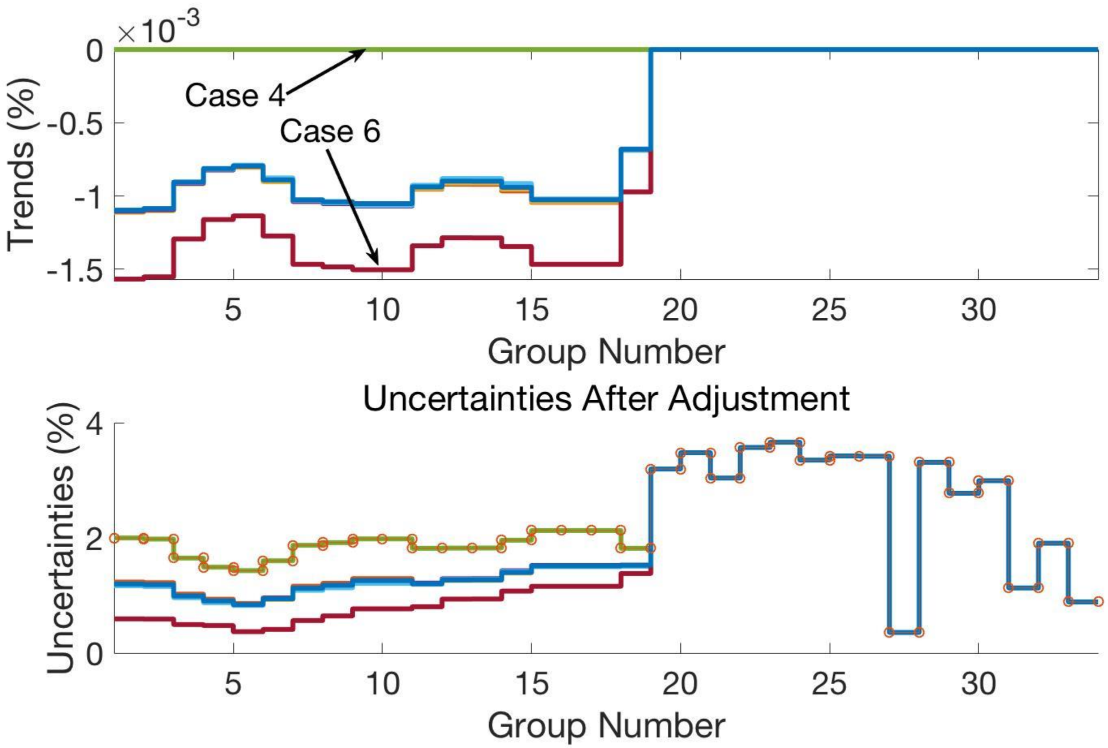


Capture data

Case1: all-Capture
Case2: all-Dissipation
Case3: all-Elastic
Case4: all-Fission
Case5: all-InElastic
Case6: all-Nu
Case7: all-NXN

- Adjusted data (trends) and uncertainties are plotted for all 7 sub cases.
- For case 4(All reaction–Fission) and 6 (All reaction–Nu) trends are highly influenced for Pu239_Capture fitted data.

Case with large Cook's distance

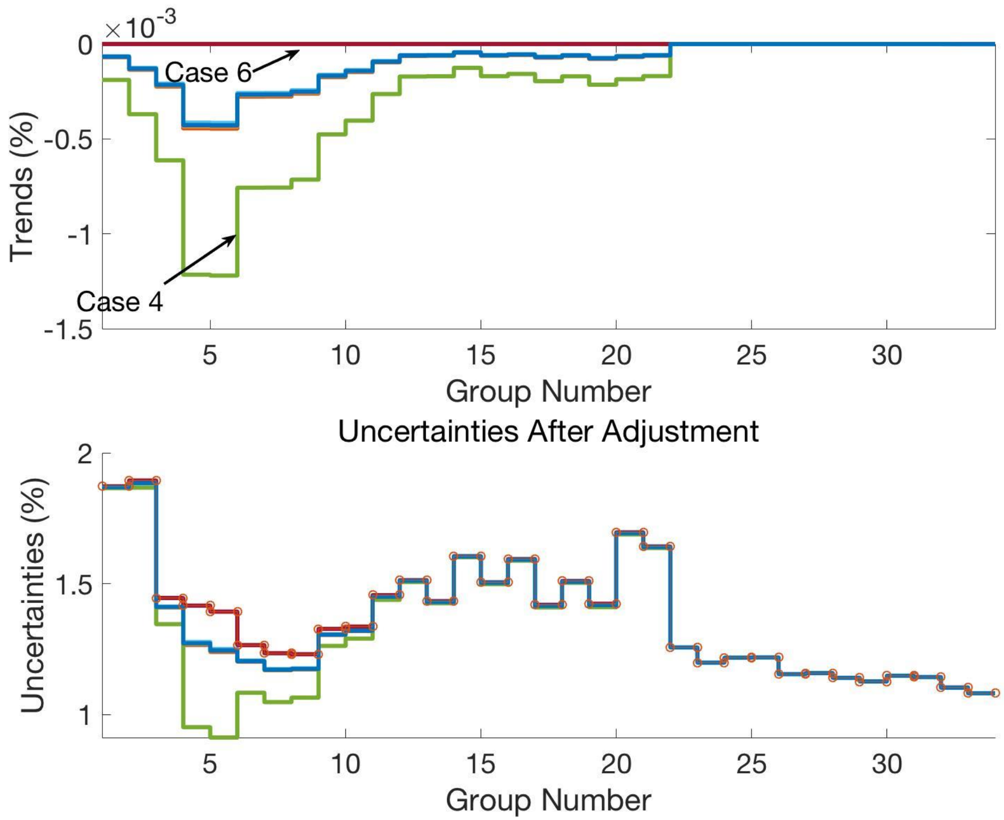


Case1: all-Capture
Case2: all-Dissipation
Case3: all-Elastic
Case4: all-Fission
Case5: all-InElastic
Case6: all-Nu
Case7: all-NXN

Fission data

- Adjusted data (trends) and uncertainties are plotted for all 7 sub cases.
- For case 4(All reaction–Fission) and 6 (All reaction–Nu) trends are highly influenced for Pu239_Fission fitted data.

Case with large Cook's distance



Case1: all-Capture
Case2: all-Dissipation
Case3: all-Elastic
Case4: all-Fission
Case5: all-InElastic
Case6: all-Nu
Case7: all-NXN

Nu data

- Adjusted data (trends) and uncertainties are plotted for all 7 sub cases.
- For case 4(All reaction–Fission) trends are highly influenced for Pu239_NU fitted data.

Conclusion

- Nuclear data uncertainties are reduced using Bayesian method with integral experiments.
- Reduction on the final uncertainties for the Concept reactor is found.
- Test for adjustment is being studied using Cook’s distance.
  - Effect of Pu isotopes is estimated on fitting.
  - Effect of Pu239 nuclear reaction is estimated on fitting.
- Pu239_Fission and Pu239_Nu are seen to be most influential datasets.

Future work

- Influence of different integral experiments

- Issues
  - Fitting test: Chi Square_opt/NDOF !=1.
  - Effective degrees of freedom

- Other statistical tests
  - Overfitting
  - Akaike information criteria (AIC)
  - Bayesian information criteria (BIC)
  - Information theory