ND Assessment alternatives: Validation Matrix instead of XS Adjustment

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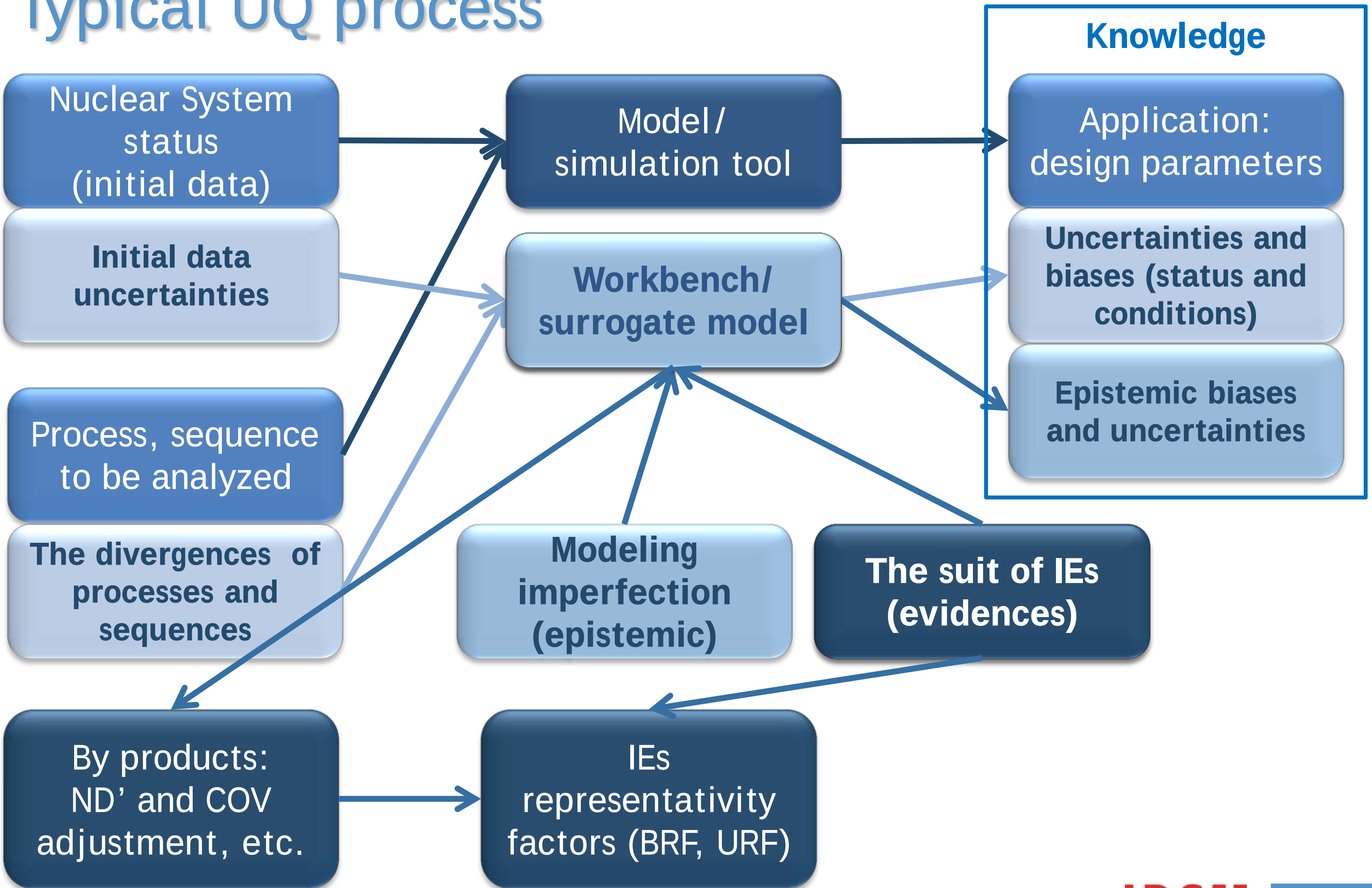
Outline

- **Introduction:**
  general remarks and validation conceptual system
- **Consistency/inconsistency of the V&UQ procedures**
- **Bayesian approach**,
  source of data and needed functionals
  characterization of the resolution factors
- **Computation of weigh factors (URF and UBF)**
- **Discussion and Conclusion**

Typical UQ process



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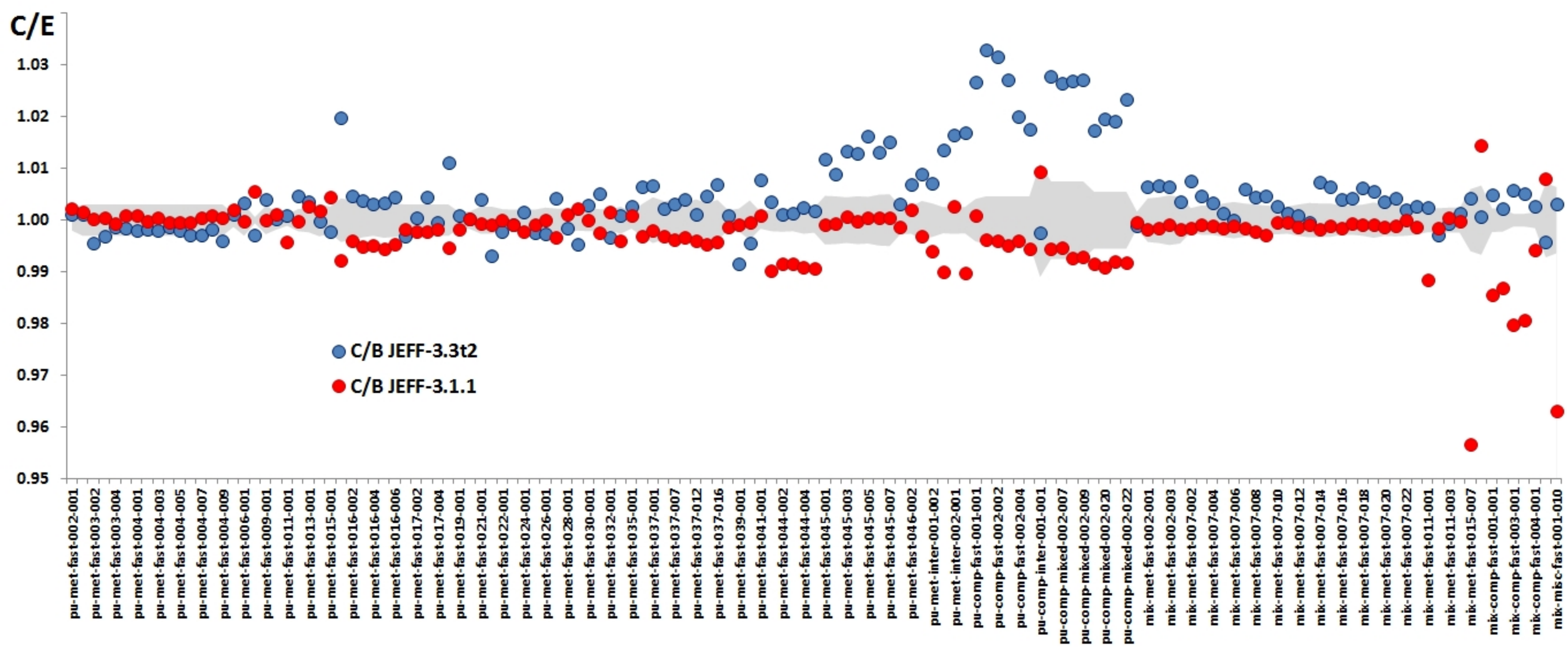
Conceptual basis (thesaurus)

- Approach:
  => the application of mathematical statistics to
  independently whether deterministic (GLLS) or random (sampling)
  => ill-posed inverse problem solution
  to build "phase space" for knowledge transpositions
  => using relevant suit of the IEs
  statistically significant, representative set
- Operated terms:
  => prior estimations
  basing on ND covariance matrices
  => observations
  C/E values
  => knowledge
  topology of the benchmarks (values together with uncertainties)
  => posterior estimations
  biases and uncertainties
  => surrogate modeling
  $\mathbf{S}_R$ sensitivity coefficients $\sigma/\mathbf{R} \cdot (\Delta\mathbf{R}/\Delta\sigma)$ or $\alpha/\mathbf{R} \cdot (\Delta\mathbf{R}/\Delta\boldsymbol{\sigma}) \cdot (\Delta\boldsymbol{\sigma}/\Delta\alpha)$

Traditional analysis: IEs with plutonium

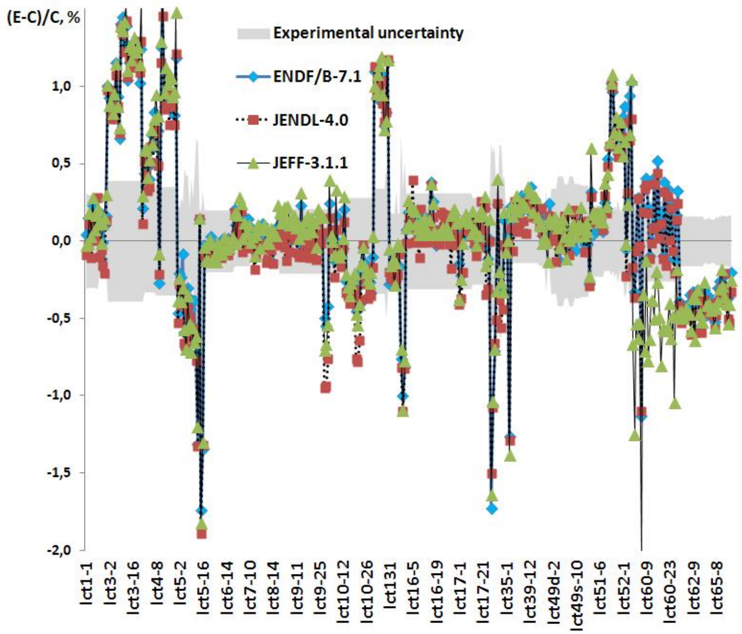
	N = 635	N = 238	N = 139
JEFF-3.3t2	-88	-297	-220
JEFF-3.1.1	-54	-205	-176
STD	10	14	21

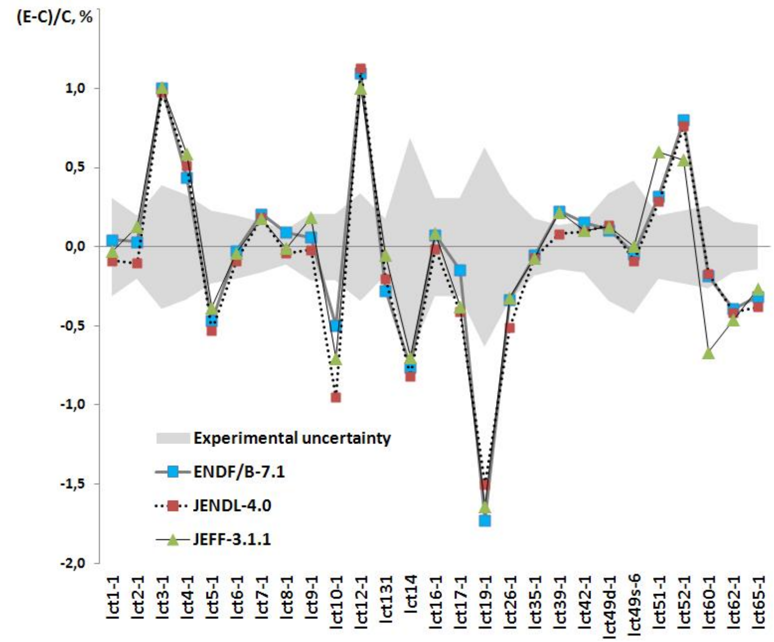
Completely withdrawing thermal spectra experiments



Traditional approach notably depends on number of benchmarks

Impact of Integral Experiments Correlations

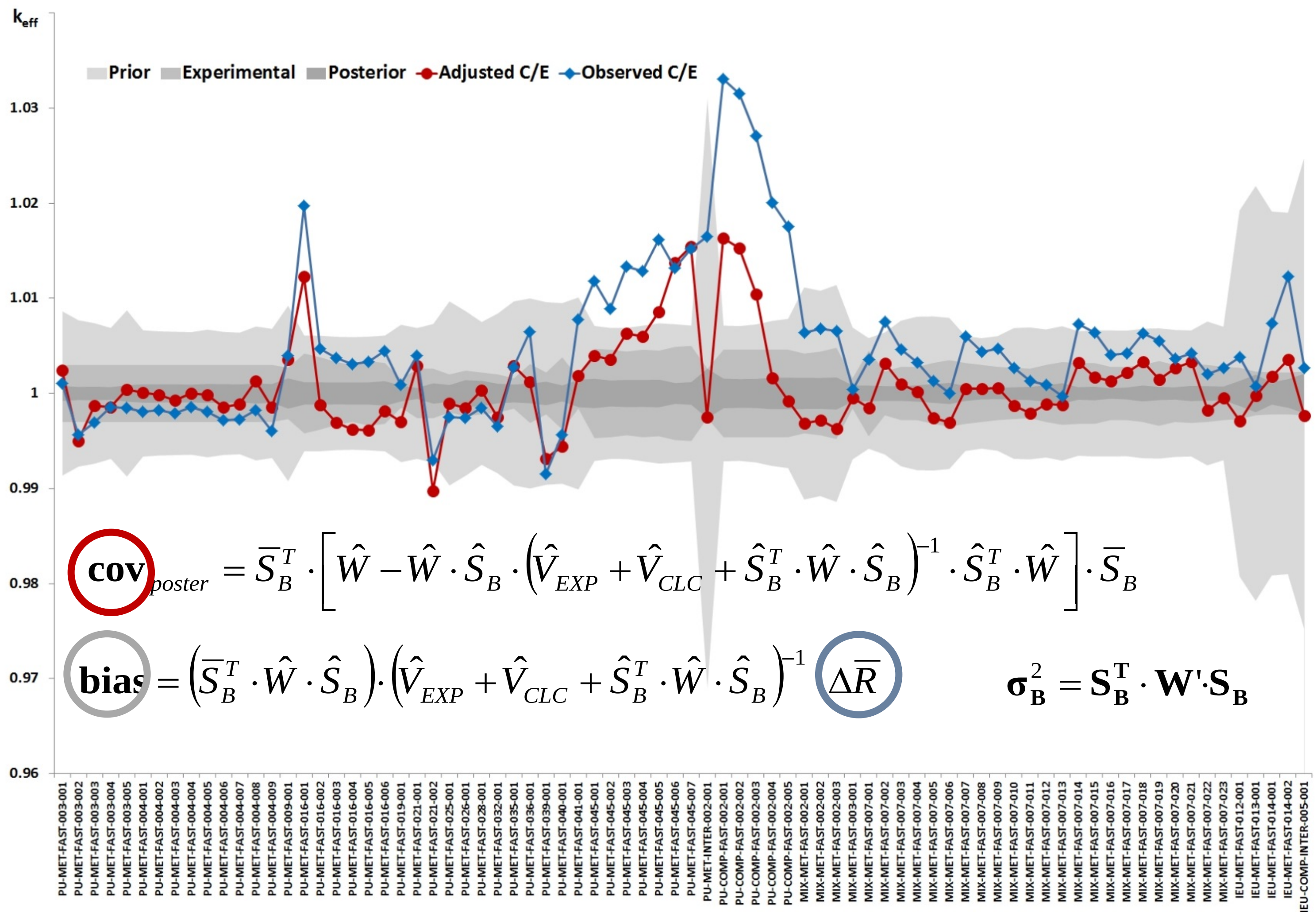




Number of LEU-COMP-THERM configurations	Weighted k_{eff} bias, pcm		
	ENDF/B-VII.1	JENDL-4.0	JEFF-3.1.1
388 configurations	-63.3	-14.9	180.0
27 configurations	53.8	113.9	183.3

Tatiana Ivanova, Evgeny Ivanov, Giulio Emilio Bianchi "Establishment of Correlations for Some Critical and Reactor Physics Experiments", Nuclear Science and Engineering, Volume 178, Number 3, November 2014

Adjustment procedure/observation correction



$$\mathbf{cov}_{poster} = \overline{S}_B^T \cdot \left[\hat{W} - \hat{W} \cdot \hat{S}_B \cdot \left(\hat{V}_{EXP} + \hat{V}_{CLC} + \hat{S}_B^T \cdot \hat{W} \cdot \hat{S}_B \right)^{-1} \cdot \hat{S}_B^T \cdot \hat{W} \right] \cdot \overline{S}_B$$

$$\mathbf{bias} = \left(\overline{S}_B^T \cdot \hat{W} \cdot \hat{S}_B \right) \cdot \left(\hat{V}_{EXP} + \hat{V}_{CLC} + \hat{S}_B^T \cdot \hat{W} \cdot \hat{S}_B \right)^{-1} \Delta \overline{R}$$

$$\boldsymbol{\sigma}_{\mathbf{B}}^2 = \mathbf{S}_{\mathbf{B}}^{\mathbf{T}} \cdot \mathbf{W'} \cdot \mathbf{S}_{\mathbf{B}}$$

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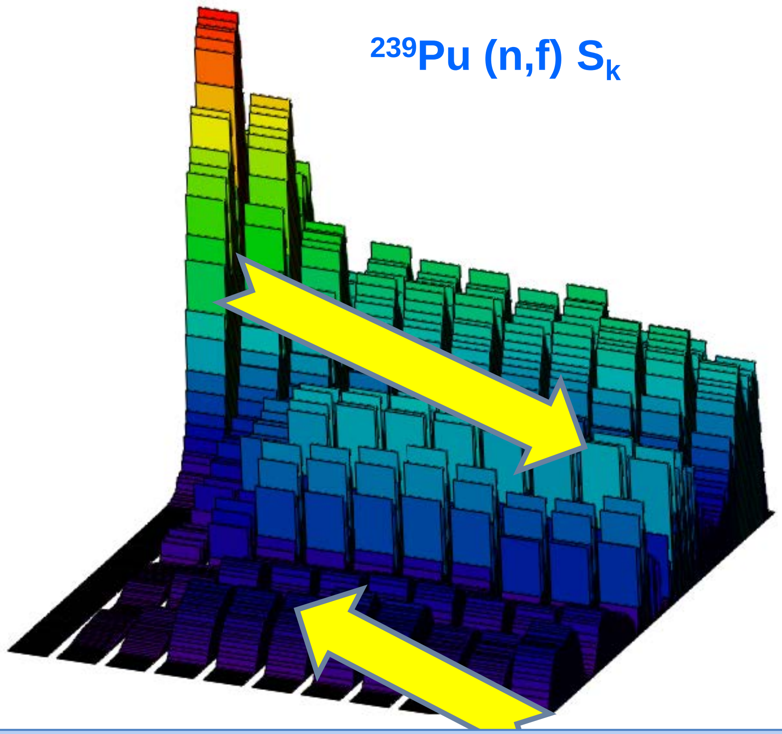
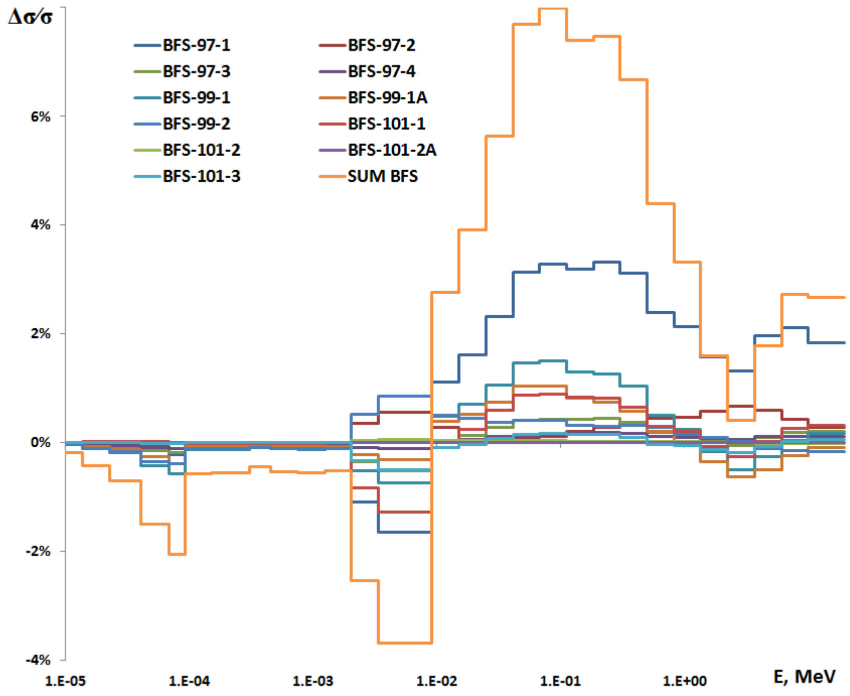
Progressive approach using dedicated IEs (BFS-MOX)

Parametrically varying spectra and energy spanned sensitivity

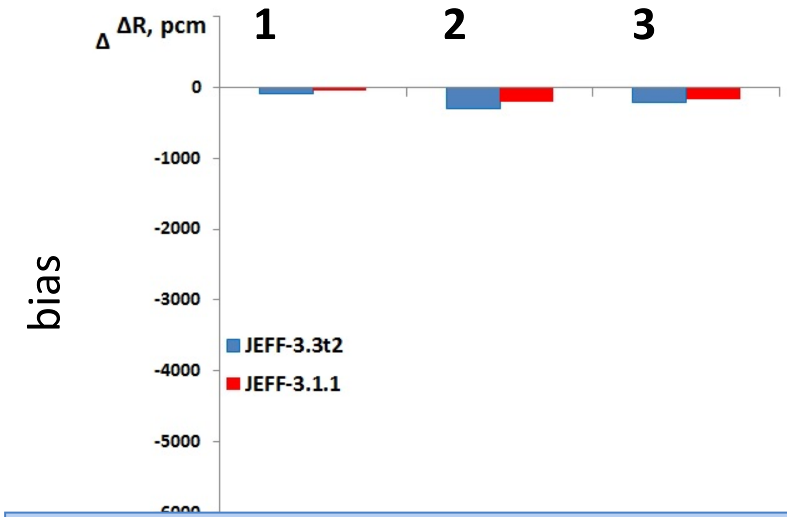


BFS-MOX integral experiments series contribution to ^{239}Pu (n,γ) cross sections



Integral experiments designed as mock-ups or dedicated to the given problem are available nowadays (using advanced analytical and statistical tools) as the experimental based benchmarks for the ND studies

Traditional approach and data assimilation

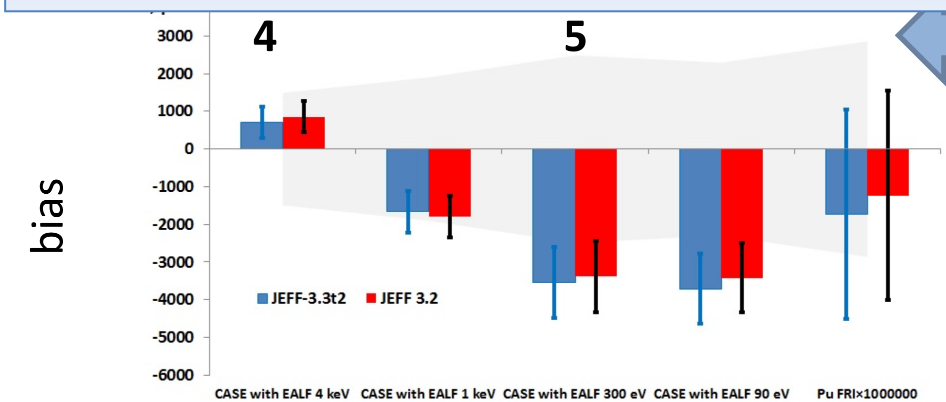


Accuracy of Pu and Mixed loaded critical systems computations

Traditional approach

1. all available benchmarks including solution experiments (N=635 cases)
2. all benchmarks except for solution experiments (N=238 cases)
3. the only fast and intermediate spectra benchmarks (N=139 cases)

The extrapolation of comfortable ~300 pcm gives ~ 4000 pcm - ~10÷15% of MCR w/o notable improvements



Data assimilation approach for different spectra

- 1÷4 criticality safety cases

4. At 4 keV EALF bias is **Positive**
5. Lower Energy EALF bias is **Negative**

- largest bias ~ **4000 pcm** (Δk_{eff})
- ^{239}Pu fission resonance integral bias and uncertainty ~ 0.12% and 0.28% (times 1M on the figure)

Bayesian approach - bias and uncertainty

- Bias – the expectation of correction factor to be associate with simulation results basing on available observations

$\Delta R \sim \mathbf{\Theta} \cdot \mathbf{\Theta_{IE}} \cdot \mathbf{S}_{AO} \cdot \mathbf{S}_{IE} \cdot \Delta \mathbf{r}_B$

depends on observations [$\Delta \mathbf{r}_B$], physics of the IEs and of application [$\mathbf{S}_{IE}$ and $\mathbf{S}_{AO}$], and basic and IE data uncertainties (freedom degree) [$\mathbf{\Theta}$] ,[$\mathbf{\Theta_{IE}}$]

- Uncertainty of the bias – the measure of the bias confidence

$\sigma(\Delta R) \sim \mathbf{\Theta} \cdot \mathbf{\Theta_{IE}} \cdot \mathbf{S}_{AO} \cdot \mathbf{S}_{IE}$

depends physics of the IEs and of application [$\mathbf{S}_{IE}$ and $\mathbf{S}_{AO}$], and basic and IE data uncertainties [$\mathbf{\Theta}$],[$\mathbf{\Theta_{IE}}$], does not depend on observations [$\Delta \mathbf{r}_B$]

Parameters to determine uncertainties and to determine the bias are different

Practical conclusions:
Space of uncertainty is orthogonal to the space of value
Model of uncertainty evolution (extrapolation) is needed

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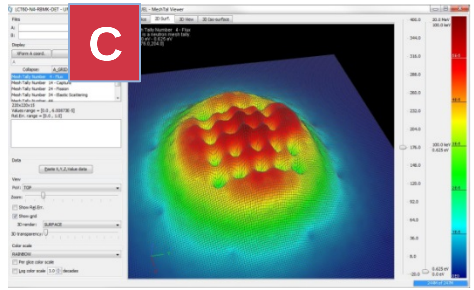
Source of data, NEA database

A

Handbook Edition	Number of Unique Cases	Sources
2012	727	TSUNAMI1D+TSUNAMI3D [VALID]+ MMK-KENO
2013	3575	Previous + Non VALID cases SCALE6.0 from Balance Inputs
2014	4011	Previous + MCNP6 + SCALE6.2BClutch

C



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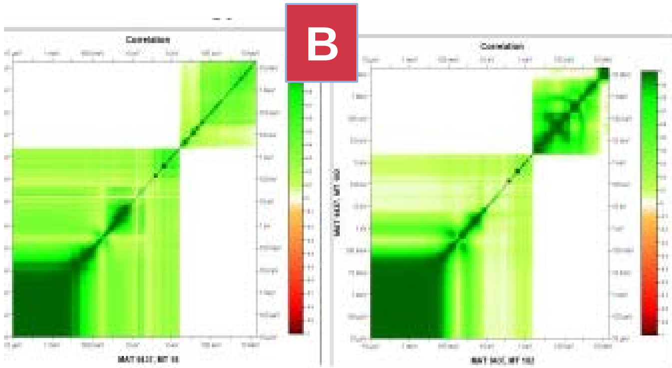
	THERM	INTER	FAST	MIXED
PU	525/608	4/10	114/121	9/9
HEU	664/895	21/32	383/403	75/84
IEU	142/180	5/21	31/43	7/23
LEU	1424/1612	0/0	1/1	5/5
U233	186/197	29/29	8/10	8/8
MIX	323/436	2/7	40/67	1/26
SPEC	0/0	0/0	4/20	0/0

D

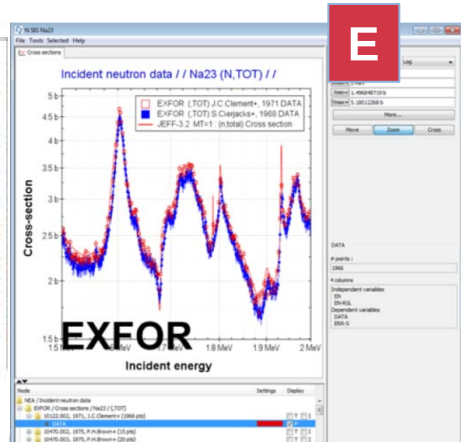
	HST 019 001	HST 025 001	HST 025 002	HST 025 004	HST 025 005
HST019-001	1000	450	450	430	410
HST025-001	450	1000	730	720	620
HST025-002	450	730	1000	720	620
HST025-004	430	720	720	1000	620
HST025-005	410	620	620	620	1000

B



ENDF/B-VII.1 JENDL-4.0

E



Openly available information in the NEA Data Bank

A. Physics (neutron status) – sensitivity coefficients (DICE,IDAT)
B. Nuclear data covariances (JANIS)
C. Benchmark models (DICE, IDAT, SINBAD, SFCOMPO)
D. Covariance of uncertainties (DICE)
E. Raw Differential Data (JANIS, EXFOR)
F. Linking (NDaST)

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Nuclide-reactions: two groups

Main group:
nuclides-reaction involved in the adjustment form the matrices of sensitivities

u-235 nubar
u-235 n,n'
u-235 elastic
u-235 fission
u-235 n,gamma
u-238 nubar
u-238 n,n'
u-238 elastic
u-238 fission
u-238 n,gamma
....

$$\mathbf{bias} = \left(\overline{S}_B^T \cdot \hat{W} \cdot \hat{S}_B\right) \cdot \left(\hat{V}_{EXP} + \hat{V}_{CLC} + \hat{V}_{RES} + \hat{S}_B^T \cdot \hat{W} \cdot \hat{S}_B\right)^{-1} \cdot \Delta\overline{R}$$

$$\mathbf{W}' = \hat{\mathbf{W}} - \hat{\mathbf{W}} \cdot \hat{S}_B \cdot \left(\hat{V}_{EXP} + \hat{V}_{CLC} + \hat{V}_{RES} + \hat{S}_B^T \cdot \hat{\mathbf{W}} \cdot \hat{S}_B\right)^{-1} \cdot \hat{S}_B^T \cdot \hat{\mathbf{W}}$$

Second group:
nuclides-reactions for which no statistically significant integral experiments data form matrix of “residual uncertainty” being added to methodological errors

....
o-16 n,alpha
....
be-9 elastic
....

$$\hat{V}_{RES} = \hat{S}_B^T \cdot \hat{\mathbf{W}} \cdot \hat{S}_B$$

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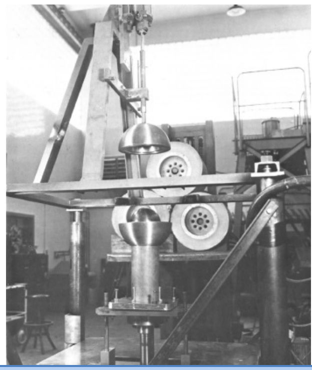
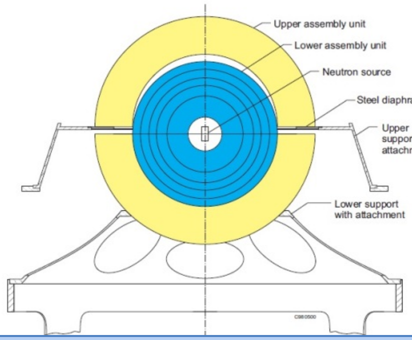
Benchmarks/residual uncertainties



◄**PMF-009-001** reflected by Al

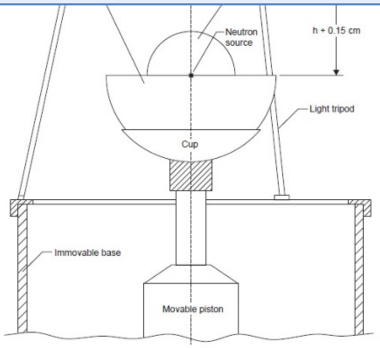
σ_{Al} ~ 100÷200 pcm



PMF-035-001 reflected by Pb►

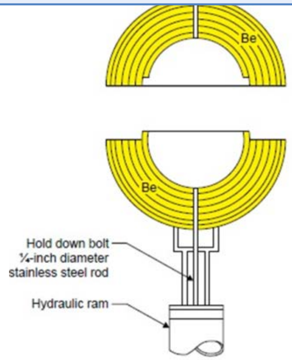
σ_{Pb} ~ 200 pcm

Nuclides-reactions should be excluded from the adjustment – if not enough statistically significant IEs cases.
Their "residual uncertainties" shall be added to the computational (C/E) uncertainties.



◄ **PMF-019-001** reflected by Be

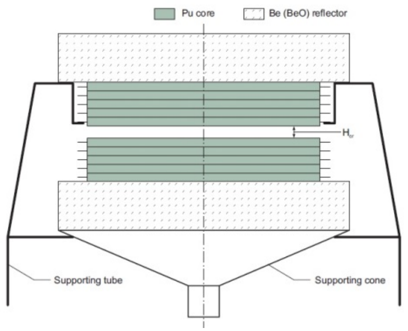
σ_{Be} ~ 200÷300 pcm



MMF-007-00X reflected by Be►

σ_{Be} ~ 500 pcm

Benchmarks/residual uncertainties, cont'd

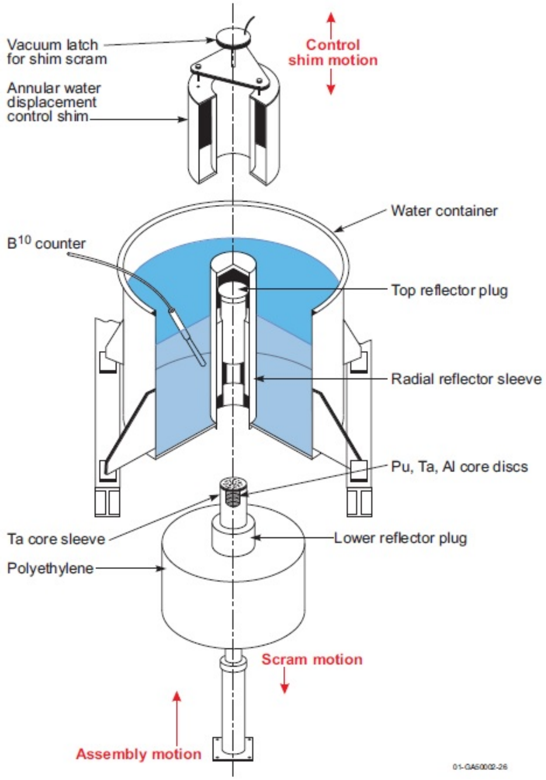


◂**PMF-021-00X** (VNIIEF) reflected by Be (BeO)

σ_{Be} ~ 600 pcm

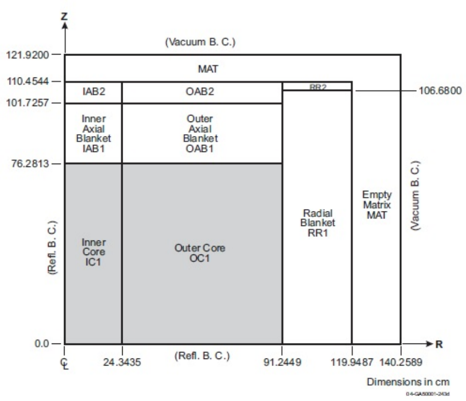
PMF-045-00X (LAMPRE) impacted by Ta and Ni▸

σ_{Ta} (unknown) ~ 600 pcm



◂ **ICI-005-001** (ZPR 6/6A) contains Na, Fe and Graphite

σ_{Na} ~ 100 pcm



Behind any case name (NMS-RRR-NNN) there is a complex configuration which detailed design, inventory and layout shall be taken into account

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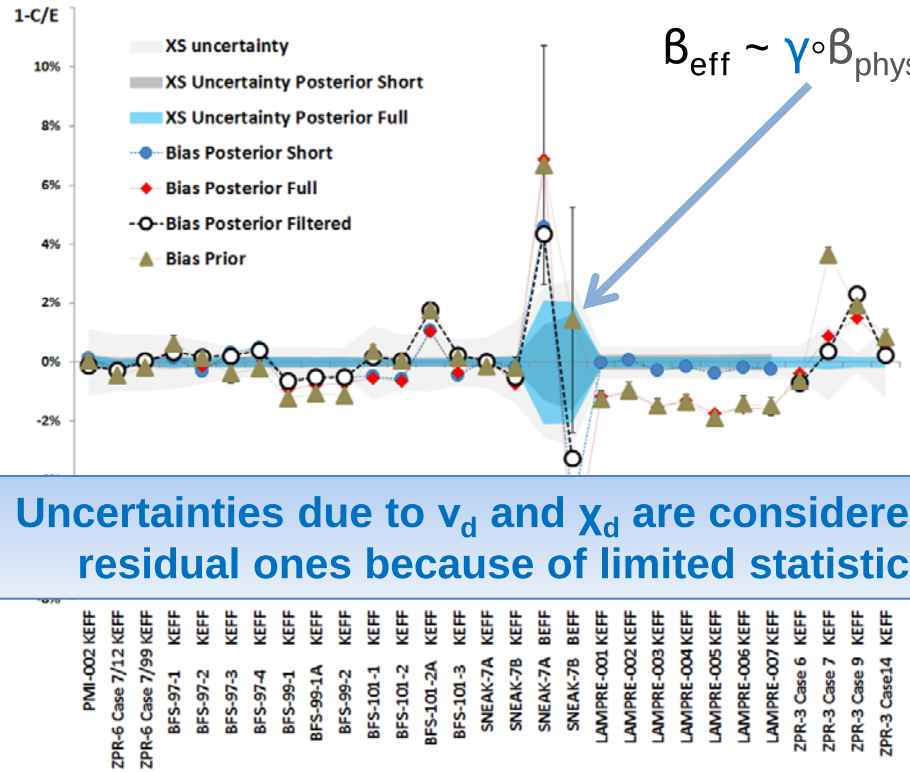
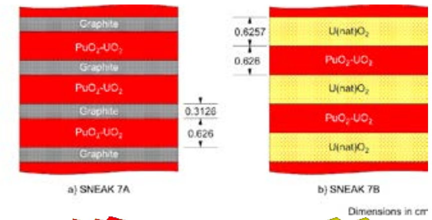
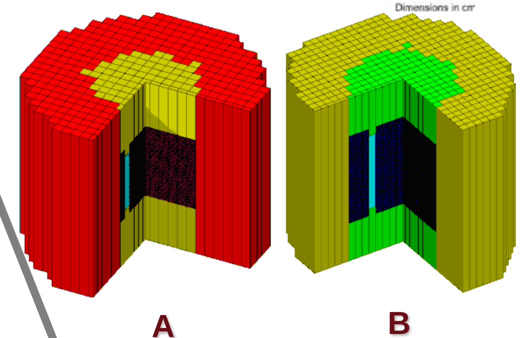
Indirectly measured values - β_{eff} and β_{phys}



$\beta_{eff} \sim \gamma \circ \beta_{phys}$

Uncertainties due to ν_d and χ_d are considered as residual ones because of limited statistics





To be used in the validation suit excluding direct ν_d and x_d (β_{phys}) contributions – analog of the reactivity benchmarks – since there is no statistically significant set of β_{eff} cases

β_{phys} can be tested against pile oscillation experiments

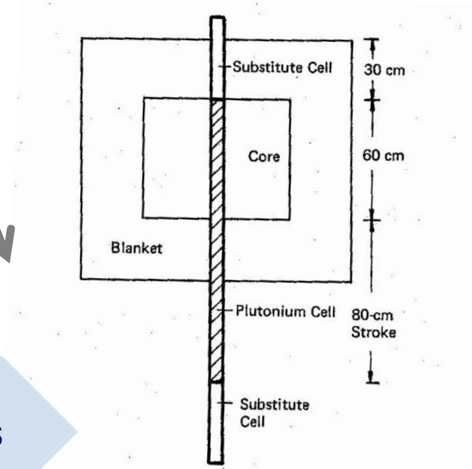


Fig. 3. Cross section of the core and the pile oscillator subassembly.

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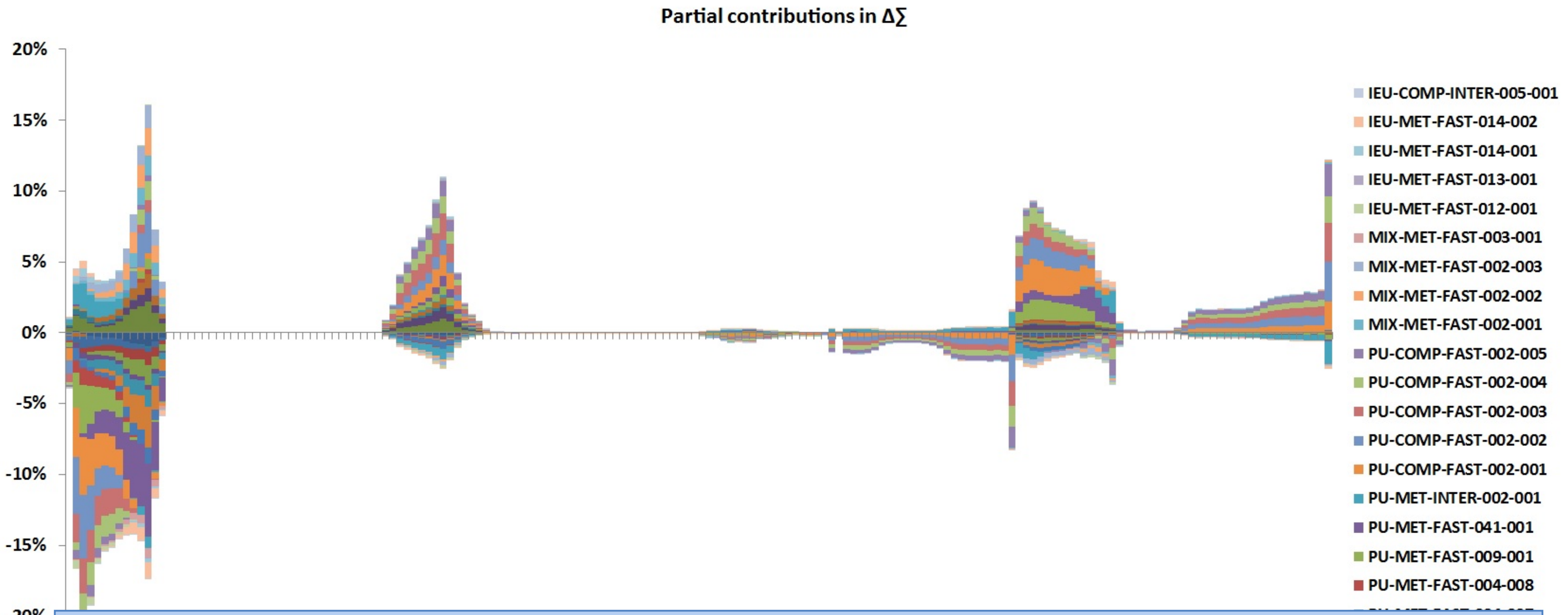
XS adjustment/correction for ^{239}Pu

Correction of the group-wise cross sections : contradictive contributions
Adjustment makes sense if the set of benchmarks is statistically significant



Note: both sensitivity coefficients and corrections can be reduced to nuclear models parameters unfolding the group-wise sensitivities $S_{R,\alpha} = \sum_m \frac{\alpha_m}{R} \cdot \frac{\partial R}{\partial \sigma_m} \cdot \frac{\partial \sigma_m}{\partial \alpha}$

However set IEs should be statistically significant for ND practical adjustment

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Resolution factor limitation

Statement concerning methodology and computations is:
new algorithms and computers enable precise comprehensive sensitivity analysis - MMKKENO, MONK, MCNP6, MCCARD, SCALE 6.2, SERPENT 2, MORET5 etc.

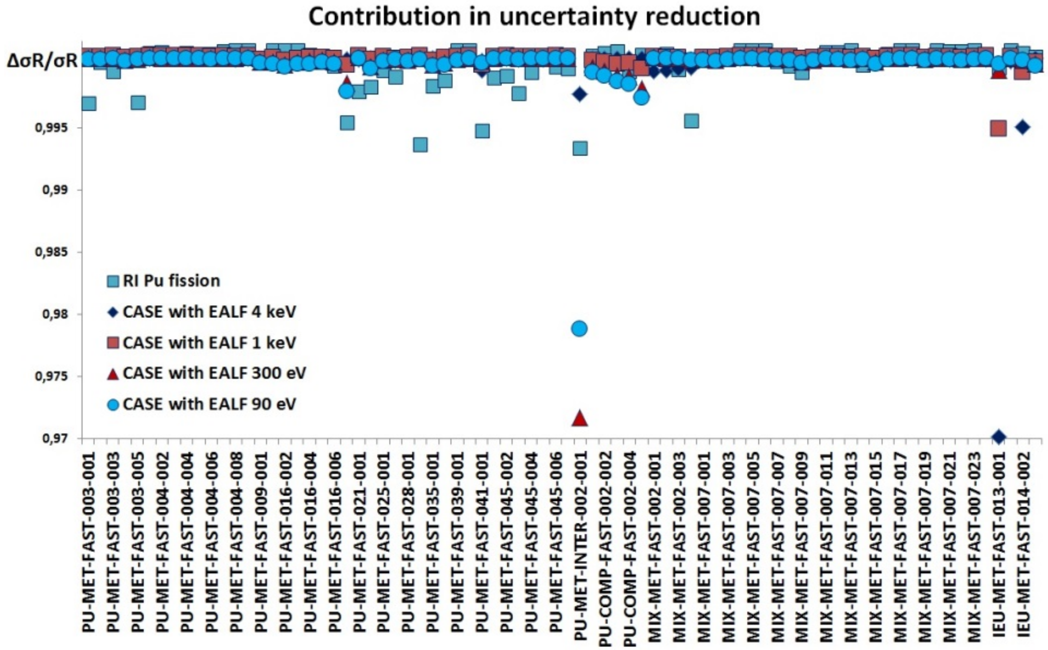
$$\mathbf{S}_k = \int \frac{\sigma(\mathbf{x})}{k_{eff}} \cdot \frac{\partial k_{eff}}{\partial \sigma(\mathbf{x})} \cdot d\mathbf{x} \neq \int \frac{\sigma(\mathbf{x})}{k_{eff}} d\mathbf{x} \cdot \int \frac{\partial k_{eff}}{\partial \sigma(\mathbf{x})} d\mathbf{x} = \frac{\Sigma}{k_{eff}} \cdot \frac{\delta k_{eff}}{\delta \Sigma}$$

Sensitivity computation approach	Forward solution, φ	Adjoint solution, ψ	Convolution, S_k	Fidelity of k_{eff} and consistency of S_k
Deterministic	Group-wise			high fidelity, non-precise k_{eff}, S_k is inconsistent
Hybrid Monte-Carlo (SCALE 6.1/ TSUNAMI-3D)	Group-wise	Group-wise approximant	Group-wise	high fidelity, non-precise k_{eff}, S_k is inconsistent
Group-wise Monte Carlo (MMKKENO)	Group-wise	-	Group-wise	high fidelity, non-precise k_{eff}, S_k is consistent
Precise Monte-Carlo (IFP and so on)	Continuous	-	Group-wise	precise k_{eff}, S_k is inconsistent

The surrogate models based on the linear response (sensitivity coefficients) have fundamentally limited resolution capabilities

Selection by contribution in uncertainty reduction

The metrics for added value - uncertainty reduction



The uncertainty reduction factors (URF)

Each benchmark contributes more or less in the reduction of prior uncertainty

Uncertainties shift factor can be computed iteratively and further corrected on χ^2.

Note: the uncertainty shift factors are independent on observations

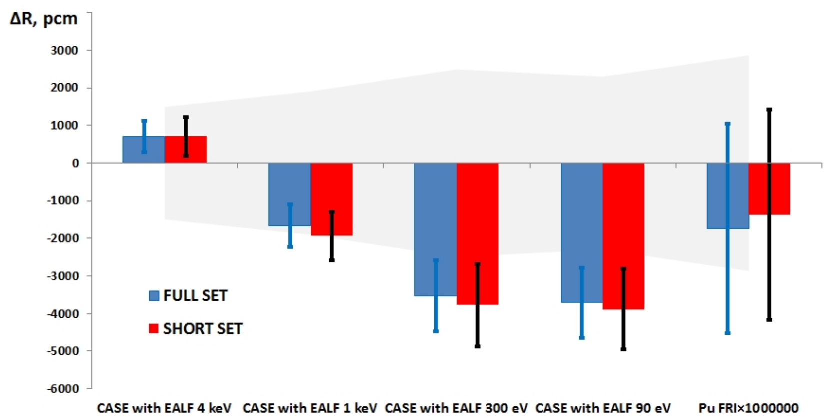
URF values can be used in express validation. URFs - independent on observations but on physics behind the test cases and applications - give enough information to design new experimental programs, if necessary

Bias and uncertainties quantification

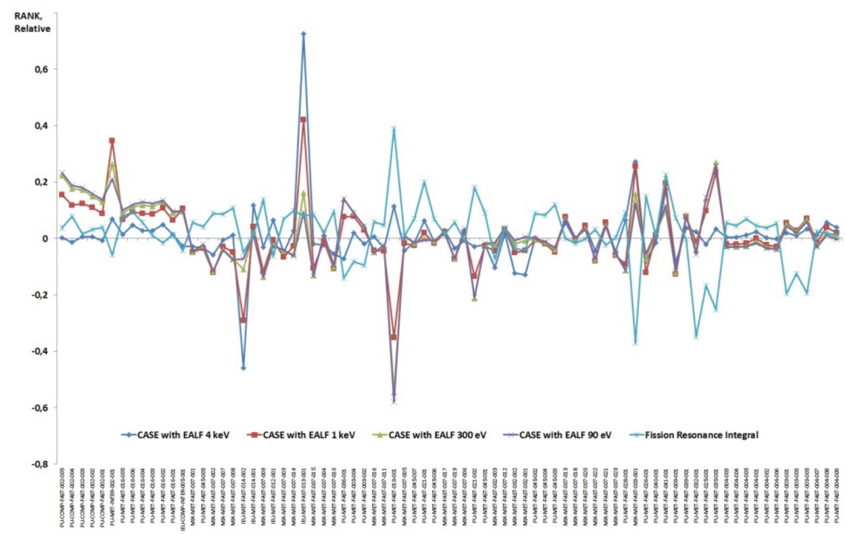
Illustration : uncertainty reduction produces bias

Bias ranking factor (BRF)

$\mathbf{\Delta R_{LIB}}$



Rank



$$\mathbf{\Delta R_{AO}} = \left(\overline{S}_{AO}^{T} \cdot \hat{W} \cdot \hat{S}_{B}\right) \cdot \left(\hat{V}_{EXP} + \hat{V}_{CLC} + \hat{S}_{B}^{T} \cdot \hat{W} \cdot \hat{S}_{B}\right)^{-1} \cdot \mathbf{\Delta R_{LIB}} \Leftrightarrow \mathbf{\Delta R_{AO}} \approx \mathbf{Rank} \cdot \mathbf{\Delta R_{LIB}}$$

$$\boldsymbol{\sigma}^{2}{}_{\mathbf{AO}} = \overline{\mathbf{S}}_{\mathbf{AO}}^{\mathbf{T}} \cdot \hat{\mathbf{W}}' \cdot \overline{\mathbf{S}}_{\mathbf{AO}}$$

The bias and the uncertainty are statistically linked as far as the bias is generated due to uncertainty reduction

Discussion: links between validation approaches

$$\left(\hat{\mathbf{V}}_{\mathbf{EXP}} + \hat{\mathbf{V}}_{\mathbf{CLC}} + \hat{S}_B^T \cdot \hat{\mathbf{W}} \cdot \hat{S}_B\right)$$ Total Covariance Matrix

***λ* – *eigenvalues* and *θ* - *eigenvectors* of Total Covariance Matrix give rotation and scaling factors for PCA**

$$\mathbf{bias} = \left(\bar{S}_{AO}^T \cdot \hat{\mathbf{W}} \cdot \hat{S}_B\right) \cdot \left(\hat{\mathbf{V}}_{\mathbf{EXP}} + \hat{\mathbf{V}}_{\mathbf{CLC}} + \hat{S}_B^T \cdot \hat{\mathbf{W}} \cdot \hat{S}_B\right)^{-1} \cdot \Delta\bar{R}$$ Expected application

$$\mathbf{bias} = RF_1 \cdot \Delta R_1 + RF_2 \cdot \Delta R_2 + \ldots + RF_N \cdot \Delta R_N$$ Mean bias ponderated using pre-computed bias ranking factors

To estimate bias using single-output analytical tool and to provide the first guess for TMC

$$\Delta\sigma_{POST}^2 = \sigma_{PRIOR}^2 - \sigma_{POST}^2 = \bar{S}_{AO}^T \cdot \hat{\mathbf{W}} \cdot \bar{S}_{AO} - \bar{S}_{AO}^T \cdot \hat{\mathbf{W}}' \cdot \bar{S}_{AO}$$ Reduction of uncertainty

$$\Delta\sigma_{POST}^2 = SF_1 + SF_2 + \ldots + SF_N$$ using pre-computed uncertainty shifting factors

$$\Delta\sigma_{POST}^2 = SF_1 + SF_2 + \ldots + SF_N + \mathbf{SF_{NEW}}$$ added value with new experiment

To design new Integral Experiments programs

Benchmarks' ranking table

Major adding value cases

	C1	C2	C3	C4	RI
PU-MET-FAST-003-001					**
PU-MET-FAST-003-003					**
PU-MET-FAST-003-005	*	*	*	*	**
PU-MET-FAST-009-001	*	**	*	*	*
PU-MET-FAST-019-001	*	***	***	***	***
PU-MET-FAST-021-001	*				**
PU-MET-FAST-021-002		**	**	**	**
PU-MET-FAST-025-001		*	*	*	**
PU-MET-FAST-026-001	*	*	*	*	**
PU-MET-FAST-032-001					***
PU-MET-FAST-035-001		**	**	**	***
PU-MET-FAST-036-001	*	*	*	*	**
PU-MET-FAST-041-001	*	**	*	*	**
PU-MET-FAST-045-003	*	*	*	*	**
PU-MET-INTER-002-001	*	***	**	**	*
PU-COMP-FAST-002-003		*	**	**	
PU-COMP-FAST-002-004		*	**	**	*
PU-COMP-FAST-002-005		**	**	**	
MIX-MET-FAST-003-001	**	***	*	*	***
MIX-MET-FAST-007-009		*	*	*	**
IEU-MET-FAST-013-001	***	***	*	*	*

Criteria of the selection

- **High fidelity evaluated integral experiment data**
- **Limited/well estimated residual uncertainty**
- **Potential contribution in uncertainty ≥ criteria based on χ^2 and 1/Number of benchmarks**

$$\overline{\mathbf{S}}^{\mathbf{T}}_{\mathbf{AO}}\hat{\mathbf{W}}\hat{\mathbf{S}}_{\mathbf{B}} \cdot \left(\hat{\mathbf{V}}_{\mathbf{EXP}} + \hat{\mathbf{V}}_{\mathbf{CLC}} + \hat{\mathbf{S}}^{\mathbf{T}}_{\mathbf{B}}\hat{\mathbf{W}}\hat{\mathbf{S}}_{\mathbf{B}}\right)^{-1} \cdot \hat{\mathbf{S}}^{\mathbf{T}}_{\mathbf{B}}\hat{\mathbf{W}}\overline{\mathbf{S}}_{\mathbf{AO}}$$

- **Visible potential contribution in the expected ultimate bias**

$$\left(\overline{\mathbf{S}}^{\mathbf{T}}_{\mathbf{B}} \cdot \hat{\mathbf{W}} \cdot \hat{\mathbf{S}}_{\mathbf{B}}\right) \cdot \left(\hat{\mathbf{V}}_{\mathbf{EXP}} + \hat{\mathbf{V}}_{\mathbf{CLC}} + \hat{\mathbf{S}}^{\mathbf{T}}_{\mathbf{B}} \cdot \hat{\mathbf{W}} \cdot \hat{\mathbf{S}}_{\mathbf{B}}\right)^{-1}$$

Table can be used for express validation (90% of success) and to provide the first guess for an estimator like TMC

Discussion

Applicants can be provided with the matrices of weighted benchmark cases instead of XS correction factors

Parameters	Potential role in the V&UQ
URF (Uncertainty reduction factors) - observation independent	**Short list of the problem oriented representative benchmarks**
Pre-computed S_k, prior ND and IEs matrices	**Establishment of the new problem-oriented IEs**
BRF (bias ranking factors) - observation dependent	**Validation of high-fidelity codes unable for PT**
The same as for URF and precisely computed ΔR	**Specification of the weighted list of cases**

Application is any given integral functional of the ND (RI, correlations etc.)

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Summary

The conceptual basis of the V&UQ

Inputs

- **A-priory available information (theoretical models and associated data)**
- **High-fidelity benchmarks – integral experiments data**
- **The topology of the benchmarks' suite and the application – the physics behind the configurations**

Outline

- **The bias associated with application and the uncertainty generated by validation**
- **Validation matrices (weighted lists of the benchmarks)**

Lessons learned

Note #1

- **The main contingencies on TMC and traditional approach => what is the criteria of success and how to reach the number of benchmarks independency**

Note #2

- **Application is flexible => it can be any linear/bilinear functional of ND (RI, etc.)**

Proposal =>

to built the comprehensive scheme of Integral Experiments Data involvement in ND elaboration using Bayesian approach and **varying the AOs**

Conclusions

- **Suggestion 1: Advanced validation should deal with assessment of the knowledge, i.e. with testing ND together with their covariances using observations and high-fidelity ND covariances, and high-fidelity IE uncertainties and correlations**

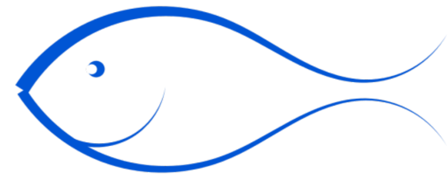
- **Suggestion 2: Further efforts on new ND evaluation and new generations of analytical tools development shall be harmonized with the establishment of ND covariance matrices, IEs covariances and with access to high-fidelity benchmarks (including proprietary)**

- **Suggestion 3: it would worth if the next generation of evaluated ND libraries will contain information about the use of IEs cases for differential experiments calibration and ND evaluation**

- **Suggestion 4: Validation process being a systematic approach should be aimed, among others, on identification of the gaps in data and models and, that is more important, on comprehensive support of the further experiments establishment**

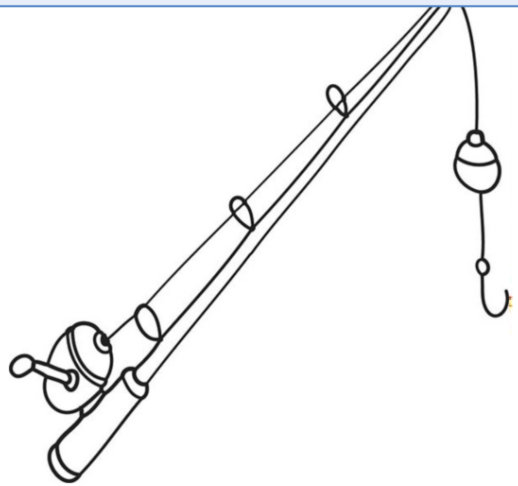
Role of the validation techniques

Raw/available data

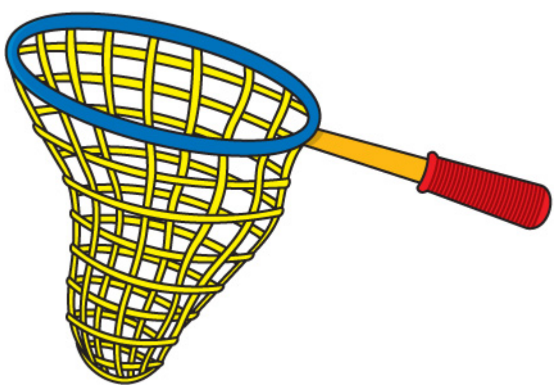


Adjusted data and/or tendency for modification

give a man a fish and feed him for a day — yet teach him to fish and feed him for life (proverb)



GLLSM (Bayesian-based) tool



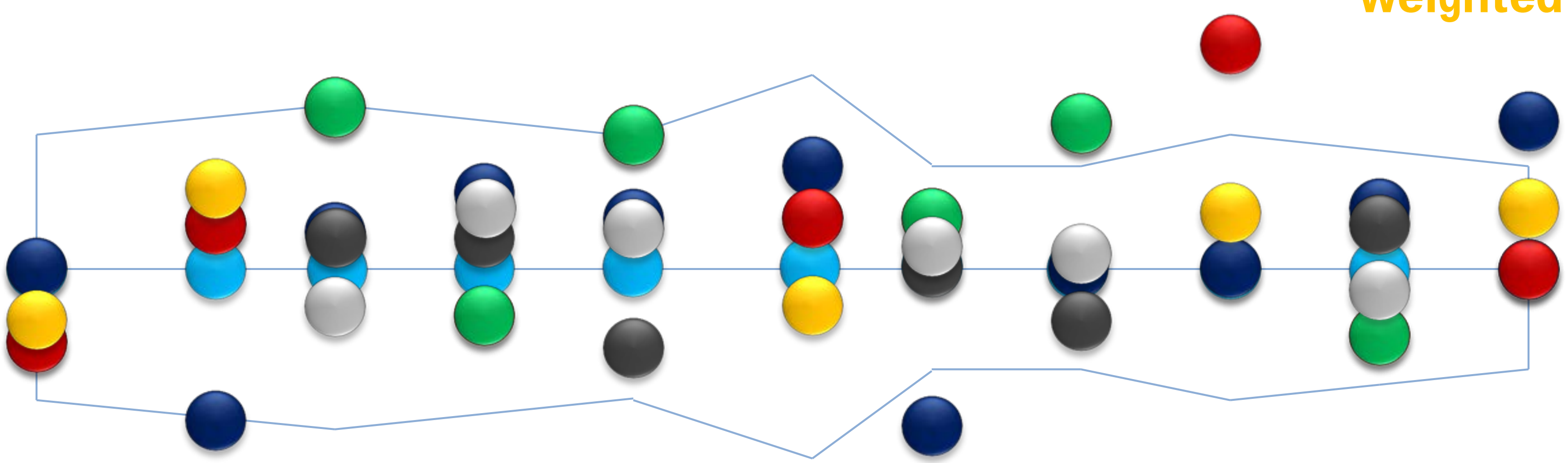
Pre-processed Validation Matrices

TMC divergence/convergence

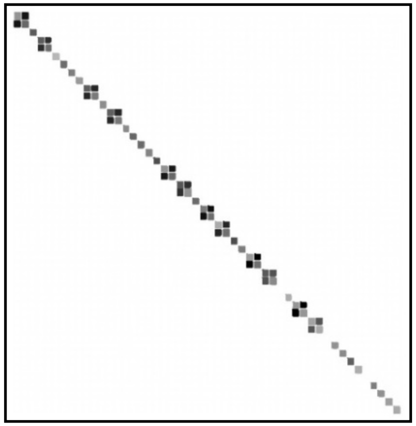
- Bayesian approach – similar weak points as in GLSSM – due to iterations and hierarchy
- Convergence : ideal – all cases are in errors bars, realistic – the most indicative are converged

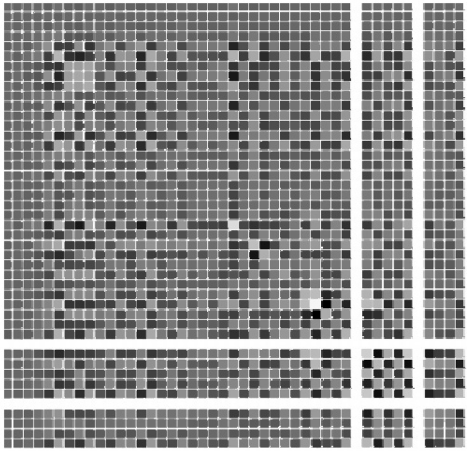
Initial state | **Ideal case** | **General case** | **Weighting** | **Weighted adjustment**

Progressive weighted



Covariance matrices correction in adjustment





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Cross-reaction and cross-material correlations always appear/be corrected while using Bayesian based data assimilation approach

Suggestion 6 : It is contended with some justification that very accurate integral data ought to be used to improve the accuracy of evaluated differential data. However, the influence of cross-reaction and cross-material uncertainty correlations in such an integrated evaluation approach should be investigated extensively before this approach could be considered as sufficiently trustworthy to be applied systematically in producing evaluated nuclear system-independent data libraries such as ENDF/B**

** D.L. Smith, Nuclear Data Uncertainty Quantification: Past, Present and Future, *Nuclear Data Sheets*, 123, pp 1-7 (2015)

* Ivanova T., Ivanov E. and Ecrabet F., "Uncertainty assessment for fast reactors based on nuclear data adjustment", *Nuclear Data Sheets*, 118, pp. 592–595 (2014).

IRSN

Summary of the Reasoning

- GLLSM to provide the first guess for further Total Monte Carlo applications

- Total Monte Carlo convergence/divergence issues

- Origin of the methodology: (Turchin, 1971)

- GLLSM = ill-posed problem solution using Frobenius simplification/ Tikhonov regularization

- Constraints: first order covariance matrices, junction of the nuclei models, statistical nature