IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Faire avancer la sûreté nucléaire

Step towards full V&UQ of Nuclear Data

Roadmap for entire Nuclear Data validation

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on behalf of

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NEA Nuclear Data Week - JEFF and WPEC SG Meetings, Sg46 (Efficient and Effective Use of Integral Experiments for Nuclear Data Validation), 27-30 November 2018 at NEA

V&UQ process, meanings of the terms

V&UQ process comprises

- (A) Application domain formalization of the model and target accuracy establishment using QPIRT
- (O) Observations, validation domain - collection and

Transposition basing on Data Assimilation - by using integral experiments (meters scales) - information is propagated back to the basic level (femto-meters in neutronics, nano-meters in material science and micrometers in thermal hydraulics) covering a range of several orders.

- *Selection of representative observations using essential information on experimental conditions and on physical phenomena of interest*
- *Data assimilation using epistemic uncertainties characterization and guidance of calculus*
- *Error propagation simultaneously of input (aleatory) and epistemic uncertainties*

- (T) Transposition methodology - knowledge propagation from Validation to Application domain

Evgeny Ivanov, IRSN

Layout

- Basic principles and “Working packages” and a “cycle of V&UQ”
- Evaluation of IEs constructing experiment-based benchmarks
- GLLSM application (as a pattern for any Bayesian-based approach)
- New kind of “representativity factors” intended to
  - facilitate validation of “client’s tools”, and
  - provide input for Hierarchic or Total Monte-Carlo
  - design a new experimental program
- Unresolved issue: ouroboros paradigm
- Conclusions

The presentation summarizes basic ideas on Nuclear Data validation using prior (differential) and integral data

(so some slides have been presented before in different contexts)

Fields/domains of a science-based V&UQ process

An application domain :

- Specification of a phase space (space of variables) identifying boundaries of a domain of interest
- Identification and quantification of a vector of Target Accuracies
- Specification of a set of Application objects (cases of interest within an Application domain)

An experimental domain :

- High-fidelity experiment-based benchmarks
- Uncertainties of benchmark values
- Correlation between uncertainties of benchmark values

Transposition technique :

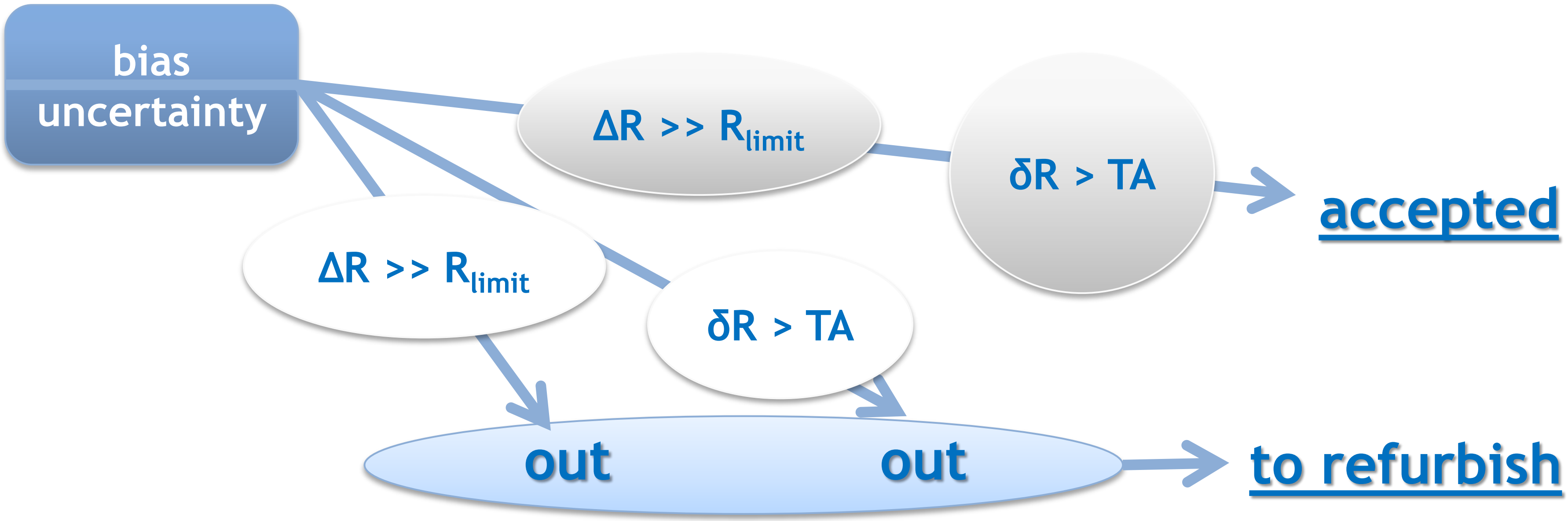
- Bayesian-based approach/process
- Progressive approach combining low-fidelity deterministic (GLLSM) and high-fidelity stochastic (Hierarchical Monte-Carlo) techniques

Decision making process

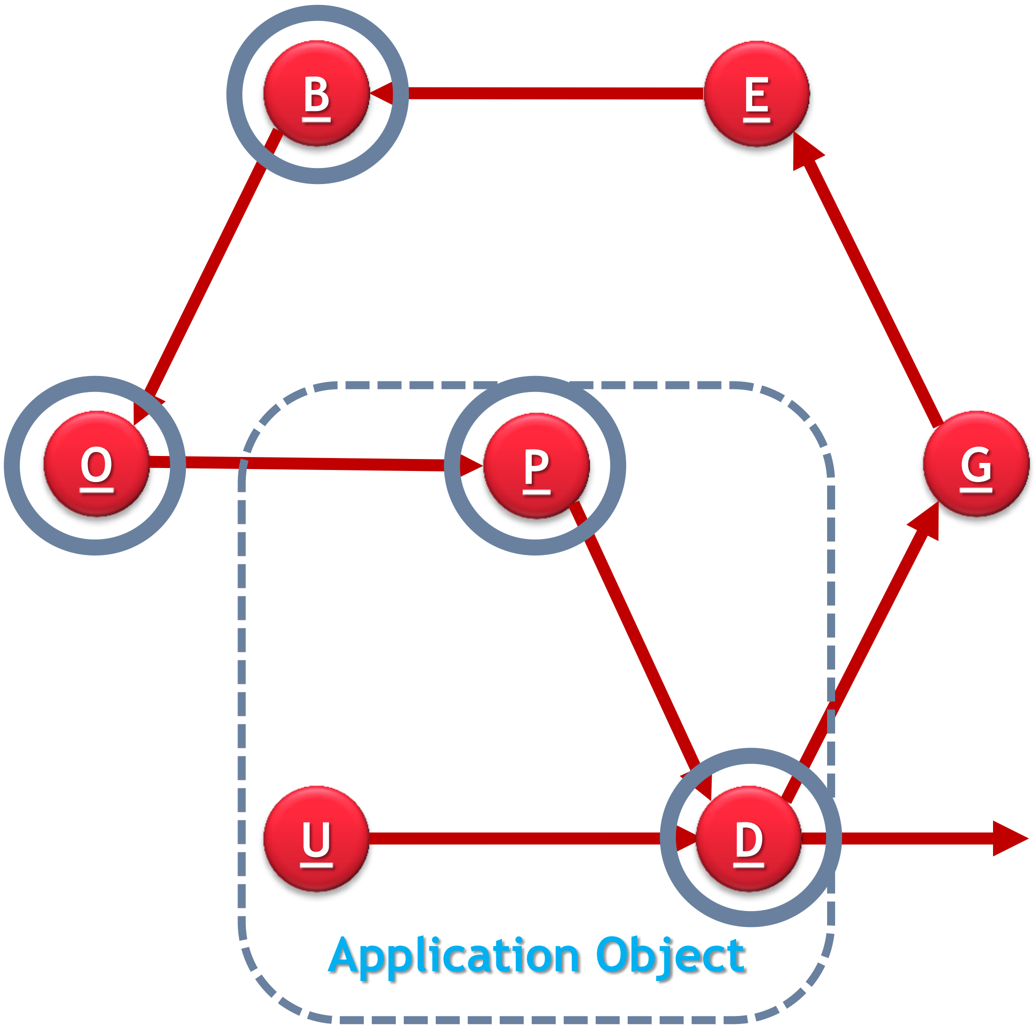
- V&UQ process assesses a “hypothesis of an accuracy” => … given Library is correct enough for … (application)
- V&UQ process => an application-dependent:

Characterizing predictive capabilities in a given domain comparing anticipated uncertainty and given Target Accuracy (TA) – as a success criterion

- V&UQ outline => a bias (ΔR) and an uncertainty of bias (δR)

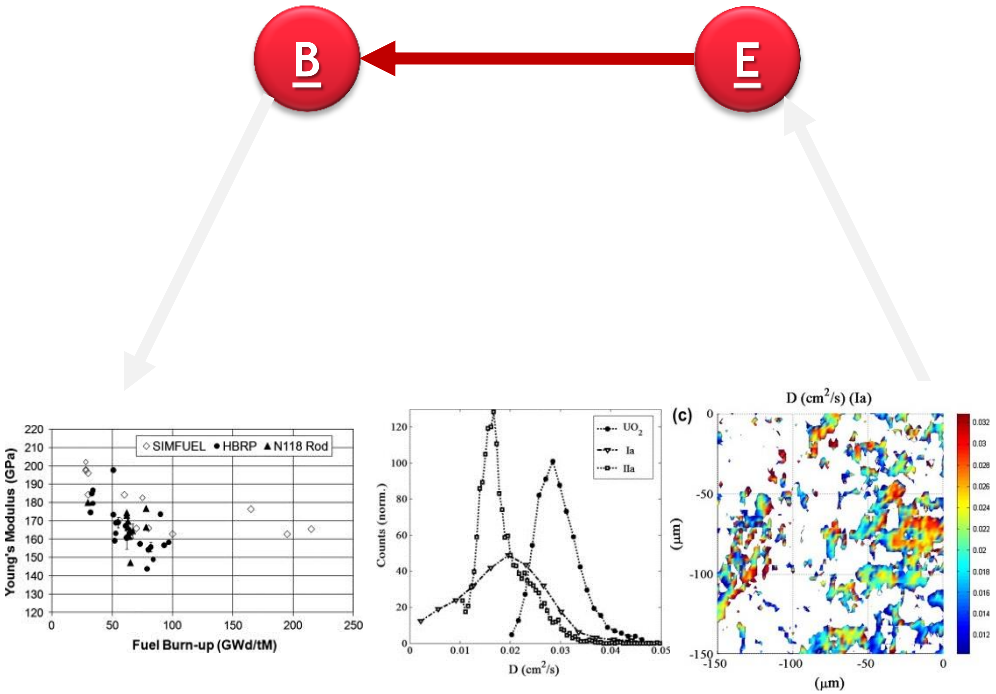


Flow sheet: entire scheme of validation



- **O** Observations
  (C/E + uncertainties)
- **B** Benchmarking
  (Database and Calculations)
- **U** Input uncertainties
  (status of Application Object)
- **P** Predictive Calculations and Data Assimilation
  (UQ for AO)
- **G** Gap analysis
- **E** Design of Experiments
  (Dedicated R&D)
- **D** Decision making process

Experiments to Benchmarks: principles



scalars vectors tensors

- **E** Design of Experiments (Dedicated R&D)
- **B** Benchmarking (Database and Calculations)

Types of experiments:

- Benchmark experiments
- Mock-ups
- PMO

Types of Data:

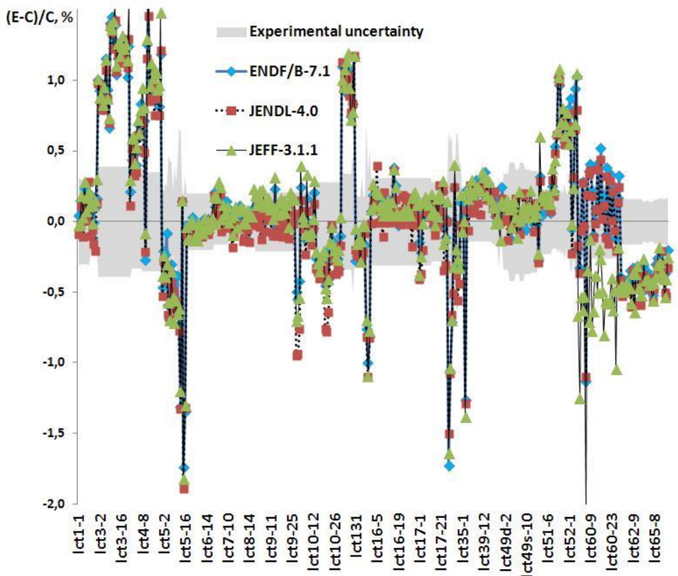
- *scalar-like,*
- *vector-like,*
- *tensor/image (patterns in a neutron noise counting)*

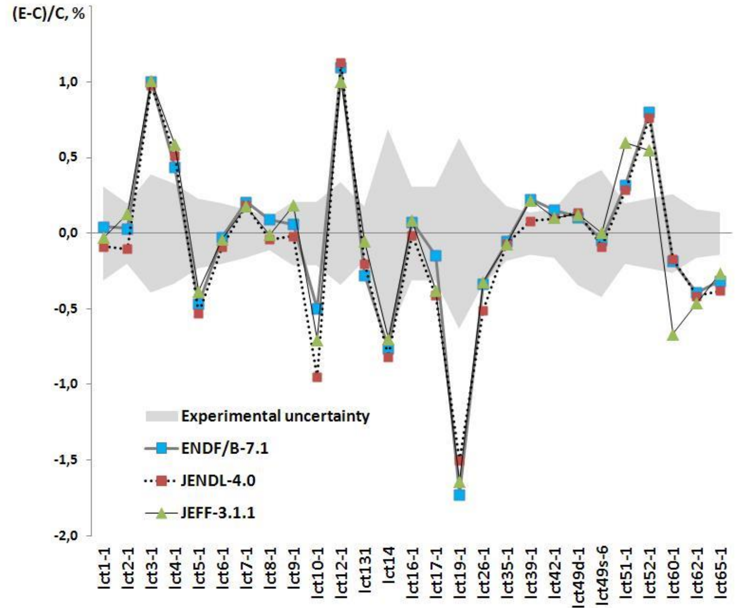
Benchmark values:

- to be done in scalar form

Needed protocol of IE evaluation:
scalar – to – scalar with uncertainty
vector – to – scalar
tensor/image – to – scalar

Integral Correlations role in assessment (Example)





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

IEs data correlate due to facilities, equipment, materials and techniques

Ignorance of correlations => under-estimation of uncertainties

Use of only non-correlated cases => over-estimation of uncertainties

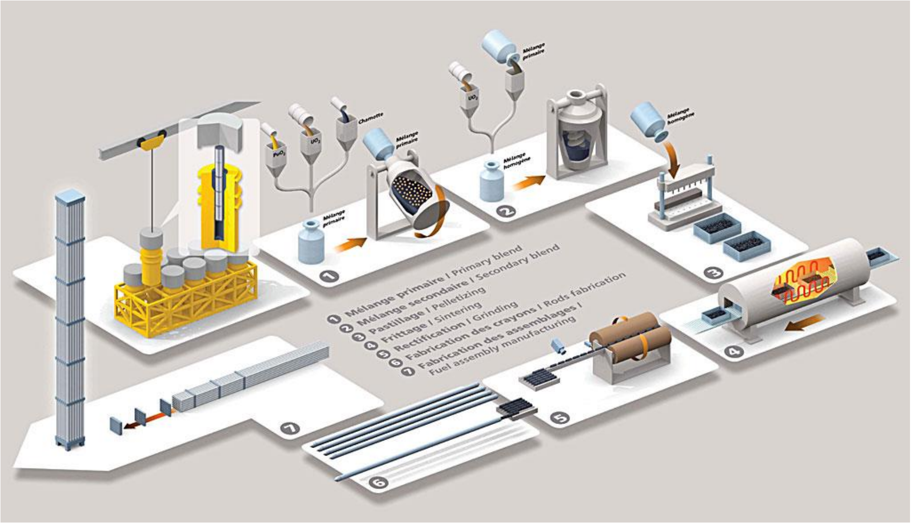
Tatiana Ivanova, Evgeny Ivanov, Giulio Emilio Bianchi "Establishment of Correlations for Some Critical and Reactor Physics Experiments", Nuclear Science and Engineering, Volume 178, Number 3, November 2014

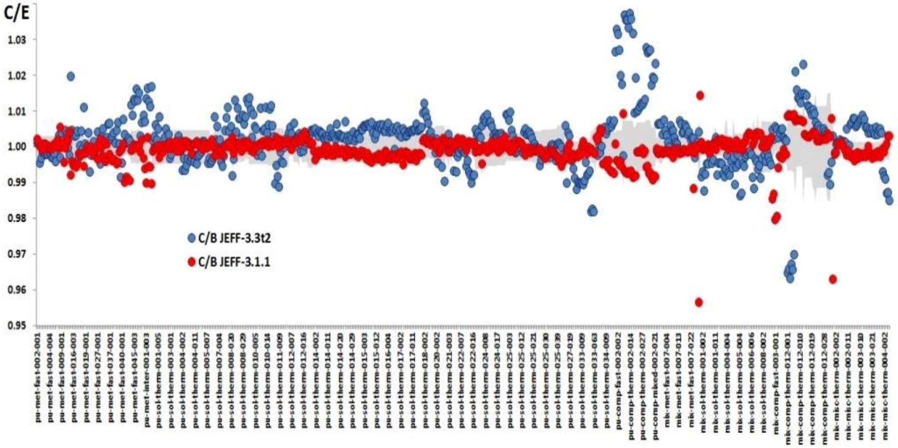
Practical application: MELOX safety assessment

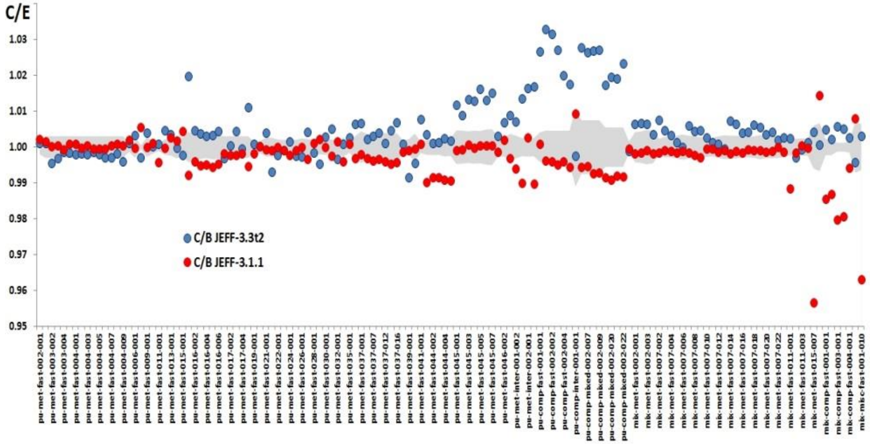
MELOX installation of fuel fabrication with Mixed Uranium-Plutonium Oxide (http://www.new.areva.com/FR/activites-4763/schma-de-fabrication-du-combustible.html?POPIN=Y)

Criticality safety case – water (moderator) in the mixture [Véronique Rouyer et al, “Towards validation of criticality calculations for systems with MOX powders”, Annals of Nuclear Energy, Volume 36, Issue 3, 2009, Pages 305-309]

Different IEs were involved in the evidence based quantification of bias and uncertainties
[T.Ivanova et al, “Methodology and issues of integral experiments selection for nuclear data validation”, *EPJ Web Conf.*, 146 (2017), Article ID 06002]







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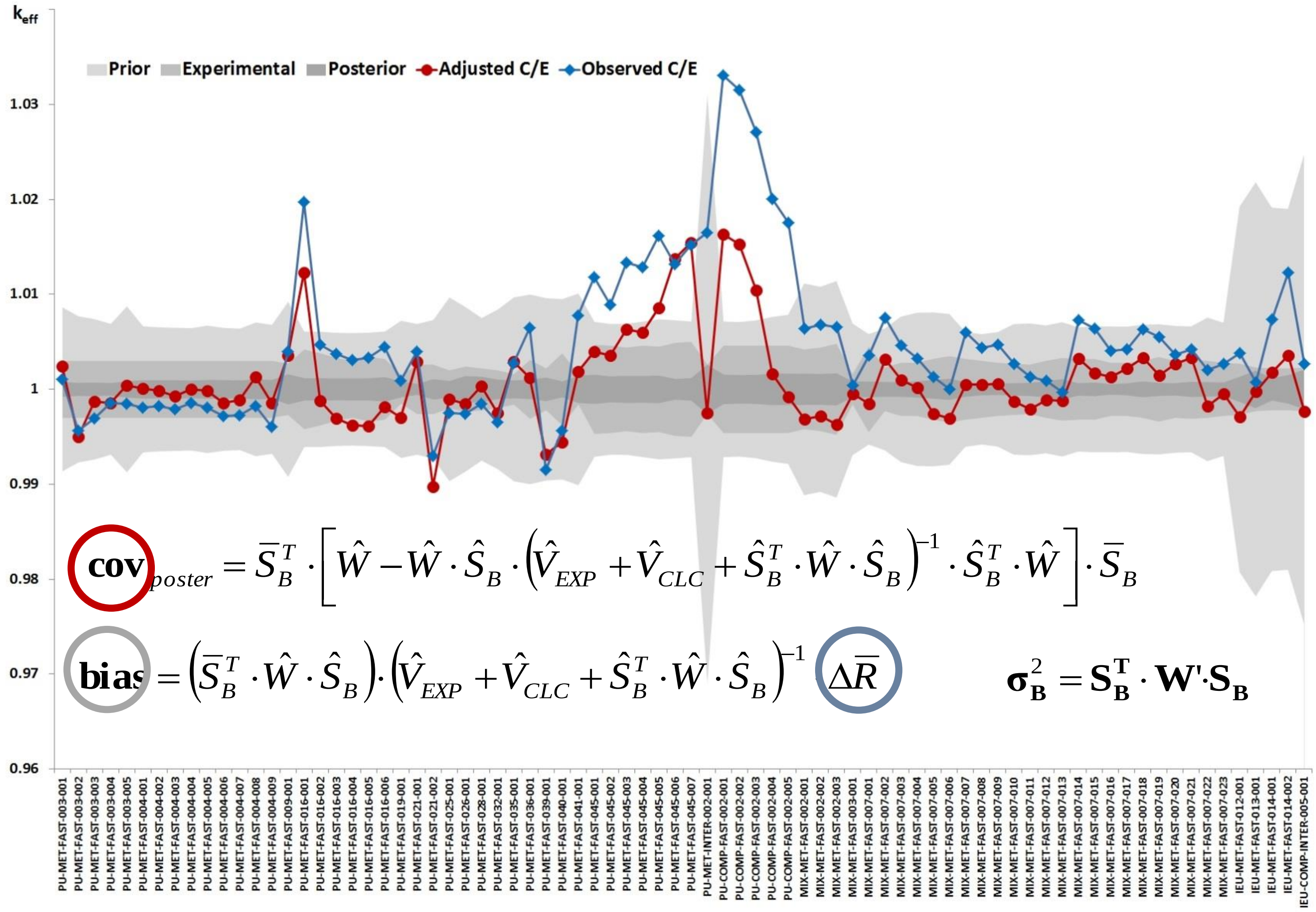
Data Assimilation: Adjustment of ND



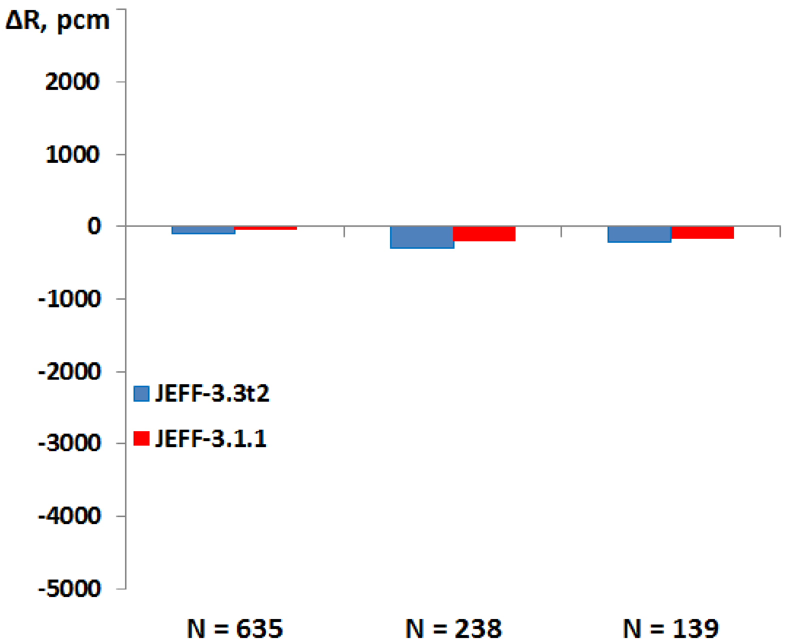
$$\mathbf{cov}_{poster} = \bar{S}_B^T \cdot \left[\hat{W} - \hat{W} \cdot \hat{S}_B \cdot \left(\hat{V}_{EXP} + \hat{V}_{CLC} + \hat{S}_B^T \cdot \hat{W} \cdot \hat{S}_B \right)^{-1} \cdot \hat{S}_B^T \cdot \hat{W} \right] \cdot \bar{S}_B$$

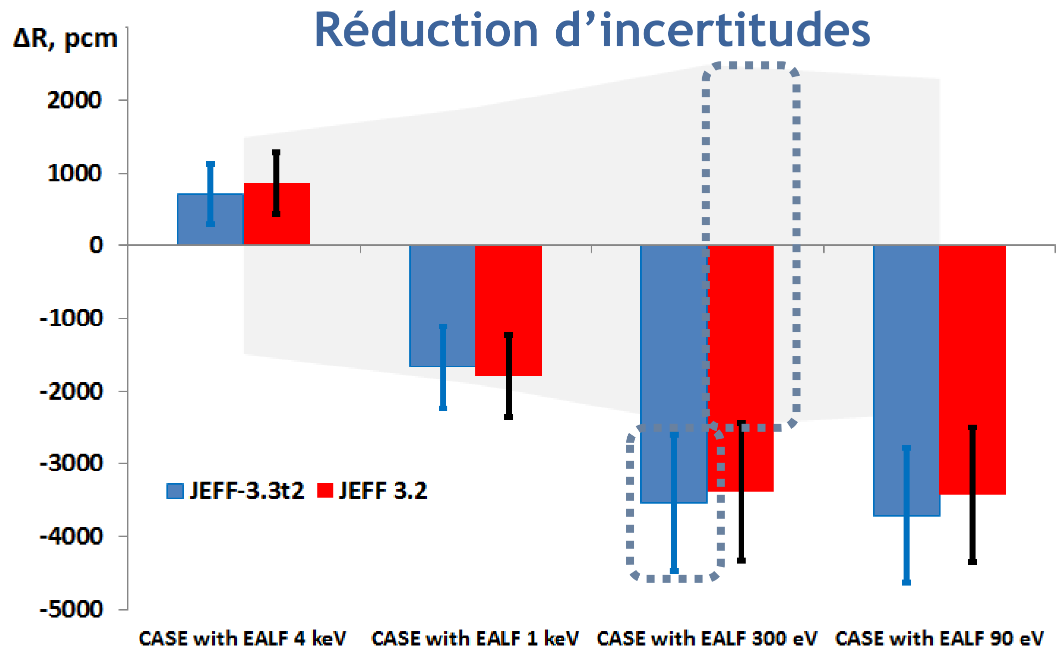
$$\mathbf{bias} = \left(\bar{S}_B^T \cdot \hat{W} \cdot \hat{S}_B \right) \cdot \left(\hat{V}_{EXP} + \hat{V}_{CLC} + \hat{S}_B^T \cdot \hat{W} \cdot \hat{S}_B \right)^{-1} \Delta \bar{R}$$

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

MELOX safety assessment basing on IEs,

T.Ivanova et al, “Methodology and issues of integral experiments selection for ND validation”, *EPJ Web Conf*, 146 (2017)





intuitive (non-stringent)

Bayesian-based judgment

Prior Weighted Average bias: expectation of ~ 300 pcm (<3% M_{CR})

The bias after Data Assimilation: ~ 4000 pcm (~ 10-15% of M_{CR})

Example: Data assimilation technique

T.Ivanova et al, "Methodology and issues of integral experiments selection for ND validation", *EPJ Web Conf*, 146 (2017)

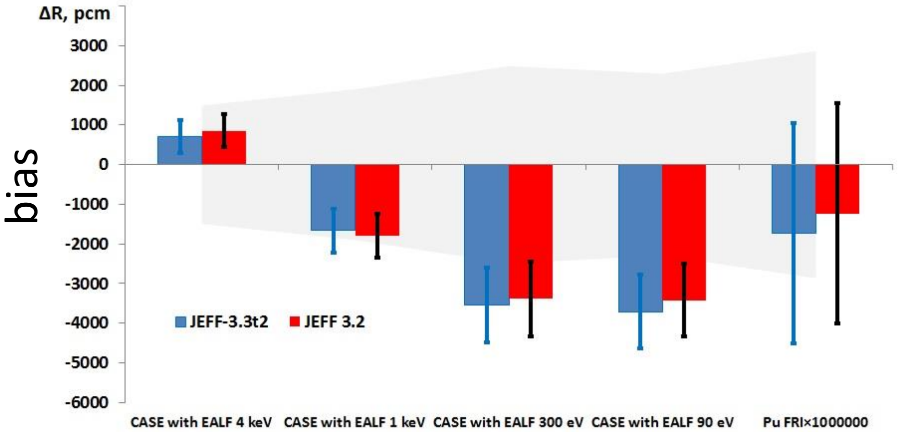
Variety of "Application objects"

Spheres of MOX powder with parametrically changing humidity surrounded by water

Integral of ^{239}Pu fission

EALF by cases **4 keV**, **1 keV**, **300 eV** and **90 eV**

$$RI = \int_{E_1}^{E_2} \sigma(E,\omega) \cdot dE d\omega$$

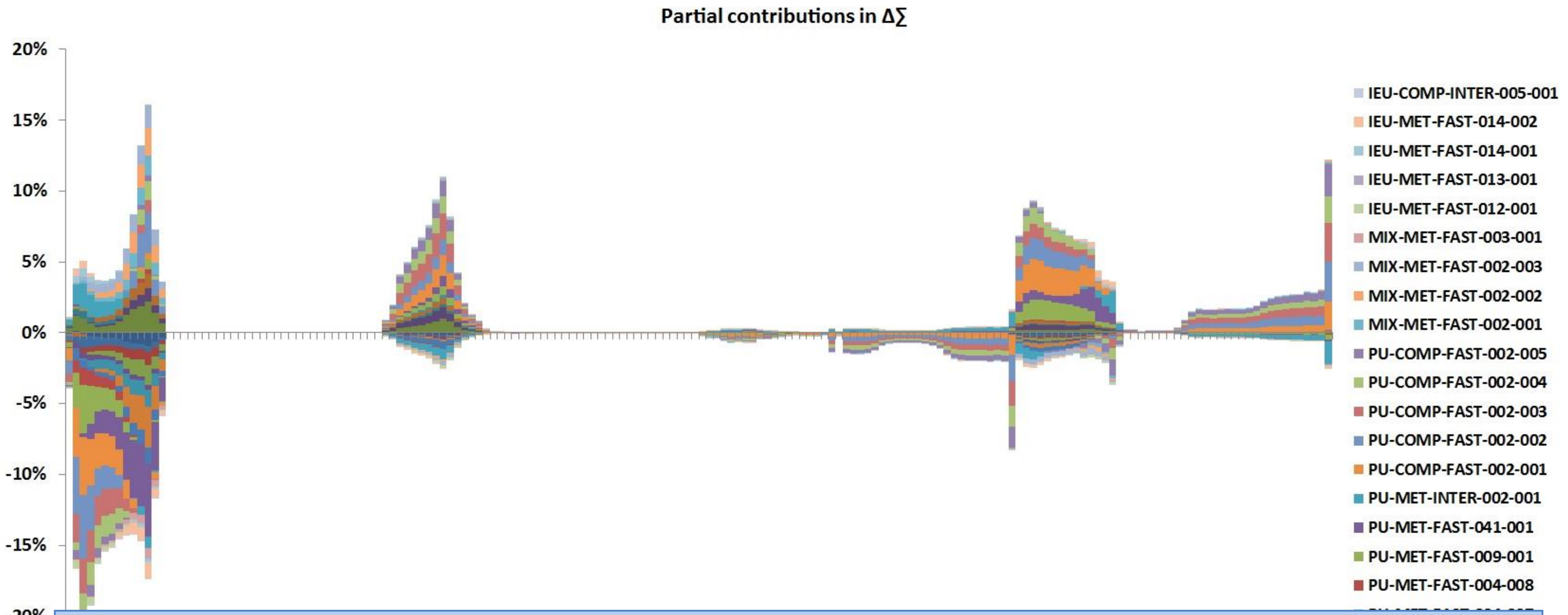


- **Data assimilation approach for different spectra**
  - 1÷4 criticality safety cases
    At 4 keV EALF bias is **Positive**
    Lower Energy EALF bias is **Negative**
  - largest bias ~ <u>**4000 pcm**</u> (Δk_{eff})
  - ^{239}Pu fission resonance integral bias and uncertainty ~ 0.12% and 0.28% (times 1M on the figure)

1) A Bayesian approach (Data Assimilation) provides predictive assessment of bias and uncertainty in a given application domain
2) Assessor may formulate any concept of an application object
(design or safety case, or any linear weighted integral functional of cross sections)

XS adjustment/correction for ^{239}Pu,

Correction of the group-wise cross sections : contradictive contributions (compensative effects similar to PREMIUM in SYSTH)
Adjustment makes sense if the set of benchmarks is statistically significant

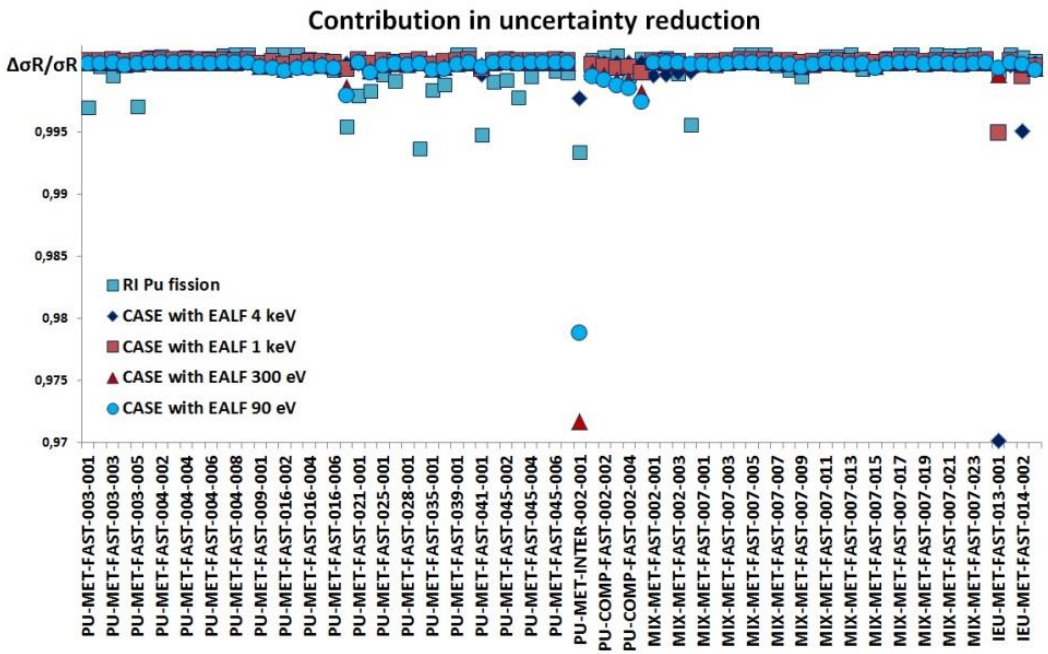


Note: both sensitivity coefficients and corrections can be reduced to nuclear models parameters unfolding the group-wise sensitivities $S_{R,\alpha} = \sum_m \frac{\alpha_m}{R} \cdot \frac{\partial R}{\partial \sigma_m} \cdot \frac{\partial \sigma_m}{\partial \alpha}$

However set IEs should be statistically significant for ND practical adjustment

To select by impact on uncertainty reduction

Uncertainty reduction as the metrics of added value



Factor of uncertainty shift (SF)

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

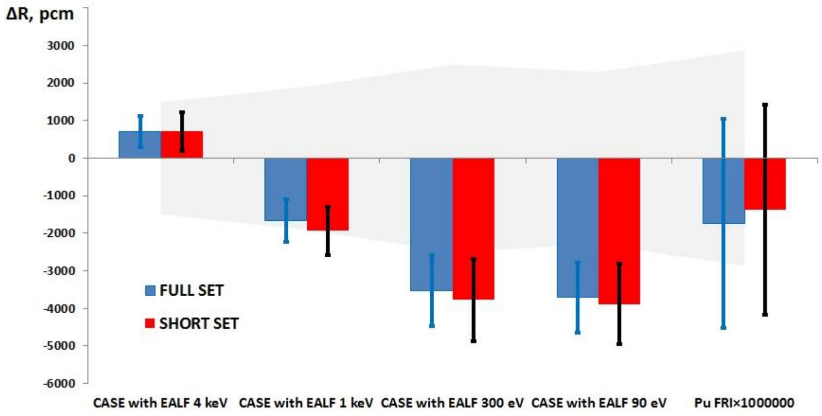
We may not exclude one or another high-fidelity evaluated benchmark from the consideration. However we may evaluate their usability for express analysis

Bias and uncertainties quantification

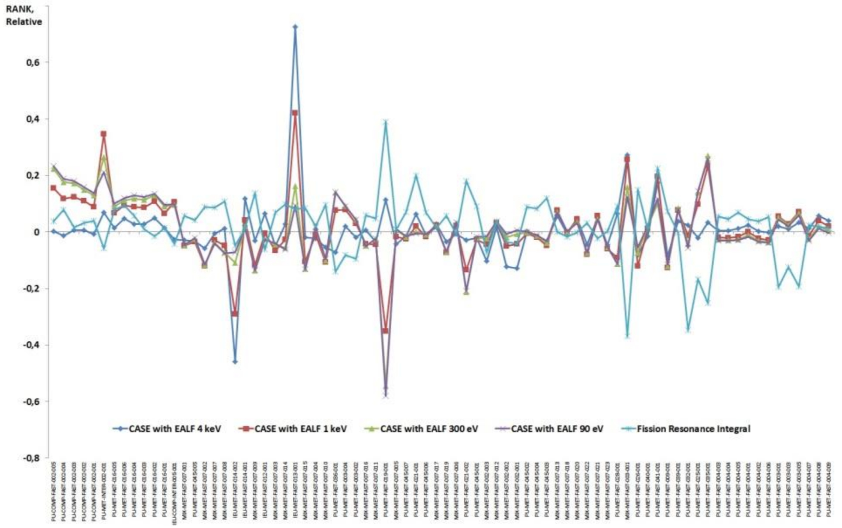
Illustration : uncertainty reduction produces bias

Bias ranking factor (RF)

ΔR_{LIB}



Rank



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

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

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

IEs selection=>
uncertainty reduction and bias conservation

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 IEs selection

- High fidelity evaluated integral experiment data
- Potential contribution in uncertainty ≥ criteria based on χ^2 and 1/Number of benchmarks
  [Factor of Representativity]

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

  [“informativeness” in SYS TH]

- Visible potential contribution in the expected ultimate bias
  [Factor of an Ultimate Bias]

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

  [“calibration” in SYS TH]

1) An express validation (90% of success), and
2) A kind of the first guess for high-fidelity Hierarchic/Total Monte-Carlo

Ouroboros paradigm (Op)

- **Ouroboros paradigm (Op)** is an inherently contradictive practice of use compromised experimental benchmarks in a validation process:

  - *ND evaluation involving Godiva, Flattop etc*
  - *Inferred experimental data*

Op *makes useless IEs on depletion, β_{eff} and some reactivity ones unless apply special techniques*

Suggestion : 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

Conclusions (roadmap's elements)

Domain of applications – a set of Application Objects (AO):

- An AO of the 1st kind: simplified design, process or safety case
- An AO of the 2nd kind: arbitrary taken weighted integral functions of XS
- Target Accuracies (TA) to be attributed to each AO [using a panel study like X-PIRT]

Validation/experimental domain:

- High-fidelity benchmarks developed using evaluated IEs: benchmark value (BV), uncertainty (UNC) of the BV and correlation of UNC between different IEs
- Prior representativity is no more a criterion for IEs selection (no rights to ignore any source of data)
- Separation of benchmarks for calibration and for V&UQ : identify in ND library which IEs have been yet used in a ND evaluation process

Transposition methodology (combining rough GLLSM and fine TMC):

- Bayesian-based (Data Assimilation) approach to solve ill-posed inverse problem
- V&UQ output: (1) posterior bias and uncertainty to meet Decision making requirements; (2) application of SF and RF to Design new Experimental programs

Thank you for your time

Questions/comments

Experiments to Benchmarks, 2/2

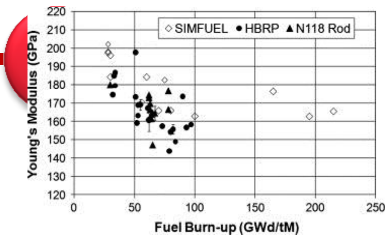
$SRQ_{BENCH} \pm \delta_{EXP} \ldots \pm \delta_{BENCH}$

B

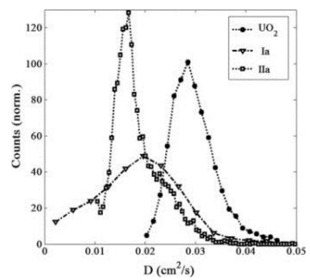
sampling

ROM

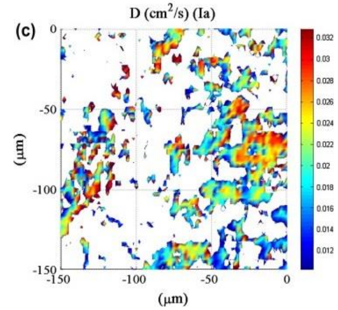
"Big Data"



scalars



vectors



tensors

- **E** Design of Experiments (Dedicated R&D)
- **B** Benchmarking (Database and Calculations)

Types of experiments:

- Benchmark experiments
- Mock-ups
- PMO

Types of Data:

- scalar,
- vector and
- tensor/image

Benchmark values:

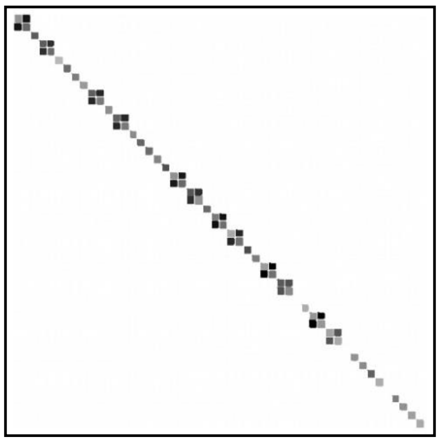
- to be done in scalar form

Generation of Images satisfies 4V's criteria

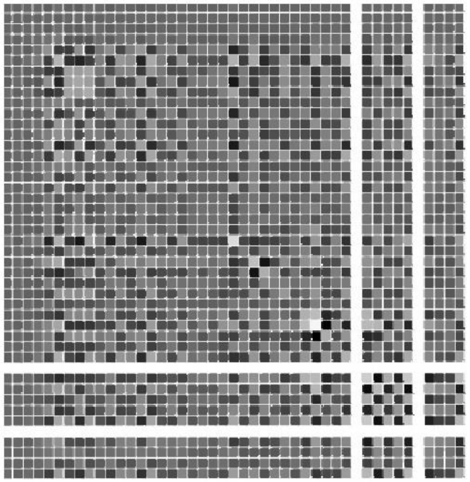
Example: V&UQ is an application-oriented item

*

Before adjustment



After adjustment



Prior covariance matrices - associated with nuclear data libraries - ENDF/B-VII.0 (COMMARA-2.0), JENDL, TENDL etc.

- Takes into account
  - similarity of sources, targets, detectors, data mining process,
  - the expert judgment
- impacted by missed data

Posterior covariance matrix – adds information on selected integral experiments (IE) data
Information about IEs compensates missed and inconsistent data filling gaps in covariance and cross-covariance elements

* 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).

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