AREVA NP

Application of Bayesian Monte Carlo Analysis to Criticality Safety Assessment

Axel Hoefer, Oliver Buss

AREVA GmbH Erlangen
Radiology, Radiation Protection & Criticality Safety Analysis

ANS Winter Meeting, Washington, D.C., October 29 - November 2, 2017

AREVA

Outline

1. **Why validation?**
2. **NUDUNA / MOCABA uncertainty propagation**
3. **Application Cases (Blind Tests)**
4. **Summary / Final remarks**

Chapter 1

Why validation?

Why validation?

What is our goal?

- **Optimum predictions (BEPU) – correct for computational bias**
  - k_{eff} of spent fuel pool
  - Power distribution of reactor / cycle prediction

What do we need?

- **Reliable uncertainty information**
  - Nuclear data covariances (ENDF)
  - Technological uncertainties (application case & benchmarks)
- **Consistent statistical framework**
  - Statistical model (Bayes)
  - Computational procedure (Sensitivity or MC)

How do we test a prediction model / procedure?

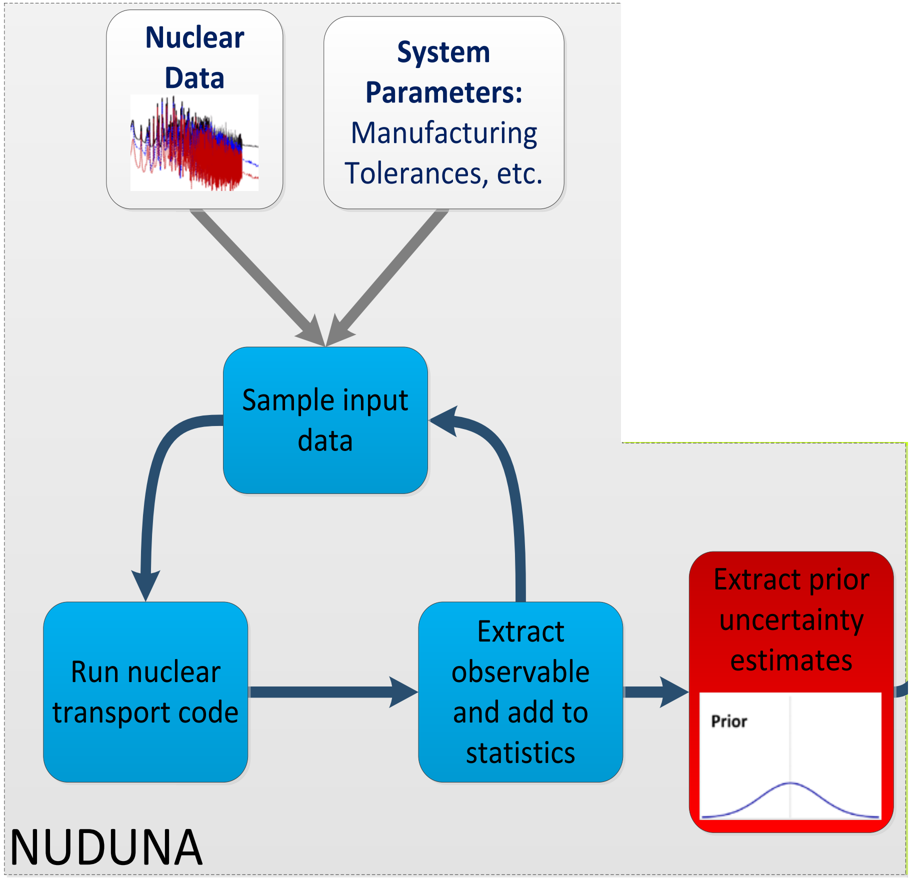
- **Blind tests: Predictions of measurements**

Chapter 2

NUDUNA / MOCABA Uncertainty propagation

Uncertainty Assessment with NUDUNA / MOCABA @AREVA

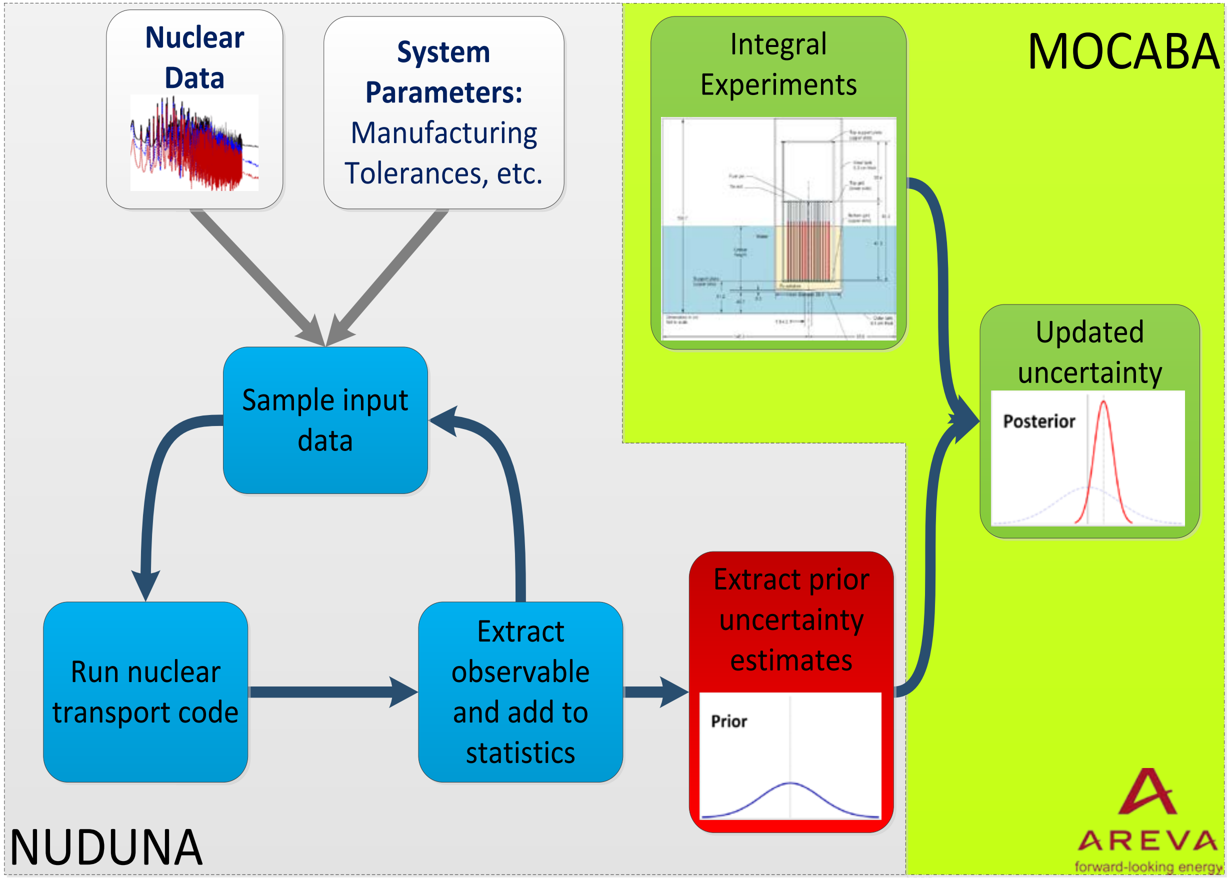
1. **NUDUNA:**
   Uncertainty assessment based on Monte Carlo



Uncertainty Assessment with NUDUNA / MOCABA @AREVA

1. **NUDUNA:**
   Uncertainty assessment based on Monte Carlo

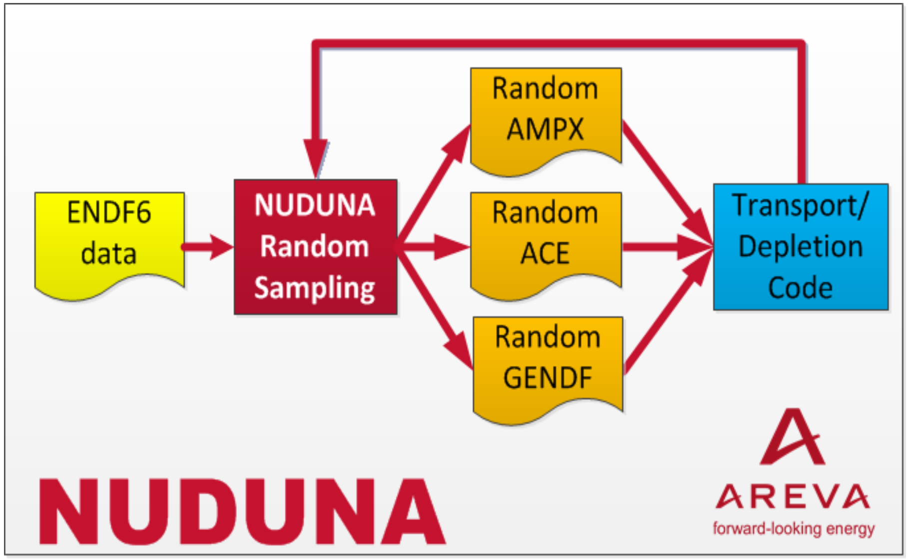
2. **MOCABA:**
   Improve predictions by adding measurements (Bayesian updating)



NUDUNA: NUclear Data UNcertainty Analysis

Annals of Nuclear Energy 77 (2015), 101ff

- Direct sampling of ENDF-6 data
  - ENDF/B, JEFF, JENDL, TENDL …
- Automatic generation of transport code libraries
  - Based on NJOY 99, PUFF IV
  - Support for MCNP, SERPENT, SCALE, WIMSD-4, ALEPH, APOLLO2-A
  - Arbitrary temperatures and broad group structures



- Current limitations (to be removed in the future)
  - No fission spectra and product yield (Files 5,8) sampling
  - No S(α,β) (File 7) sampling
  - No isotope-isotope correlations

MOCABA:
Monte Carlo based Bayesian updating

Annals of Nucl. Energy 77 (2015), 514ff

1. **MC sampling of nuclear data (*NUDUNA*):**

$$\boldsymbol{\alpha}_{MC} \propto p(\boldsymbol{\alpha}) = N(\hat{\boldsymbol{\alpha}}, \boldsymbol{\Sigma}_{\alpha})$$

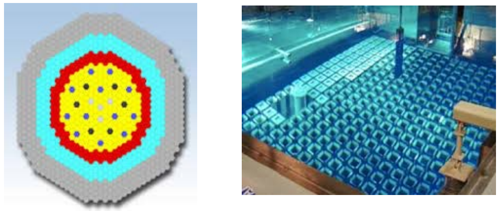
mean vector *covariance matrix*

2. **Calculation of integral quantities:**

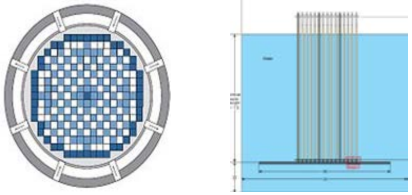
MC draws of system parameters

$$\mathbf{y}_{MC} := \left(y_{A,1}(\boldsymbol{\alpha}_{MC}, \mathbf{x}_{MC}), \ldots, y_{A,n_A}(\boldsymbol{\alpha}_{MC}, \mathbf{x}_{MC}) \;,\; y_{B,1}(\boldsymbol{\alpha}_{MC}, \mathbf{x}_{MC}), \ldots, y_{B,n_B}(\boldsymbol{\alpha}_{MC}, \mathbf{x}_{MC}) \right)^T$$

Appl. Case



Benchmarks



3. **Calculation of prior mean and prior covariance matrix:**

$$\mathbf{y}_0 = \frac{1}{n_{MC}} \sum_i \mathbf{y}_{MC,i} \qquad \boldsymbol{\Sigma}_0 = \frac{1}{n_{MC} - 1} \sum_i (\mathbf{y}_{MC,i} - \mathbf{y}_0)(\mathbf{y}_{MC,i} - \mathbf{y}_0)^T$$

Σ_{0A}	Σ_{0AB}
Σ_{0AB}^T	Σ_{0B}

Prior distribution: $p(\mathbf{y}) = N(\mathbf{y}_0, \boldsymbol{\Sigma}_0)$

reflects integral uncertainties due to nuclear data uncertainties

AREVA NP

MOCABA:
Monte Carlo based Bayesian updating

Annals of Nucl. Energy 77 (2015), 514ff

4. Evaluation of likelihood function of integral measurements / constraints

$$p(\mathbf{v_B} \,|\, \mathbf{y_B}) \propto N(\mathbf{v_B}, \mathbf{\Sigma_{vB}})$$

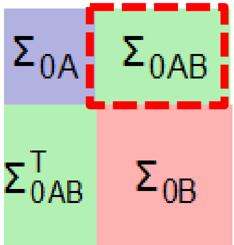
Covariance matrix of integral quantities

Measurement vector / linear constraint vector

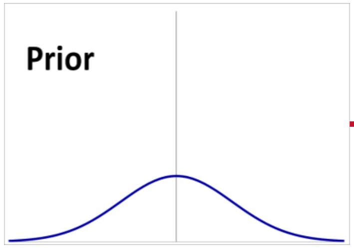
5. Bayesian updating

Updated model parameters

$$p(\mathbf{y} \,|\, \mathbf{v_B}) \propto p(\mathbf{v_B} \,|\, \mathbf{y_B})\, p(\mathbf{y}) = N(\mathbf{y}^*, \mathbf{\Sigma}^*)$$

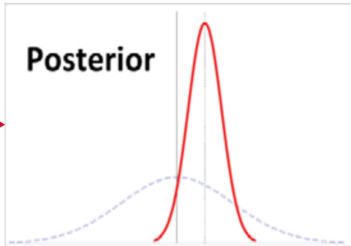


Σ_{0A}	Σ_{0AB}
Σ_{0AB}^T	Σ_{0B}



$$\mathbf{y}_{0A/B} \rightarrow \mathbf{y}^*_{A/B}$$

$$\mathbf{\Sigma}_{0A/B} \rightarrow \mathbf{\Sigma}^*_{A/B}$$



Impact of benchmark information determined by similarities to application cases
→ Correlations due to common input parameter uncertainties

MOCABA:
Monte Carlo based Bayesian updating

Annals of Nucl. Energy 77 (2015), 514ff

Special case: normal distribution model, no constraints

- **Prior**

$$p(\mathbf{y}) \propto \exp\left(-Q_0/2\right)$$

$$Q_0 = \left(\mathbf{y}-\mathbf{y}_0\right)^T \boldsymbol{\Sigma}_0^{-1}\left(\mathbf{y}-\mathbf{y}_0\right)$$

$$\mathbf{y}_0 = \left(\mathbf{y}_{0A}^T, \mathbf{y}_{0B}^T\right)^T \qquad \boldsymbol{\Sigma}_0 = \begin{pmatrix} \boldsymbol{\Sigma}_{0A} & \boldsymbol{\Sigma}_{0AB} \\ \boldsymbol{\Sigma}_{0AB}^T & \boldsymbol{\Sigma}_{0B} \end{pmatrix}$$

- **Likelihood**

$$p(\mathbf{v}\,|\,\mathbf{y}) \propto \exp\left(-Q_V/2\right)$$

$$\mathbf{v}_0 = \left(\mathbf{v}_{0A}^T, \mathbf{v}_{0B}^T\right)^T \qquad \boldsymbol{\Sigma}_V^{-1} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Sigma}_{VB}^{-1} \end{pmatrix}$$

$$Q_V = \left(\mathbf{y}-\mathbf{v}\right)^T \boldsymbol{\Sigma}_V^{-1}\left(\mathbf{y}-\mathbf{v}\right)$$

- **Posterior**

$$p(\mathbf{y}\,|\,\mathbf{v}) \propto \exp\left(-Q^*/2\right)$$

$$\mathbf{y}^* = \left(\mathbf{y}_A^{*T}, \mathbf{y}_B^{*T}\right)^T \qquad \boldsymbol{\Sigma}^* = \begin{pmatrix} \boldsymbol{\Sigma}_A^* & \boldsymbol{\Sigma}_{AB}^* \\ \boldsymbol{\Sigma}_{AB}^{*T} & \boldsymbol{\Sigma}_B^* \end{pmatrix}$$

$$Q^* = Q_0 + Q_V = \left(\mathbf{y}-\mathbf{y}^*\right)^T \boldsymbol{\Sigma}^{*-1}\left(\mathbf{y}-\mathbf{y}^*\right)$$

$$\mathbf{y}_A^* = \mathbf{y}_{0A} + \boldsymbol{\Sigma}_{0AB}\left(\boldsymbol{\Sigma}_{0B}+\boldsymbol{\Sigma}_{VB}\right)^{-1}\left(\mathbf{v}_B-\mathbf{y}_{0B}\right) \qquad \boldsymbol{\Sigma}_A^* = \boldsymbol{\Sigma}_{0A} - \boldsymbol{\Sigma}_{0AB}\left(\boldsymbol{\Sigma}_{0B}+\boldsymbol{\Sigma}_{VB}\right)^{-1}\boldsymbol{\Sigma}_{0AB}^T$$

GLLS = 1st order approximation of MOCABA

Annals of Nucl. Energy 77 (2015), 514ff

- **Apply 1st order series expansion to MOCABA updating formulas**

$$\mathbf{y}(\boldsymbol{\alpha}) \approx \mathbf{y}(\boldsymbol{\alpha}_0) + \mathbf{S}(\boldsymbol{\alpha} - \boldsymbol{\alpha}_0) + \xcancel{\ldots}$$

GLLS: posterior distribution of nuclear data vector

Prior $p(\boldsymbol{\alpha}) = N(\boldsymbol{\alpha}_0, \boldsymbol{\Sigma}_\alpha)$

Posterior $p(\boldsymbol{\alpha} \mid \mathbf{v}_B) = N(\boldsymbol{\alpha}^*, \boldsymbol{\Sigma}^*_\alpha)$

$$\mathbf{y}^*_A \approx \mathbf{y}_{0A} + \mathbf{S}_A(\boldsymbol{\alpha}^* - \boldsymbol{\alpha}_0) + \xcancel{\ldots}$$

$$\boldsymbol{\alpha}^* = \boldsymbol{\alpha}_0 + \boldsymbol{\Sigma}_\alpha \mathbf{S}_B^T \left(\mathbf{S}_B \boldsymbol{\Sigma}_\alpha \mathbf{S}_B^T + \boldsymbol{\Sigma}_{VB}\right)^{-1} \left(\mathbf{v}_B - \mathbf{y}_{0B}\right)$$

$$\boldsymbol{\Sigma}^*_A \approx \mathbf{S}_A \boldsymbol{\Sigma}^*_\alpha \mathbf{S}_A^T + \xcancel{\ldots}$$

$$\boldsymbol{\Sigma}^*_\alpha = \boldsymbol{\Sigma}_\alpha - \boldsymbol{\Sigma}_\alpha \mathbf{S}_B^T \left(\mathbf{S}_B \boldsymbol{\Sigma}_\alpha \mathbf{S}_B^T + \boldsymbol{\Sigma}_{VB}\right)^{-1} \mathbf{S}_B \boldsymbol{\Sigma}_\alpha$$

MOCABA: Monte Carlo based Bayesian updating

Annals of Nucl. Energy 77 (2015), 514ff

General MOCABA Framework

Linear constraints → Generalization of Likelihood (Linear Combinations)

$$p(\mathbf{v}\,|\,\mathbf{y}) \propto \exp\left(-Q_V / 2\right) \qquad Q_V = (\mathbf{U}\mathbf{y}-\mathbf{v})^T \Sigma_V^{-1} (\mathbf{U}\mathbf{y}-\mathbf{v})$$

- Sum rules for ND updating, e.g. total XS as sum of contributions
- Fixed total power of reactor as sum FA power contributions

➔ Generalized Updating Formulas

Extension to more general distribution models (e.g. Johnson)

- Useful for strongly non-linear responses to variations in nuclear data, e.g. for transients
- Procedure: Invertible transformation to normal data → Application of MOCABA to transformed data → Back-transformation

AREVA

MOCABA vs. GLLS

GLLS	MOCABA
Adjoint-based PT (internal)	Monte Carlo (external – black box)
1st order approximation	Non-perturbative
Updating of nuclear data	Direct updating of integral observables or nuclear data
Efficient algorithms for sensitivity computations	Higher computational costs for precise Sensitivities
Unfavorable for large number of responses	Any number of responses

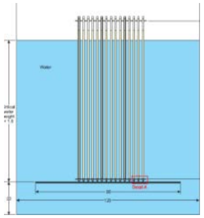
MOCABA:
Monte Carlo based Bayesian updating

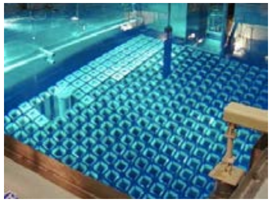
Random Input

Black Box

Physical Model

Benchmark
& Appl. Case

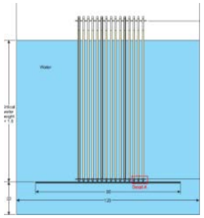




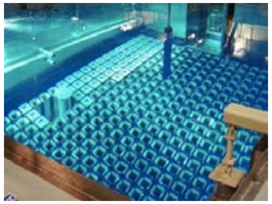
Random Output

MOCABA

Measurements,
Constraints



Prediction

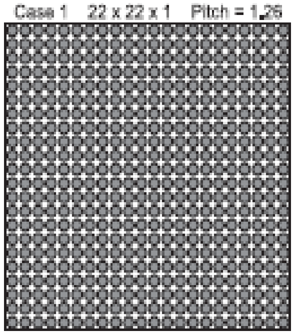


Chapter 3

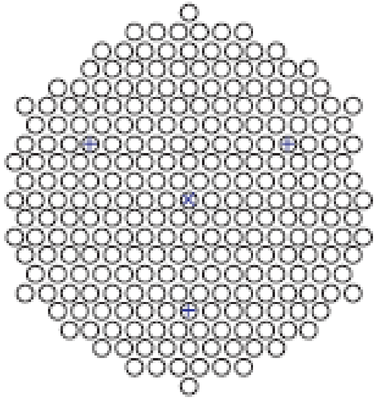
Application Cases (Blind Tests)

Application to UACSA Benchmark 4

- **UACSA Benchmark 4**
  - **Role of Integral Experiment Covariance Data for Criticality Safety Validation**
- **21 Benchmark Experiments**
  - **LCT 07 & LCT 39 (ICSBEP)**
    - Rectangular UO_2 Lattices
    - e=4.738 wt.-%
    - Pitch:
      - LCT07: 1.26-2.52 cm
      - LCT39: 1.26 cm
- **Application Cases:**
  - **LCT 79 Case 1 & 6 (ICSBEP)**
    - Hexagonal UO_2 Lattices
    - e=4.31 wt.-%
    - Pitch:
      - 2 cm for case 1
      - 2.8 cm for case 6



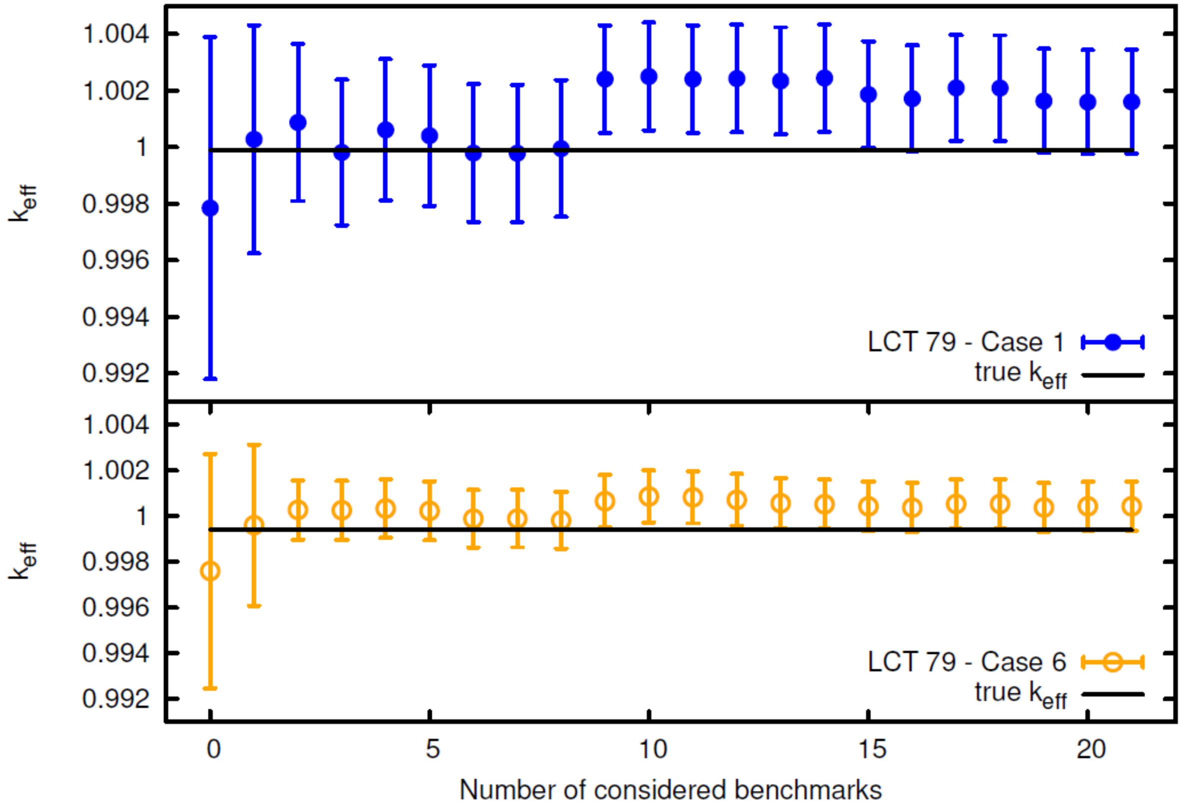
LCT 39- Case 1



LCT 79- Case 1

Application to UACSA Benchmark 4

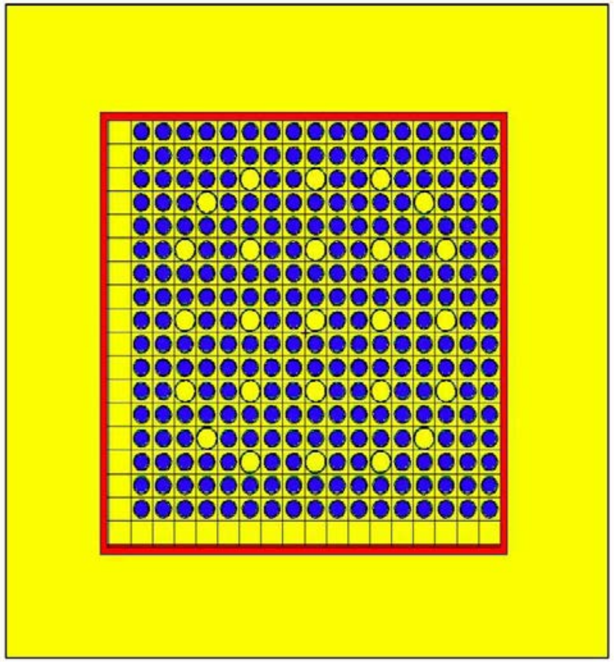
- **SCALE 6.0 / NITAWL / ENDF/B VII.1 / NUDUNA / MOCABA**



- **MOCABA leads to improved mean values and to a massive reduction of uncertainties!**

Application to wet storage of fuel assemblies

- **"Uncertainties for the Ringhals fuel storage due to nuclear data"**
  - D.A. Rochman and A.J. Koning
  - ftp://ftp.nrg.eu/pub/www/talys/bib_rochman/vattenfall.ringhal.pdf

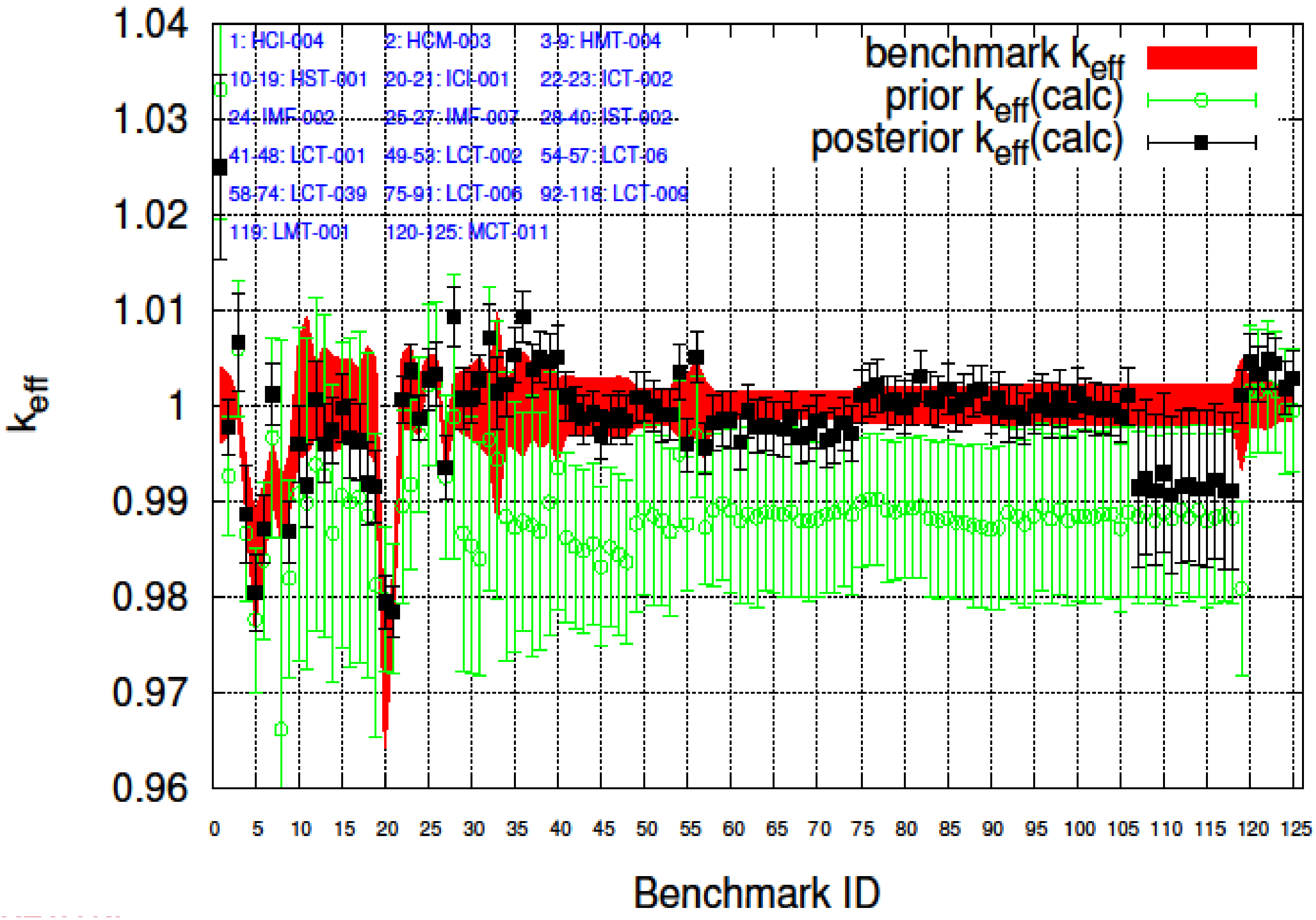


- **MCNP model for criticality calculations**
  - AREVA HTP 17x17-24-1 FA
  - 4.65 wt. % U-235
  - Eccentric positioning within stainless steel channels

- **Nuclear Data Simulations with fast TMC (NRG)**
  - **TMC sampling of U-235 (598 samples)**
  - **For each ND sample MCNP calculations for**
    - Ringhals storage pool
    - 125 ICSBEP benchmarks (17 sets)

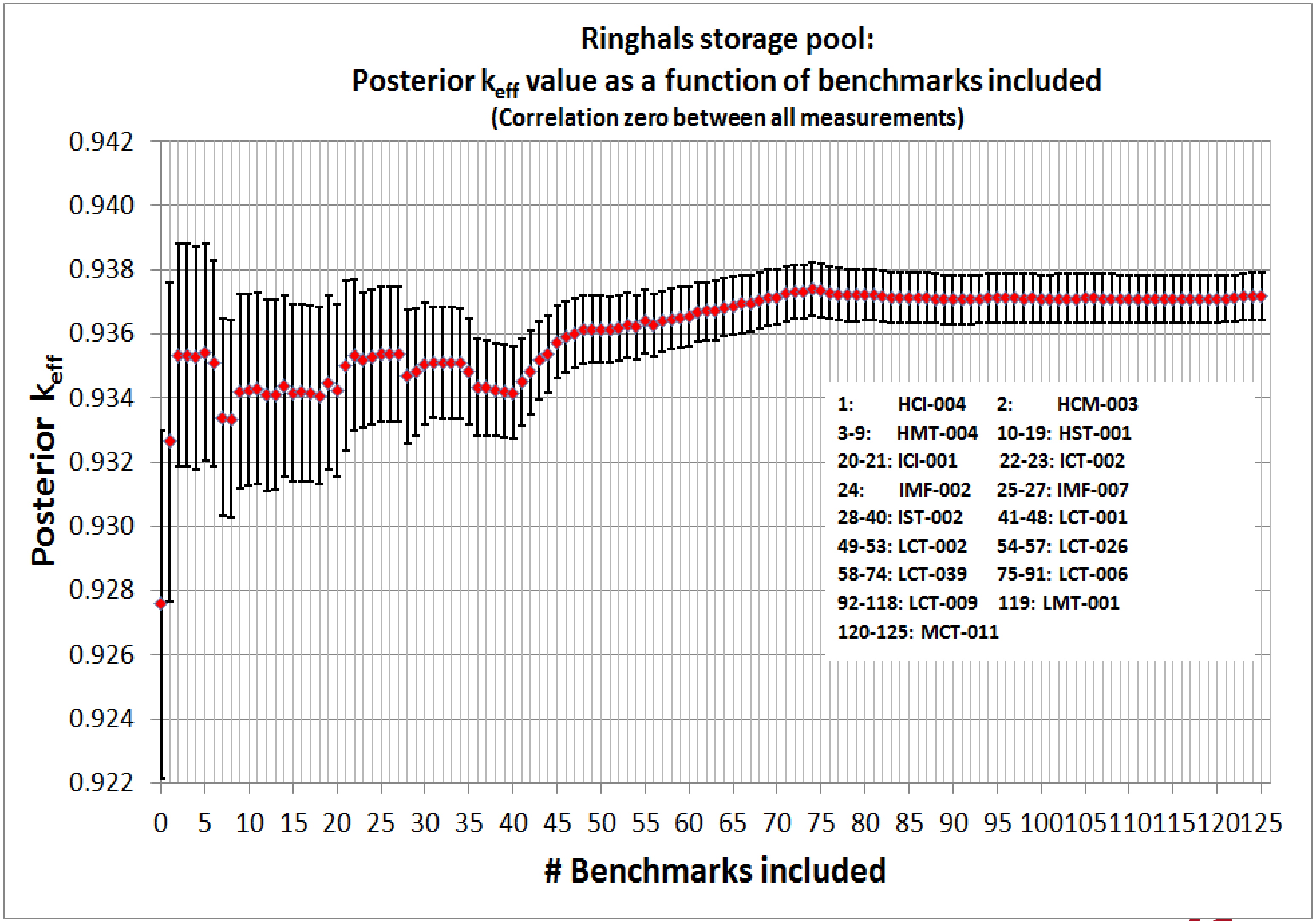
Application to wet storage of fuel assemblies

Prediction of the keff values for 17 sets of criticality benchmarks based on the other 16 benchmark sets respectively



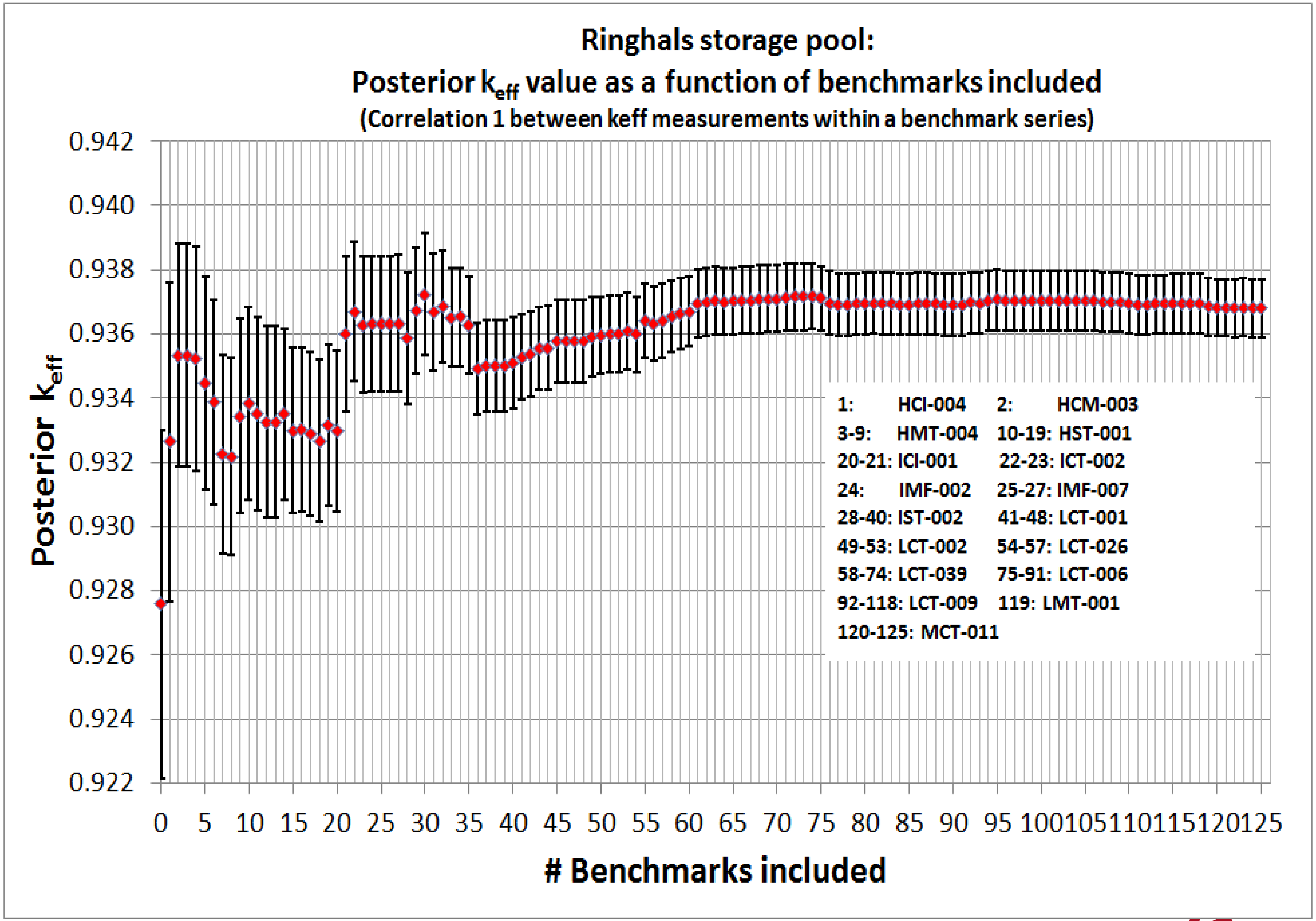
Application to wet storage of fuel assemblies

Corr = 0 within series



Application to wet storage of fuel assemblies

Corr = 1 within series

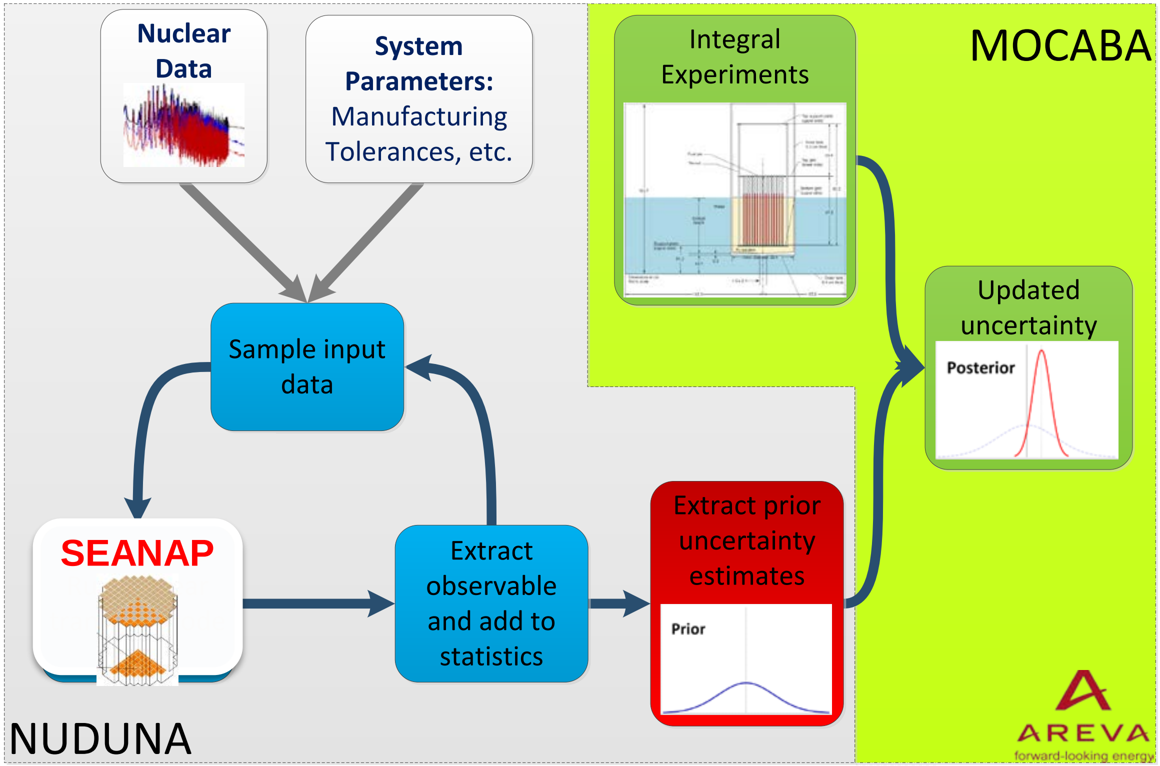


Application to Core Simulation

- **Blind test:**

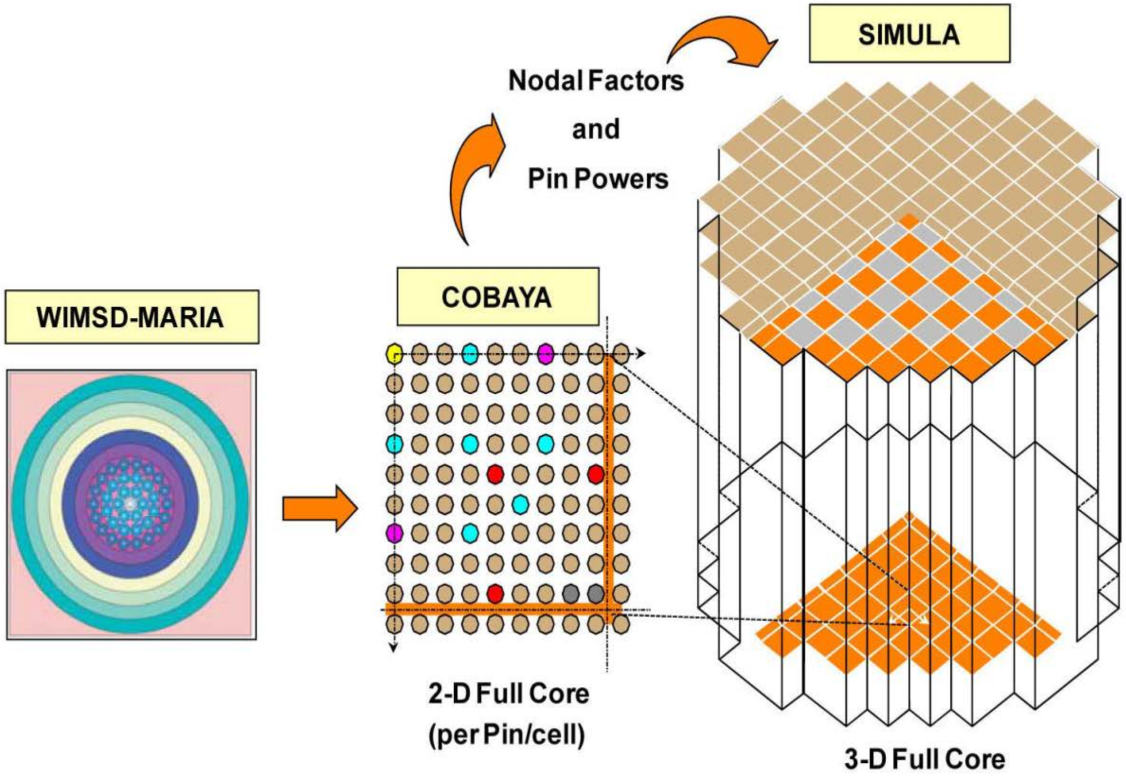
Annals of Nucl. Energy 95 (2016), 148ff

- **MOCABA predictions of Cycle B based on measurements of previous Cycle A**
- **Compare Cycle B predictions to Cycle B measurements**
  → test predictive power of MOCABA framework



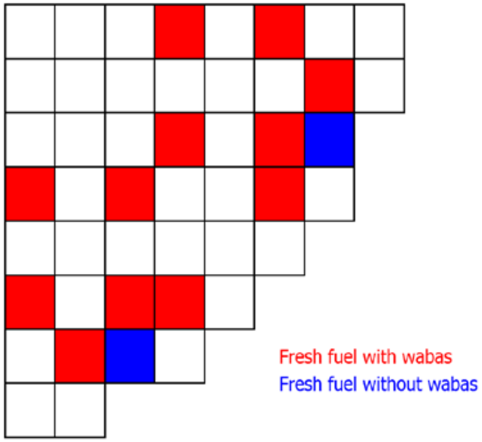
Application to Core Simulation

- **SEANAP: Sistema Español de Análisis de Núcleos de Agua a Presión. System developed at Universidad Politécnica de Madrid for the analysis of PWR reactors**
  - Applied by facilities in many cycles of Spanish PWR for the last 25 years



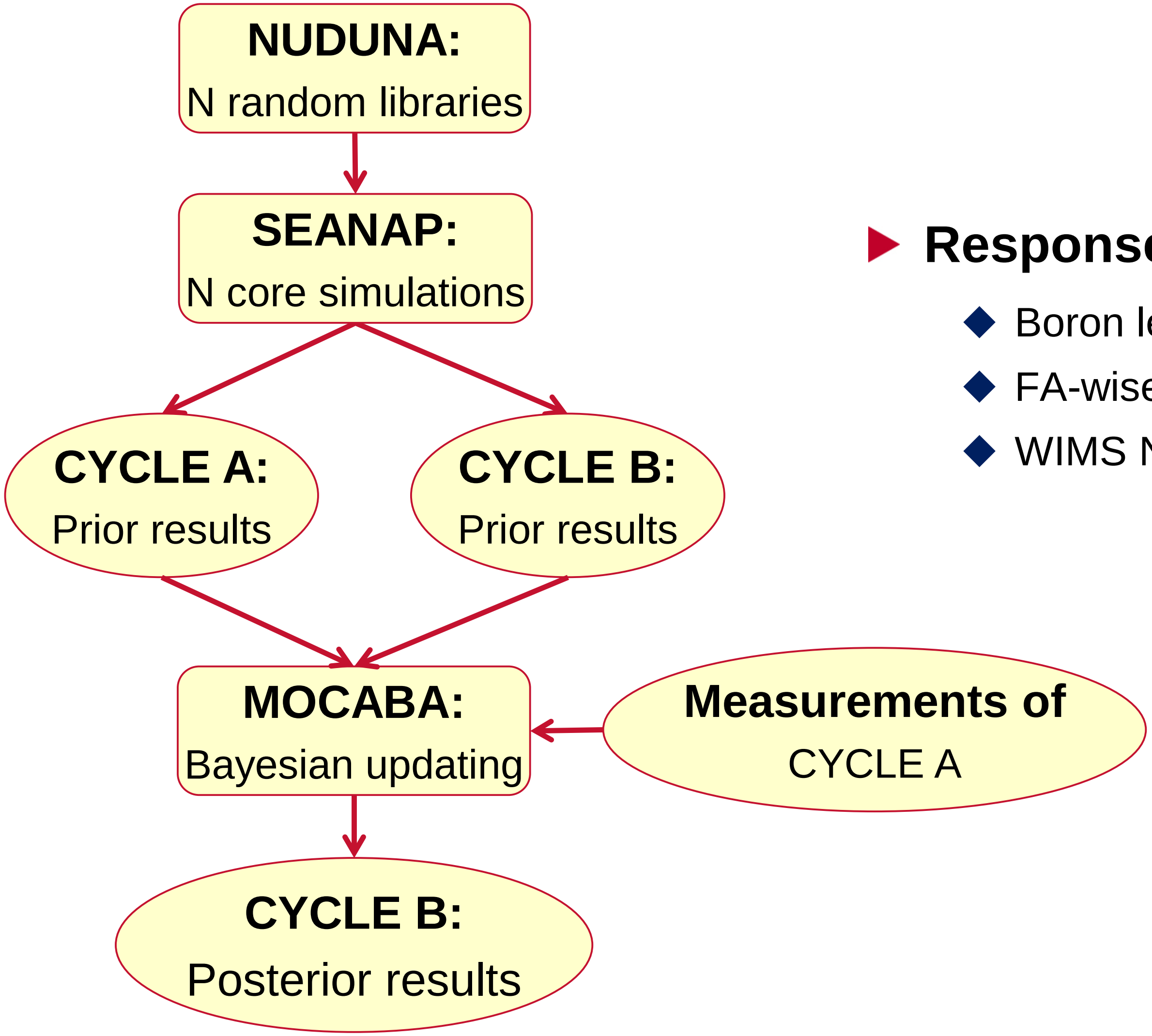
Application to Core Simulation

- **PWR core specifications cycle B:**
  - 157 Fuel Assemblies
  - 2775 MW_t
  - Fresh and used fuel
  - Wabas as burnable absorber.



- **Random libraries generated with NUDUNA from ENDF/B-VII.1:**
  - U-235 and U-238, Pu-239, Hydrogen, B-10, O-16

Application to Core Simulation



NUDUNA:
N random libraries

SEANAP:
N core simulations

CYCLE A:
Prior results

CYCLE B:
Prior results

MOCABA:
Bayesian updating

Measurements of
CYCLE A

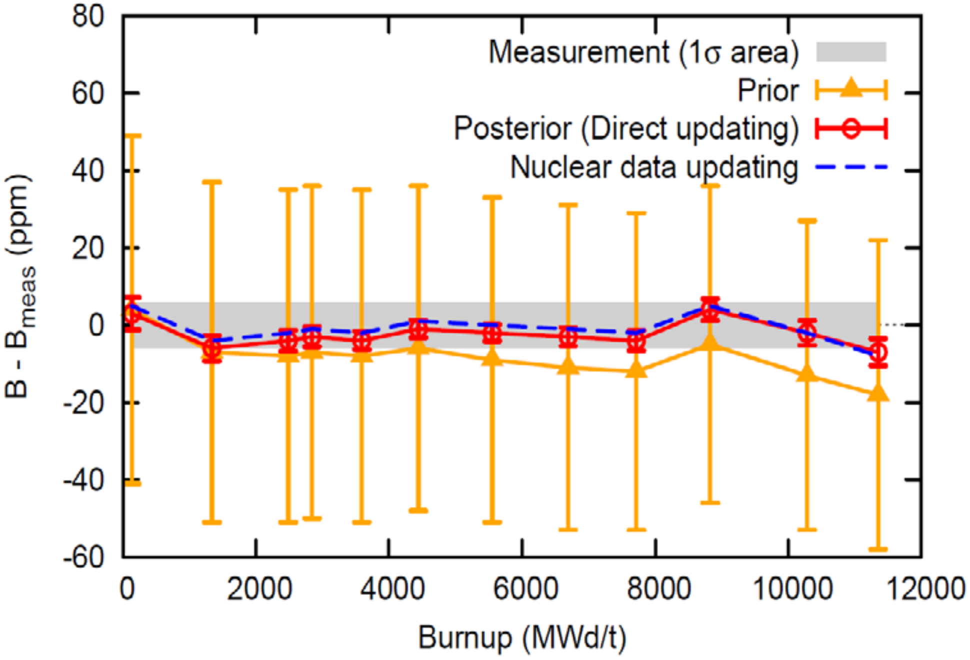
CYCLE B:
Posterior results

- **Responses:**
  - Boron letdown curve
  - FA-wise power distribution
  - WIMS Nuclear Data Library

Application to Core Simulation

- **B = boron concentration / ppm σ = one standard deviation (ppm)**

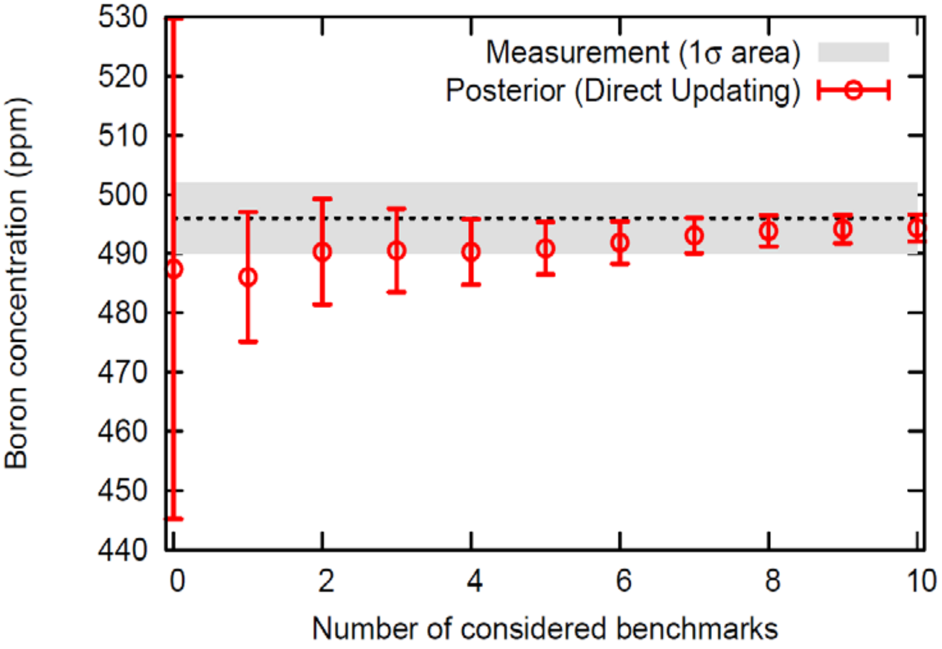
MWd/t	B_{prior}	σ_{prior}	B_{post}	σ_{post}	$\sigma_{prior} / \sigma_{post}$
135	987	45	986	4.2	10.7
1340	867	44	868	3.3	13.3
2487	763	43	767	2.7	15.9
2842	733	43	737	2.6	16.5
3591	664	43	668	2.4	17.9
4441	590	42	595	2.3	18.3
5549	487	42	494	2.2	19.1
6692	383	42	391	2.4	17.5
7716	290	41	298	2.6	15.8
8823	197	41	206	2.8	14.6
10284	74	40	85	3.2	12.5
11351	-15	40	-4	3.5	11.4



Application to Core Simulation

B = boron concentration / ppm **σ = 1 standard deviation / ppm**

MWd/t	B_{prior}	σ_{prior}	B_{post}	σ_{post}	σ_{prior} / σ_{post}
135	987	45	986	4.2	10.7
1340	867	44	868	3.3	13.3
2487	763	43	767	2.7	15.9
2842	733	43	737	2.6	16.5
3591	664	43	668	2.4	17.9
4441	590	42	595	2.3	18.3
5549	487	42	494	2.2	19.1
6692	383	42	391	2.4	17.5
7716	290	41	298	2.6	15.8
8823	197	41	206	2.8	14.6
10284	74	40	85	3.2	12.5
11351	-15	40	-4	3.5	11.4



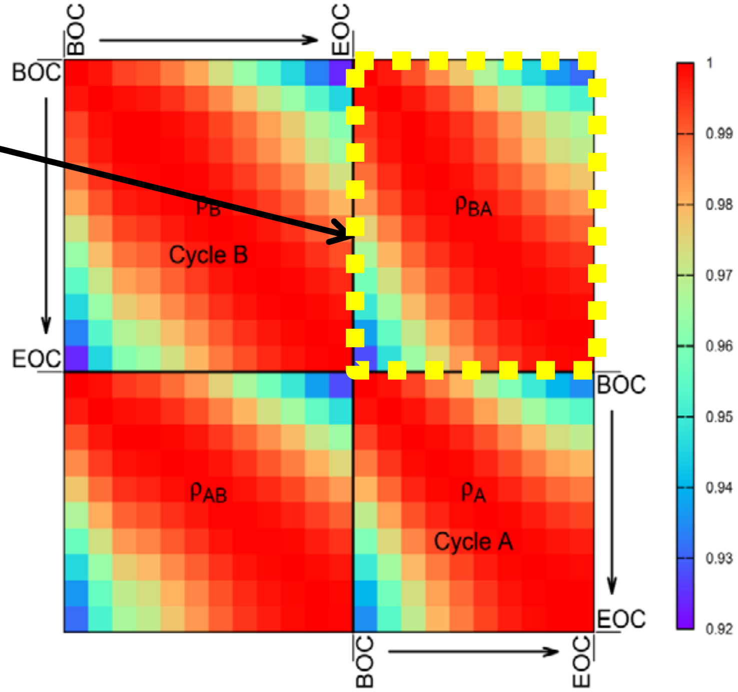
Application to Core Simulation

Large ND correlations between Cycle A and B

> 0.92

↓

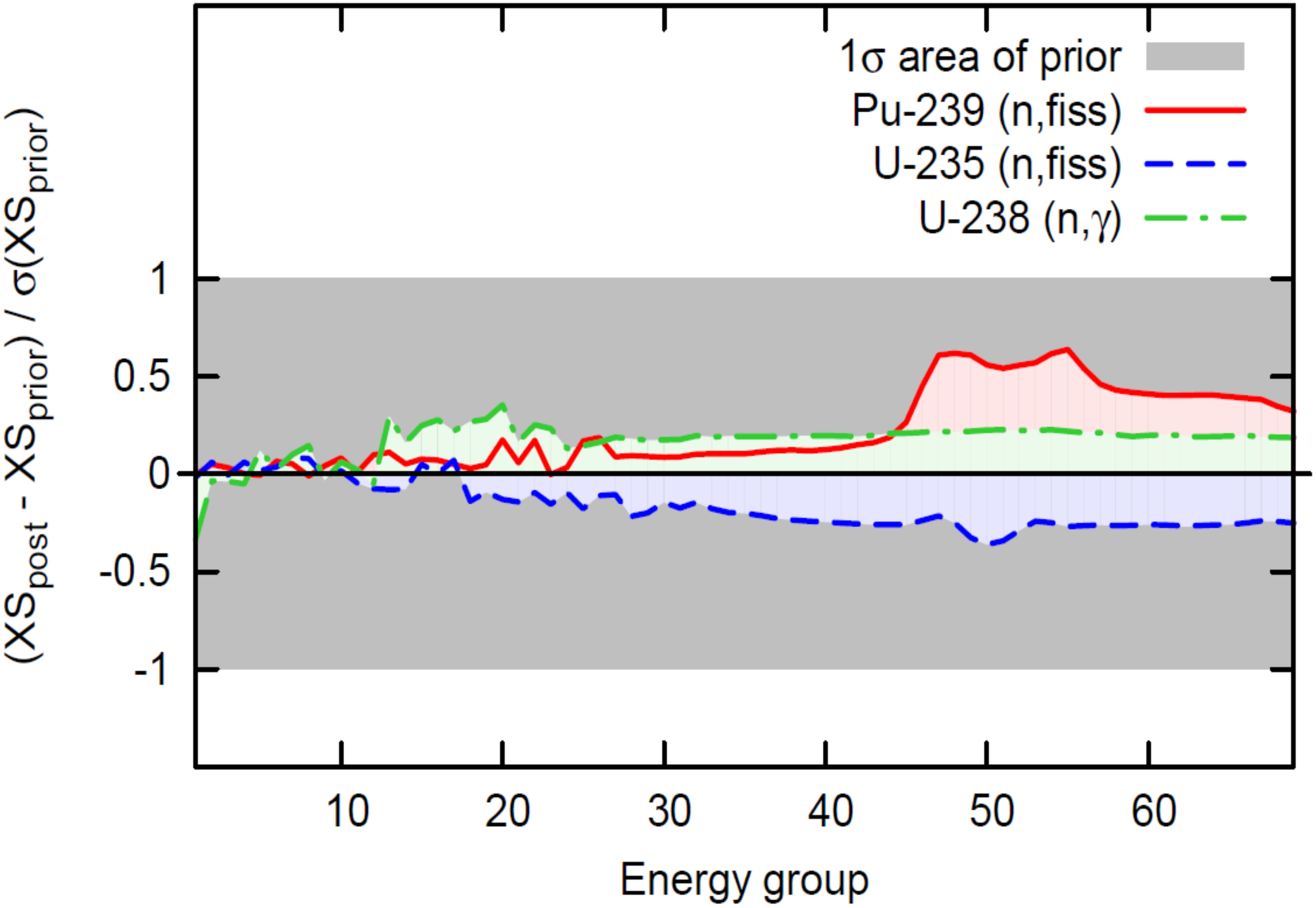
Large impact of the Bayesian updating



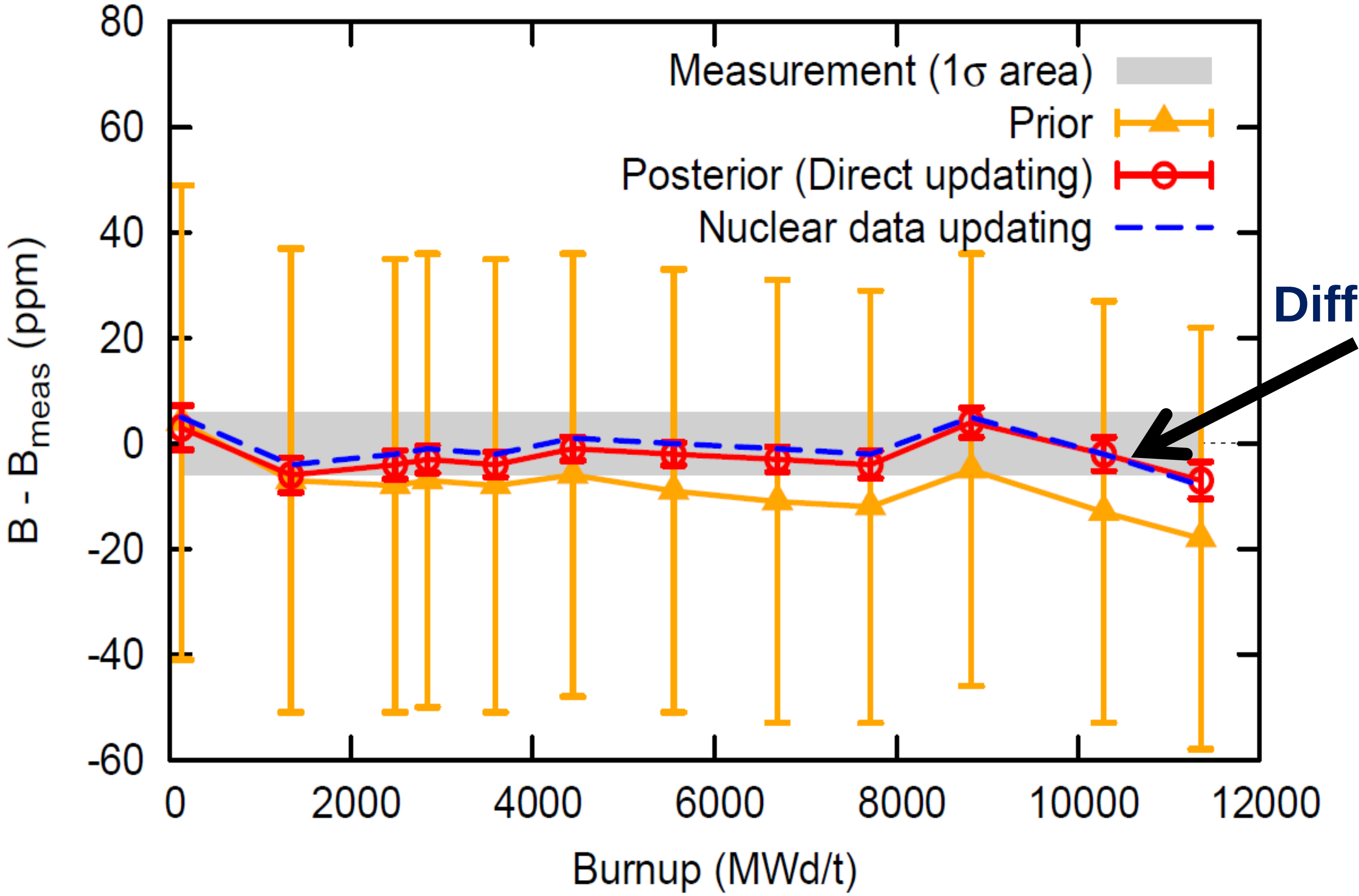
- **Posterior boron concentration improves in all cases**
- **Posterior uncertainty is reduced by one order of magnitude**
- **All posterior results are within the error band of the measurements**

Application to Core Simulation

MOCABA updating of 69 group WIMS ND library



Application to Core Simulation



Differences < 2ppm

Consistent results with both updating schemes: direct vs. nuclear data updating

Chapter 4

Summary / Final Remarks

Summary / Final Remarks

- **MOCABA: Powerful and flexible MC-based Bayesian updating framework**
  - **Non-perturbative alternative to GLLS**
  - **Direct updating of integral observables**
  - **Transport code as black box**
  - **Arbitrarily complex calculation procedures**
  - **Can be combined with any ND MC program**
    - NUDUNA, TMC, XSUSA, SAMPLER, NUSS, SANDY …

- **Applied by different institutions to CSA and reactor physics**
  - **AREVA, GRS, AMEC Foster Wheeler, PSI, EPFL**

- **Request to ND community**
  - **Keep high quality benchmarks for validation**

References

[1] A. Hoefer, O. Buss, M. Hennebach, M. Schmid, D. Porsch

MOCABA: A general Monte Carlo-Bayes procedure for improved predictions of integral functions of nuclear data
Annals of Nuclear Energy Volume 77, March 2015, Pages 514-521

[2] O. Buss O., A. Hoefer, J. Neuber

NUDUNA – nuclear data uncertainty analysis.
Proc. International Conference on Nuclear Criticality (ICNC 2011), Edinburgh, Scotland.

[3] C. J. Diez, O. Buss, A. Hoefer, D. Porsch, O. Cabellos

Comparison of nuclear data uncertainty propagation methodologies for PWR burn-up simulations
Annals of Nuclear Energy Volume 77, March 2015, Pages 101–114

[4] E. Castro, C. Ahnert, O. Buss, N. García-Herranz, A. Hoefer, D. Porsch

Improving PWR core simulations by Monte Carlo uncertainty analysis and Bayesian inference

Annals of Nuclear Energy Volume 95, May 2016, Pages 148–156

[5] D.J. Siefman, M. Hursin, P. Grimm, A. Pautz

Case Study of Data Assimilation Methods with the LWR-Proteus Phase II Experimental Campaign

M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering,

Jeju, Korea, April 16-20, 2017, on USB (2017)