AREVA

MOCADATA

Monte Carlo Aided Design and Tolerance Analysis

General hierarchical Bayesian procedure for calculating the bias and the a posteriori uncertainty of neutron multiplication factors

Usage of TSUNAMI in a hierarchical Bayesian procedure for calculating the bias and the a posteriori uncertainty of keff

Jens Christian Neuber and Axel Hoefer

AREVA NP GmbH Germany
Department NEEA-G

jens-christian.neuber@areva.com

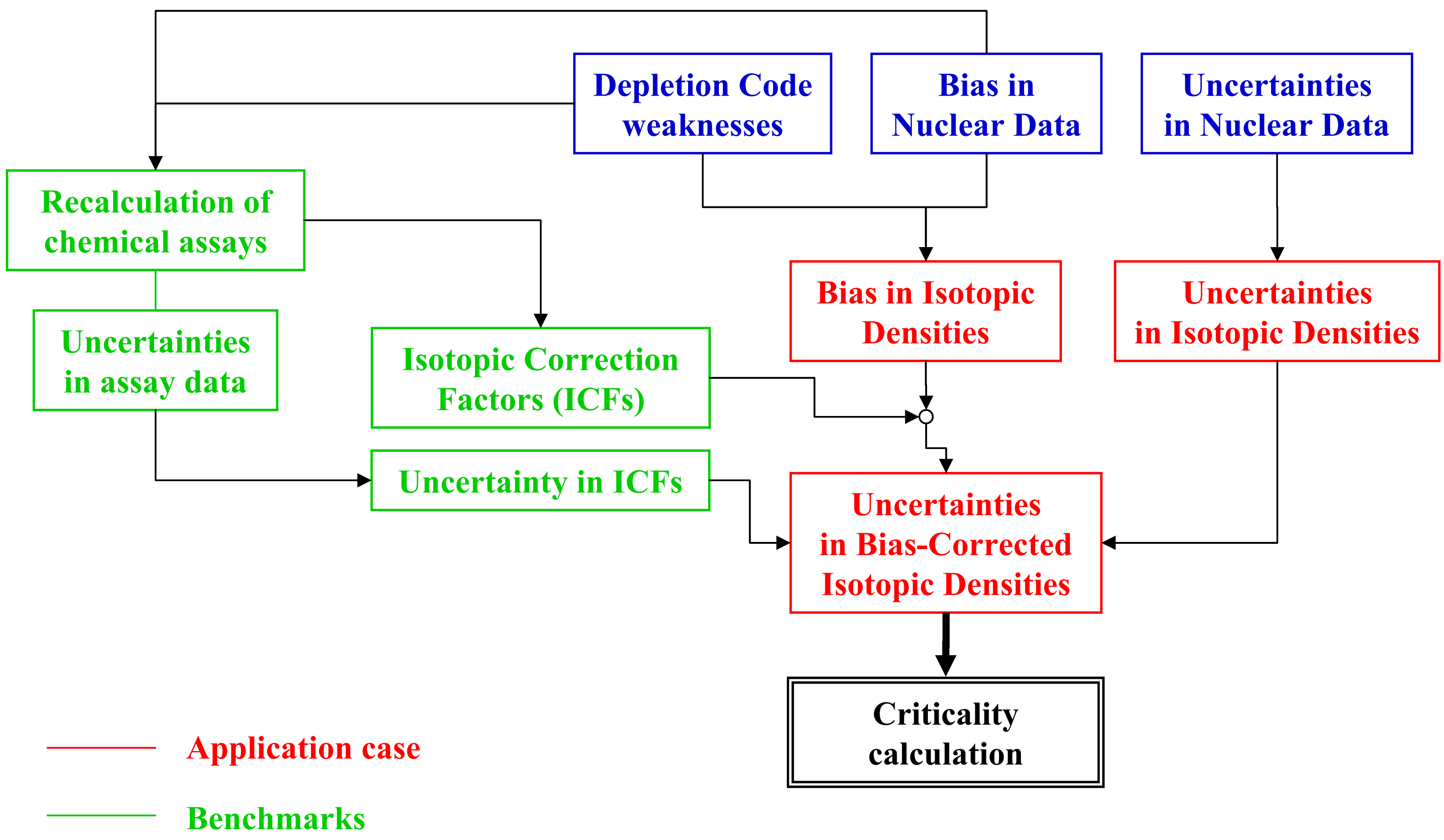
axel.hoefer@areva.com

Overview

- **Observations: Sources of Uncertainty**
- **Observation: Hierarchy of Uncertainties**
- **Bayesian Hierarchical Procedures**
  - Depletion Calculation and Validation
  - Criticality Calculation and Validation
- **Conclusions**

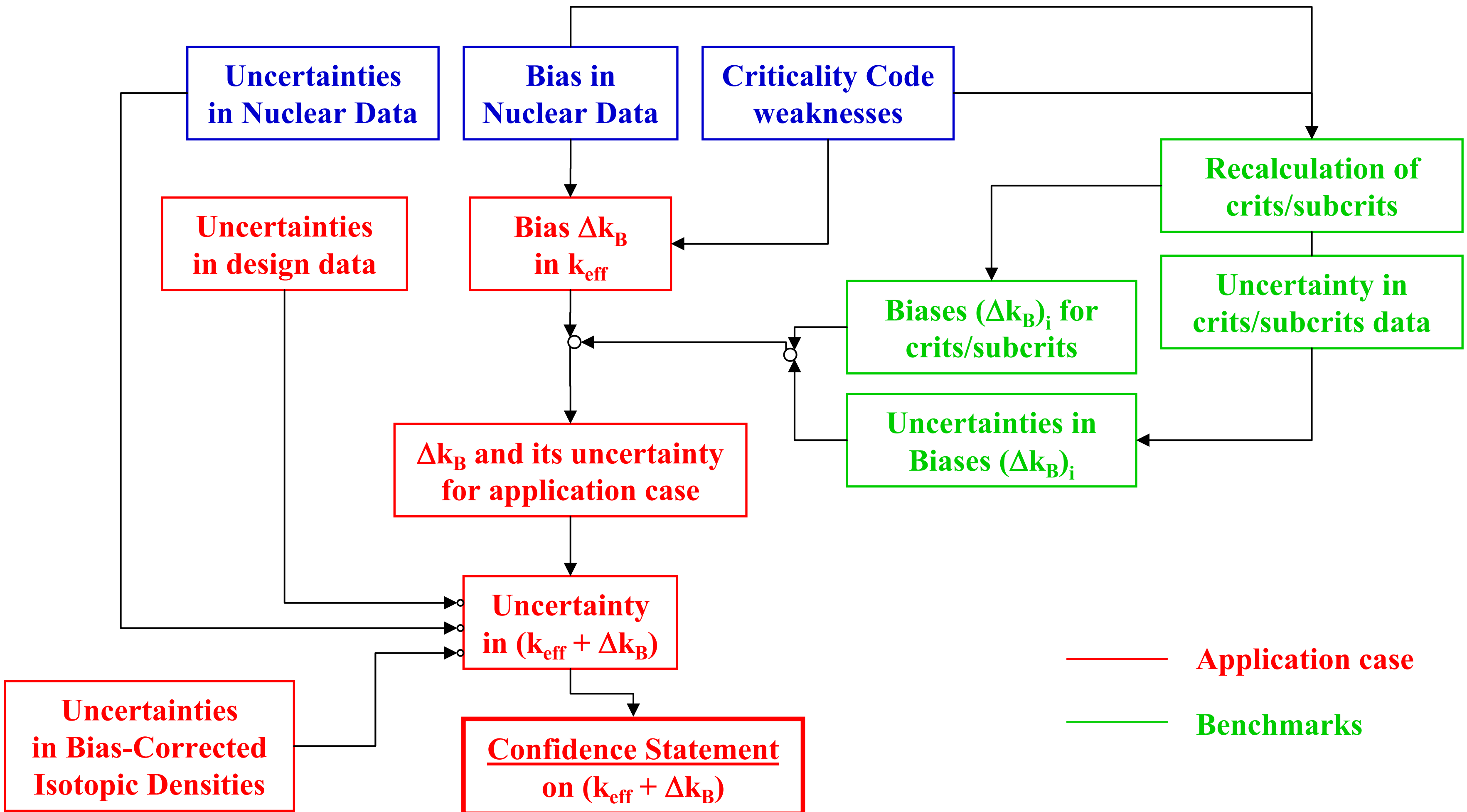
Observations: Sources of Uncertainty

Depletion Calculation and Validation



Observations: Sources of Uncertainty

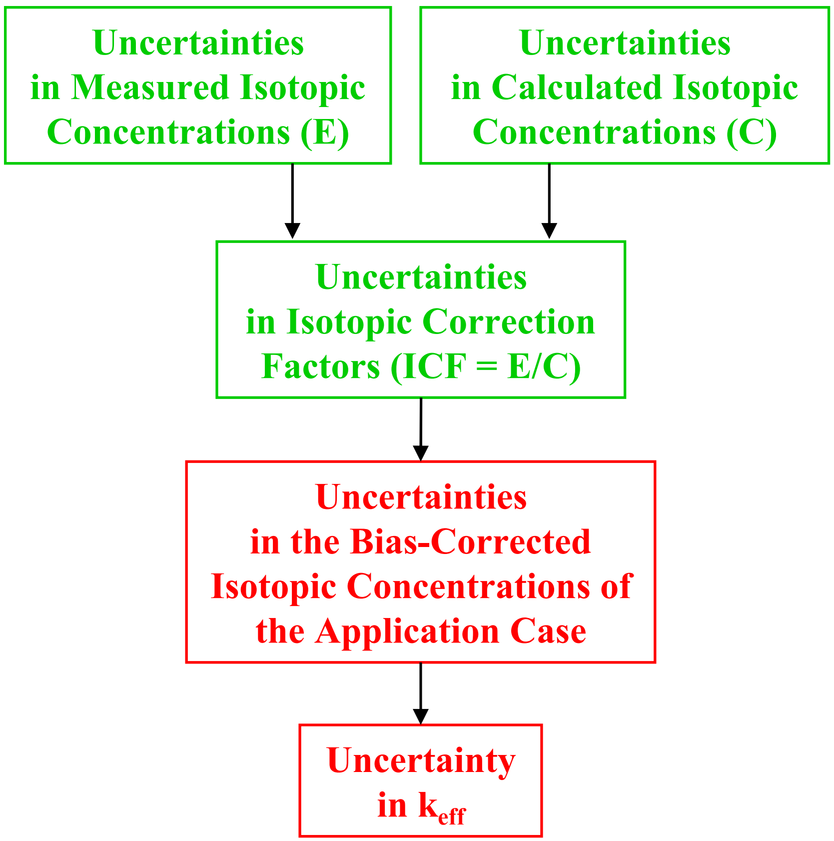
Criticality Calculation and Validation



AREVA

Observation: Hierarchy of Uncertainties

Example



Application case

Benchmarks

Statements

- Observed data (E, C, …) are random numbers, i.e. outcomes from random variables (vectors)
- Random variables (vectors) x are completely defined by probability distributions:

$$P(x \leq x_0) = \int_{x_{min}}^{x_0} dx\, p(x\,|\,\Theta)$$

p(x|Θ):= probability density function (pdf) of x,
Θ:= parameter characterizing the pdf
(e.g.: p(x|Θ) = multivariate normal distribution,
Θ → mean vector and covariance matrix)

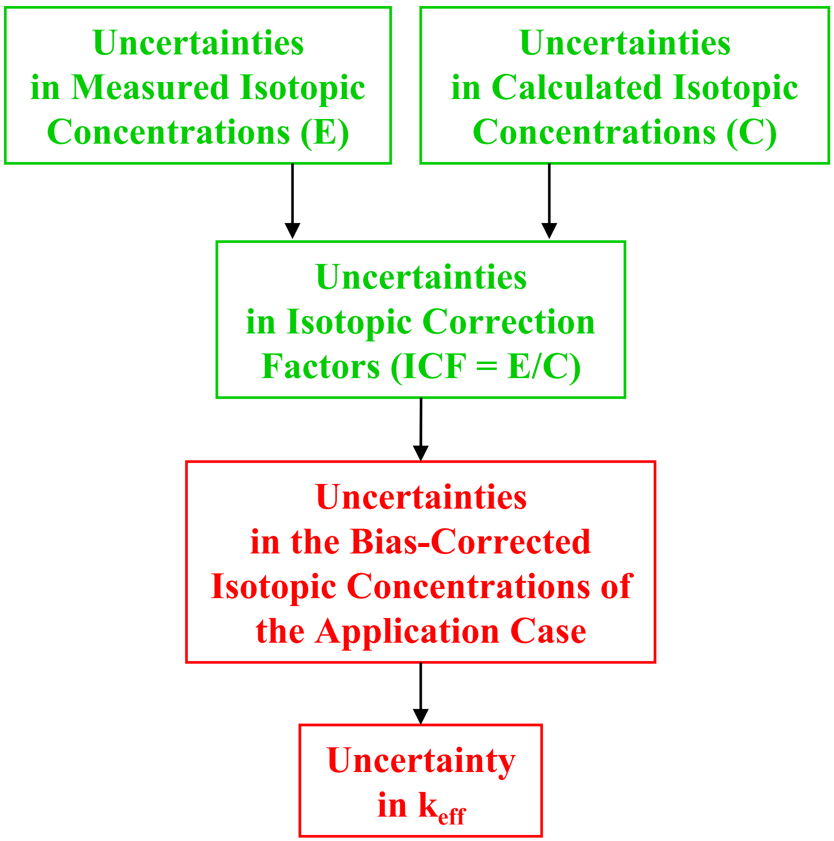
- Problem: p(x|Θ) often unknown, only available: empirical data (e.g.: E) or observations (e.g.: C)

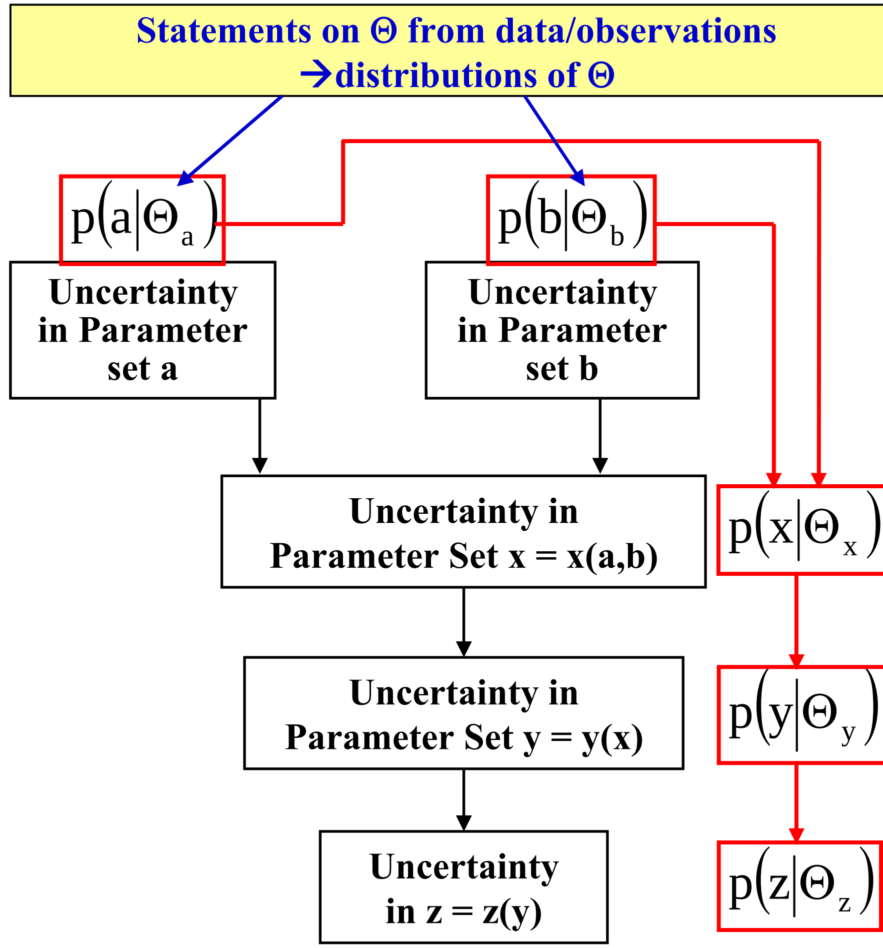
Tasks:

- Derive from empirical data/observations on x statements about Θ
- Bearing the uncertainties in the variable/vector x from one level to the next one

Observation: Hierarchy of Uncertainties

Example



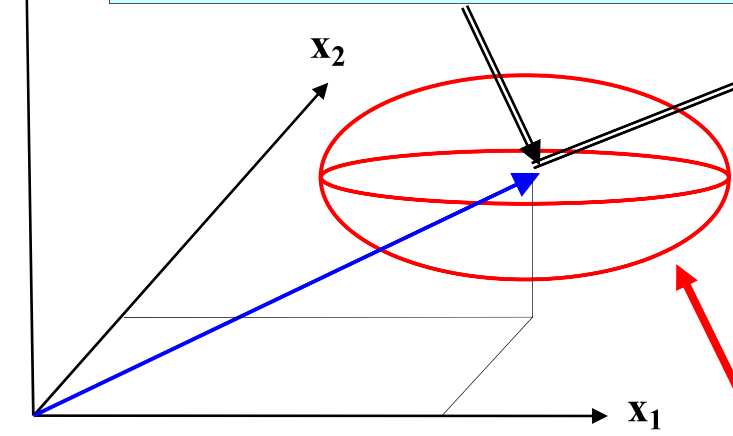


Most powerful tool of bearing the uncertainties from one level to the next one:
→ Bayesian Monte Carlo hierarchical procedures

← NCSD 2009 Topical Meeting, Sept. 13-17, 2009 Paper #33 (Neuber, Hoefer)

Monte Carlo Sampling at given level → pdf of the succeeding level

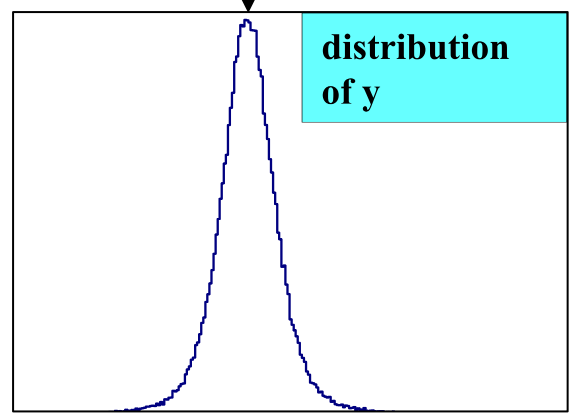
Monte Carlo (MC) sampling on the parameter region



Sets of MC sampled parameter values $(x_s)_i = (x_{s1}, x_{s2}, x_{s3}, \ldots)_i$, $i = 1,\ldots,\kappa$

Set of MC sampled parameter values

$(y_s)_i = y((x_s)_i)$, $i = 1,\ldots,\kappa$



- **MC sampling on a parameter region from the joint probability density function (pdf) $p(x|\Theta)$ of the parameters**

- **Problem: pdf usually unknown**
- **Necessary: *pdf model derived from empirical data***

Monte Carlo Sampling at given level

→Generate MC samples x_s under the condition of empirical data X:

Posterior predictive

$$p(x_s|X) = \int p(x_s|\Theta)\, p(\Theta|X)\, d\Theta$$

n x m *data matrix* of n independent identically distributed (iid) m-variate data $x_i = (x_{i1}, x_{i2}, \ldots, x_{im})$

$$\begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1,m-1} & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2,m-1} & x_{2m} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{n-1,1} & x_{n-1,2} & \cdots & x_{n-1,m-1} & x_{n-1,m} \\ x_{n,1} & x_{n,2} & \cdots & x_{n,m-1} & x_{n,m} \end{pmatrix}$$

Θ → probability distribution model

e.g. normal distribution: Θ = (μ,Σ)

parameter Θ unknown

→MC sampling on Θ under the condition of the data X

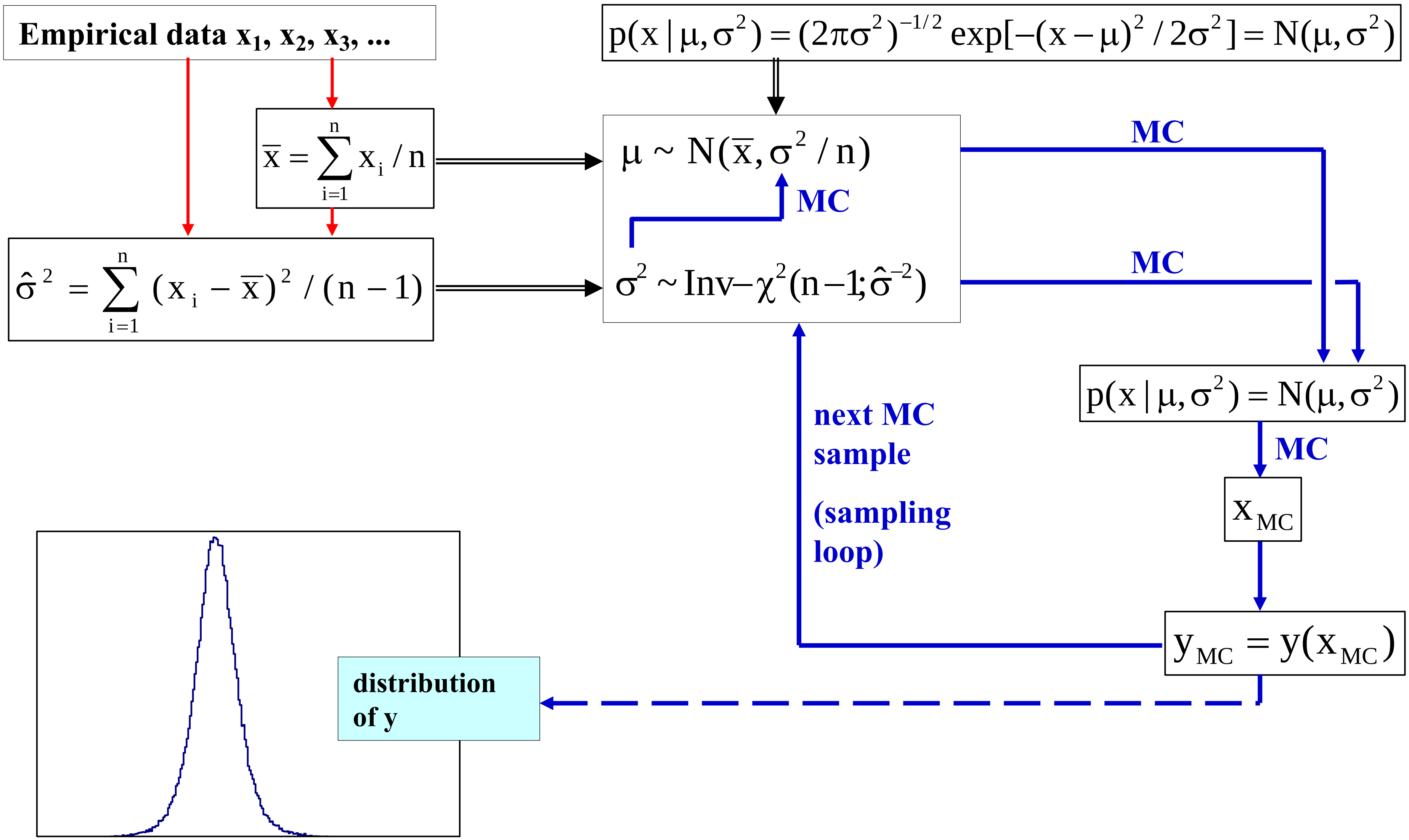
$$p(\Theta|X) \propto p(X|\Theta)\, p(\Theta)$$

posterior know-ledge about Θ

Likelihood of X under Θ

prior knowledge about Θ

Simple example for Monte Carlo Sampling at given level



Depletion Validation: Evaluation of Assay Data

First step: Evaluation of the results from one lab for one sample

Measured Isotopic Concentrations (E)

Calculated Isotopic Concentrations (C)

Required: Burnup of the fuel sample

Isotopic Correction Factors (ICF = E/C)

$$\mathbf{E}_{JL} = (\ldots, E_{IJL}, \ldots)^T$$

- **J:= number of the fuel sample**
- **L(J):= number of the lab (→J-th sample is divided in L(J)-th subsamples which are independently analyzed by the L(J)-th labs)**
- **I=I(L(J)):= number of the isotope (number can differ from lab to lab at given J)**

$$\mathbf{S}_{JL} \text{ with } \operatorname{cov}(E_{iJL}, E_{kJL}) = \sum_{\nu,\mu} \frac{\partial E_{iJL}}{\partial p_\nu} \frac{\partial E_{kJL}}{\partial p_\mu} \operatorname{cov}(p_\nu, p_\mu)$$

$$= \sum_{\nu} \frac{\partial E_{iJL}}{\partial p_\nu} \frac{\partial E_{kJL}}{\partial p_\nu} \sigma^2(p_\nu), \text{ if } \operatorname{cov}(p_\nu, p_\mu) = 0 \text{ for } \nu \neq \mu$$

- **Vector p: experimental parameters impacting the results E_{IJL}**

assumption on pdf:

$$N(\mathbf{E}_{JL}, \mathbf{S}_{JL})$$

(normal distribution)

Monte Carlo (MC) sample

$$\mathbf{E}_{JL}^{MC}$$

Depletion Validation: Evaluation of Assay Data

Second step: Evaluation of the sample's burnup

Measured Isotopic Concentrations (E)

Calculated Isotopic Concentrations (C)

Required: Burnup of the fuel sample

Isotopic Correction Factors (ICF = E/C)

Different cases possible:

a) **Each lab has estimated the burnup value from burnup indicators**

b) **Burnup only calculated (not any measurement at any lab)**

c) **a) and b) mixed**

Case a1): Burnup indicators for which a MC sample is included in E_{JL}^{MC}:

$$B_{\nu}^{MC} = f(E_{\nu JL}^{MC}),\ \nu = 1,\ldots,\nu_m$$

Case a2): Burnup indicators for which a MC sample is not included in E_{JL}^{MC}:

Draw MC sample

$$B_{\mu}^{MC} \text{ from } N\left((\overline{B}_{\mu}, s^2(\overline{B}_{\mu})\right),\ \mu = 1,\ldots,\mu_m$$

$$\overline{B}_{JL} = \frac{1}{\nu_m + \mu_m}\left(\sum_{\nu=1}^{\nu_m} B_{\nu}^{MC} + \sum_{\mu=1}^{\mu_m} B_{\mu}^{MC}\right),$$

$$\hat{\sigma}^2(\overline{B}_{JL}) = \frac{1}{(\nu_m + \mu_m) - 1}\left(\sum_{\nu=1}^{\nu_m}(B_{\nu}^{MC} - \overline{B}_{JL})^2 + \sum_{\mu=1}^{\mu_m}(B_{\mu}^{MC} - \overline{B}_{JL})^2\right)$$

Depletion Validation: Evaluation of Assay Data

Second step: Evaluation of the sample's burnup / case a)

Measured Isotopic Concentrations (E)

Calculated Isotopic Concentrations (C)

Required: Burnup of the fuel sample

Isotopic Correction Factors (ICF = E/C)

$$\sigma_{JL}^2 \leftarrow \mathrm{Inv}-\chi^2\left((\nu_m+\mu_m)-1;\hat{\sigma}^2\left(\bar{B}_{JL}\right)\right)$$

$$\mathrm{MC\,sample}(\sigma_{JL}^2)^{MC}$$

$$E[B_{JL}] \leftarrow N\left(\bar{B}_{JL}, \frac{\sigma_{JL}^2}{\nu_m+\mu_m}\right)$$

$$\mathrm{MC\,sample}\,E[B_{JL}]^{MC}$$

$$B_{JL} \leftarrow N\left(E[B_{JL}], \sigma_{JL}^2\right)$$

$$\mathrm{MC\,sample}\,B_{JL}^{MC}$$

Depletion Validation: Evaluation of Assay Data

Second step: Evaluation of the sample's burnup / case b) (Burnup only calculated)

Measured Isotopic Concentrations (E) → Isotopic Correction Factors (ICF = E/C)

Calculated Isotopic Concentrations (C) → Isotopic Correction Factors (ICF = E/C)

Required: Burnup of the fuel sample → Calculated Isotopic Concentrations (C)

In analogy to case a2): Draw MC sample

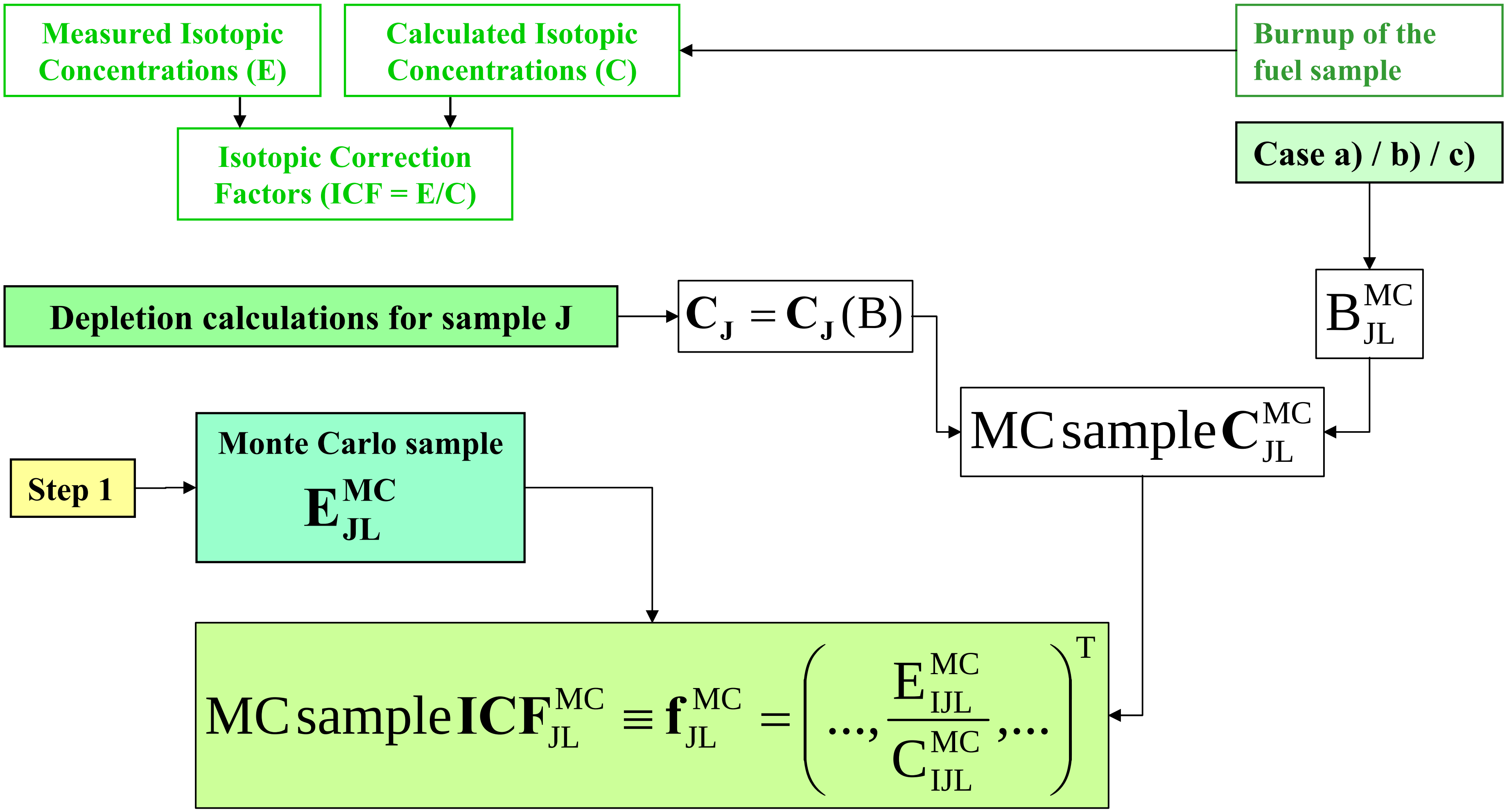
$$B_{JL}^{MC} \text{ from } N\left(\left(\overline{B}_J, s^2(\overline{B}_J)\right)\right), \forall L(J)$$

Second step: Evaluation of the sample's burnup / case c) (mixed case)

- **For Labs to which case a) applies use a) → lab-specific MC sample** B_{JL}^{MC}
- **For Labs to which case b) applies use b) → one MC sample for all labs**

Depletion Validation: Evaluation of Assay Data

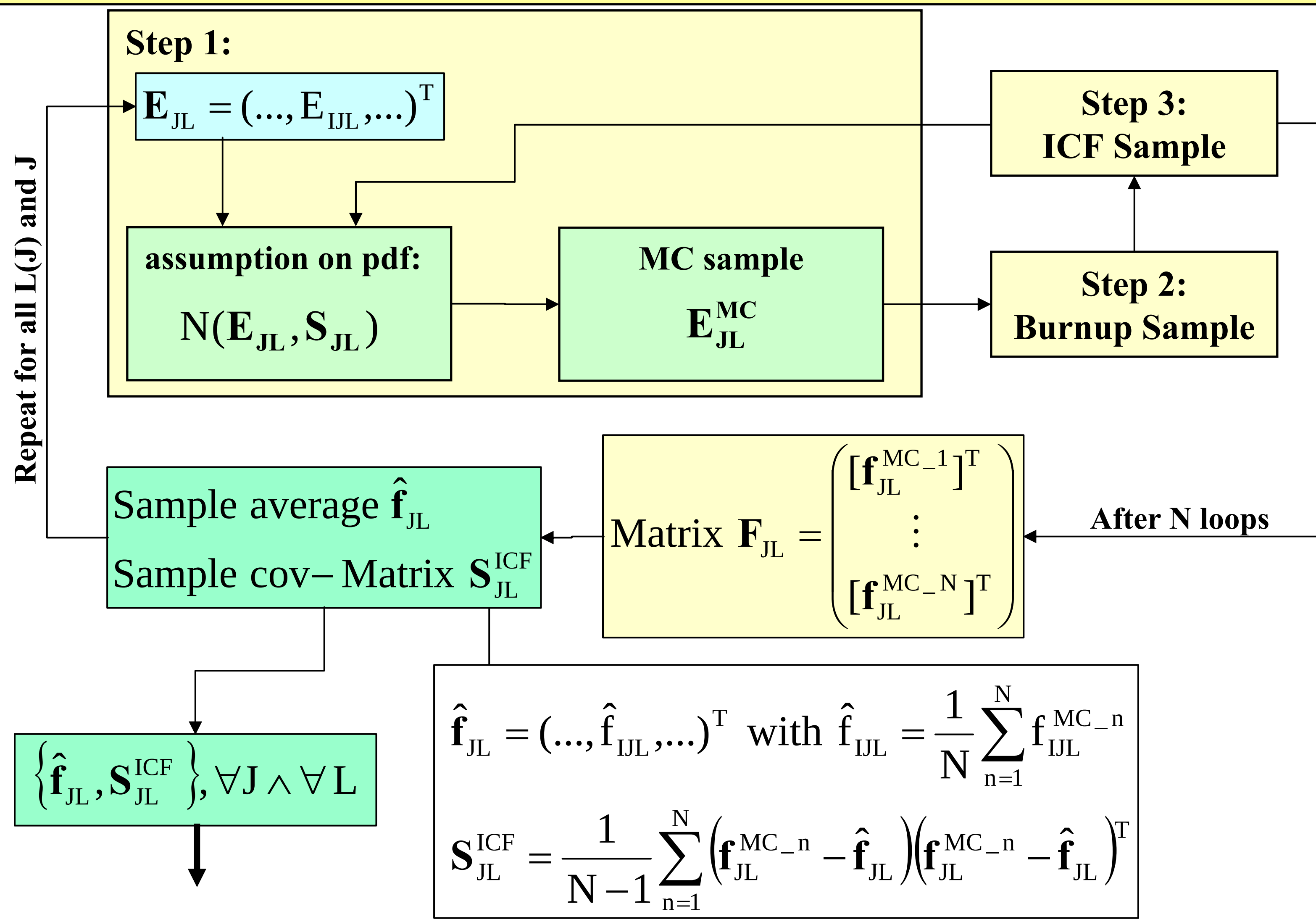
Third step: Evaluation of the calculated isotopic concentration and the ICF



AREVA

Depletion Validation: Evaluation of Assay Data

Sampling MC-ICF values for fuel sample J analyzed in lab L



Depletion Validation: Application of ICFs

Step 4: Selection of the ICFs for the isotopes selected for the BUC application case

$\left\{\hat{\mathbf{f}}_{JL}, \mathbf{S}_{JL}^{ICF}\right\}, \forall J \wedge \forall L$ pool (set) for selecting the ICFs for a specific BUC application case

Set of BUC isotopes to be used in the application case

↓

Reduction to BUC isotopes (to be used in application case)

$\left\{\hat{\mathbf{f}}_{JL}^{BUC}{}_{JL}, \mathbf{S}_{JL}^{BUC}\right\}, \forall J \wedge \forall L$ **"BUC AC working pool"**

(AC: application case)

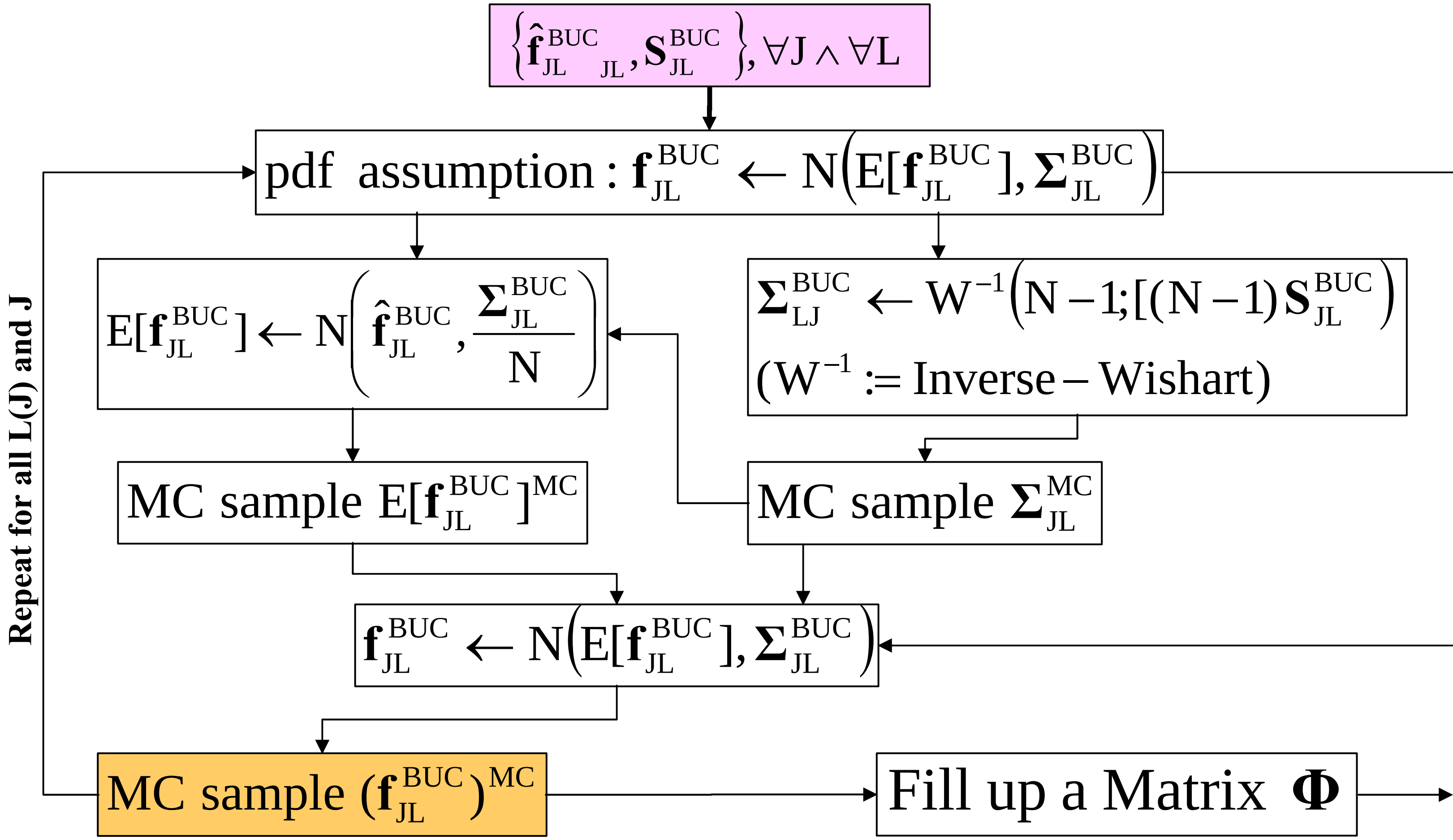
↓

MC sampling on BUC isotopes' ICFs

AREVA

Depletion Validation: Application of ICFs

Step E1: Evaluation of the BUC AC working pool



AREVA

Depletion Validation: Application of ICFs

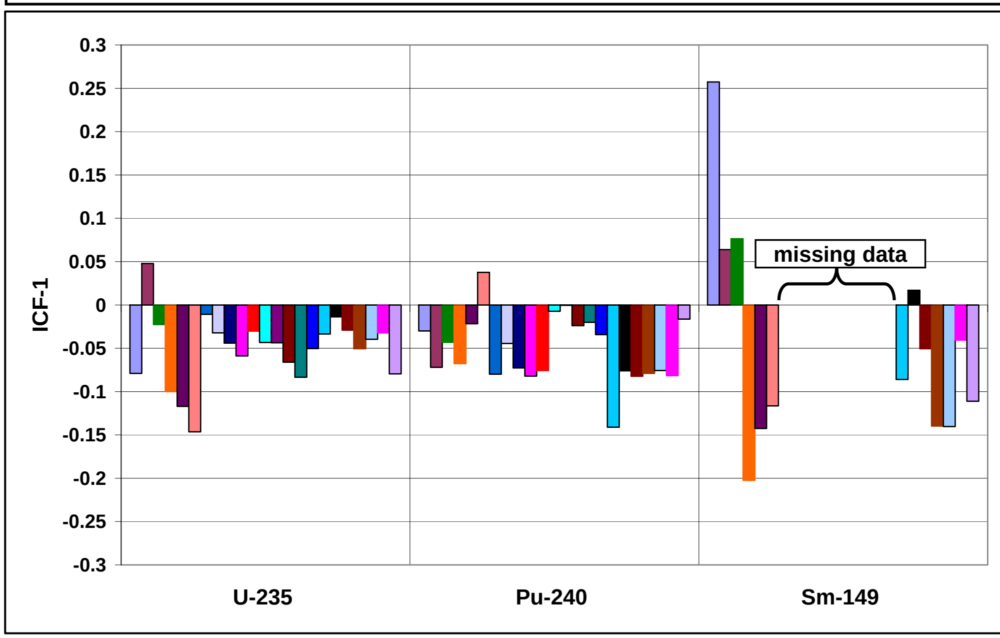
Step E2: Evaluation of the matrix Φ

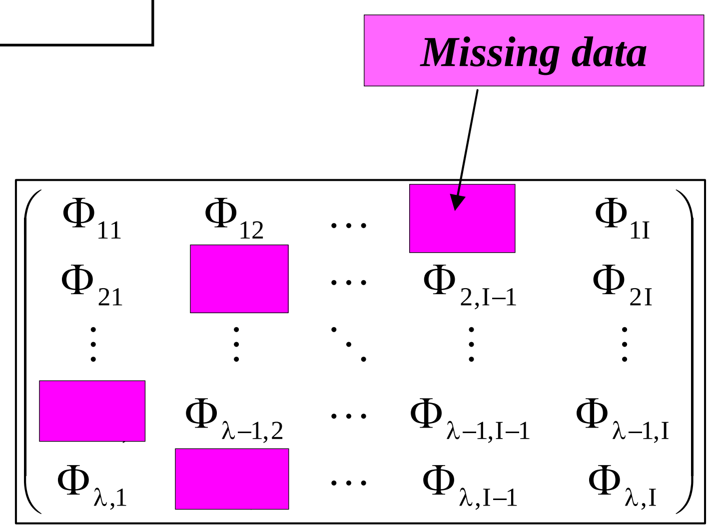
Matrix Φ

$$\text{Number of lines}: \lambda = \sum_{j=1}^{J_{tot}} L(j)_{tot}$$

$$\text{Number of columns} = \text{Number of BUC Isotopes to be used}$$

Matrix is usually <u>incomplete</u>, since not all of the isotopes to be used are measured for all J and L(J)





AREVA

Depletion Validation: Application of ICFs

Step E2: Evaluation of the matrix Φ: Solution of the missing data problem

- **By construction, the matrix elements Φ_{ji} are possible outcomes for the random variables Φ_{ji}.**
- **Therefore, each line vector f_λ is a sample on the pdf $p(f|\Theta)$ of the random vector f**
- **If the matrix Φ were complete, the elements Φ_{ji} would be completely defined by the pdf $p(\Phi|\Theta)$, called "complete-data pdf" in the following.**

Complete-data pdf can be written:

$$p(\boldsymbol{\Phi}|\boldsymbol{\Theta}) = p(\boldsymbol{\Phi}_{miss}, \boldsymbol{\Phi}_{obs}|\boldsymbol{\Theta}) = \underbrace{p(\boldsymbol{\Phi}_{miss}|\boldsymbol{\Phi}_{obs}, \boldsymbol{\Theta})}_{\text{predictive distribution of missing data}}\, p(\boldsymbol{\Phi}_{obs}|\boldsymbol{\Theta})$$

predictive distribution of missing data

Solution of the missing data problem → Data augmentation

Depletion Validation: Application of ICFs

Step E2: Evaluation of the matrix Φ:
Solution of the missing data problem by data augmentation (principle)

Given a guess $\boldsymbol{\Theta}_{(i)} \rightarrow p\left(\boldsymbol{\Phi}_{mis} \middle| \boldsymbol{\Phi}_{obs}, \boldsymbol{\Theta}_{(i)}\right) \rightarrow \boldsymbol{\Phi}_{mis}^{(i+1)}$

"Imputation step"

i = i+1

"complete-data posterior pdf" $p\left(\boldsymbol{\Theta} \middle| \boldsymbol{\Phi}_{obs}, \boldsymbol{\Phi}_{mis}^{(i+1)}\right) \rightarrow \boldsymbol{\Theta}_{(i+1)}$

"Posterior step"

$$p\left(\boldsymbol{\Theta} \middle| \boldsymbol{\Phi}\right) \propto p\left(\boldsymbol{\Phi} \middle| \boldsymbol{\Theta}\right) p\left(\boldsymbol{\Theta}\right)$$

convergence achieved

Sufficient number of iterations →
MC samples f_{MC} can be drawn from
the model p(f|Θ) after each posterior step:

$$p\left(\mathbf{f} \middle| \boldsymbol{\Theta}_{(i)}\right) \rightarrow \mathbf{f}_{MC}^{(i)}$$

Starting parameter vector $\Theta_{(1)}$ can be generated by using the "Expectation Maximizing (EM) algorithm"; the data augmentation procedure is performed by means of Markov chain Monte Carlo techniques

J.C. Neuber, A. Hoefer, ICNC 2007, paper 223

Depletion Validation: Application of ICFs

Step E2: Evaluation of the matrix Φ: Solution of the missing data problem by data augmentation (performance)

- **Each line vector f_λ of Φ is a sample on a multivariate normal distribution p(f|Θ)=N(E[f], cov(f)) with unknown expectation E[f] and unknown covariance matrix cov(f)**
- **No prior information about E[f] and cov(f) available → using a non-informative prior (e.g. $p(\Theta) = [\det(\mathrm{cov}(f))]^{-(m+1)/2}$)**

Posterior Step becomes

$$\mathrm{cov}(\mathbf{f}) \leftarrow W^{-1}\left(\lambda-1, \boldsymbol{\Psi}_{(i)}\right) \text{ with } \boldsymbol{\Psi}_{(i)} = (\lambda-1)^{-1}\left[\mathbf{S}\left(\boldsymbol{\Phi}_{\mathbf{obs}}, \boldsymbol{\Phi}_{\mathbf{mis}}^{(i)}\right)\right]^{-1} \Rightarrow \mathrm{cov}(\mathbf{f})_{(i)}$$

Inverted Wishart Distribution (W)

Sample covariance matrix (S)

and

$$E[\mathbf{f}] \leftarrow N\left(\hat{\mathbf{f}}_{(i)}, \lambda^{-1}\,\mathrm{cov}(\mathbf{f})_{(i)}\right) \text{ with } \hat{\mathbf{f}}_{(i)} = \hat{\mathbf{f}}\left(\boldsymbol{\Phi}_{\mathrm{obs}}, \boldsymbol{\Phi}_{\mathrm{mis}}^{(i)}\right) \Rightarrow E[\mathbf{f}]_{(i)}$$

Sample mean ($\hat{\mathbf{f}}_{(i)}$)

→ MC samples f_{MC} drawn after each posterior step:

$$N\left(\mathbf{f} \,\middle|\, E[\mathbf{f}]_{(i)}, \mathrm{cov}(\mathbf{f})_{(i)}\right) \Rightarrow \mathbf{f}_{MC}^{(i)}$$

J.C. Neuber, A. Hoefer, J.M. Conde Lopez, ICNC 2007, paper 243

J.C. Neuber, A. Hoefer, PHYSOR 2008, Paper 525

Depletion Validation: Application of ICFs

Sampling MC-ICFs for the BUC application case

Generation of the BUC AC working pool

$$\left\{\hat{\mathbf{f}}_{JL}^{BUC}, \mathbf{S}_{JL}^{BUC}\right\}, \forall J \wedge \forall L$$

Step E1: Evaluation of the BUC AC working pool → Matrix Φ

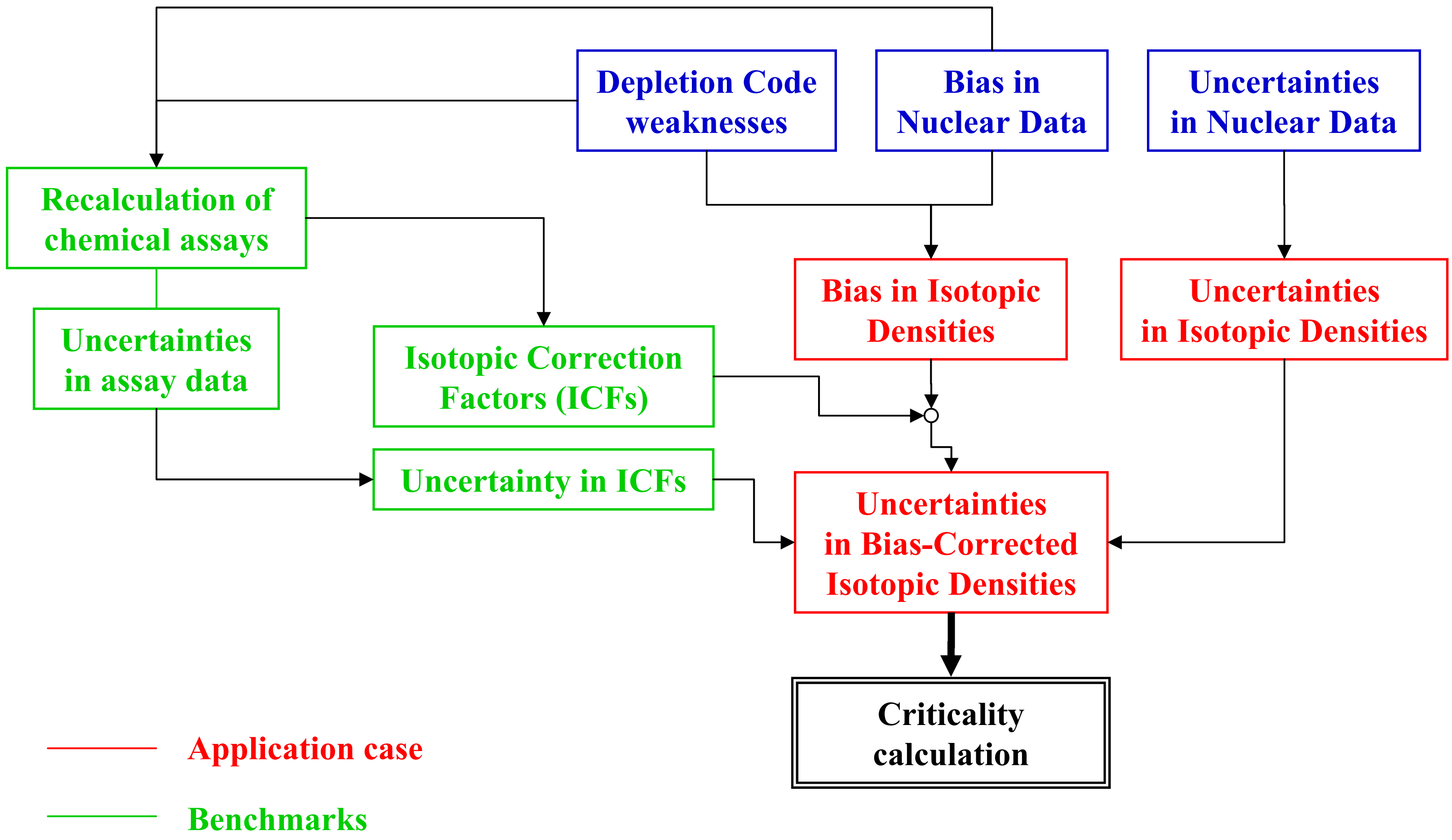
Step E2:

- **Matrix Φ complete**
- **Matrix Φ incomplete → solution of the missing data problem**

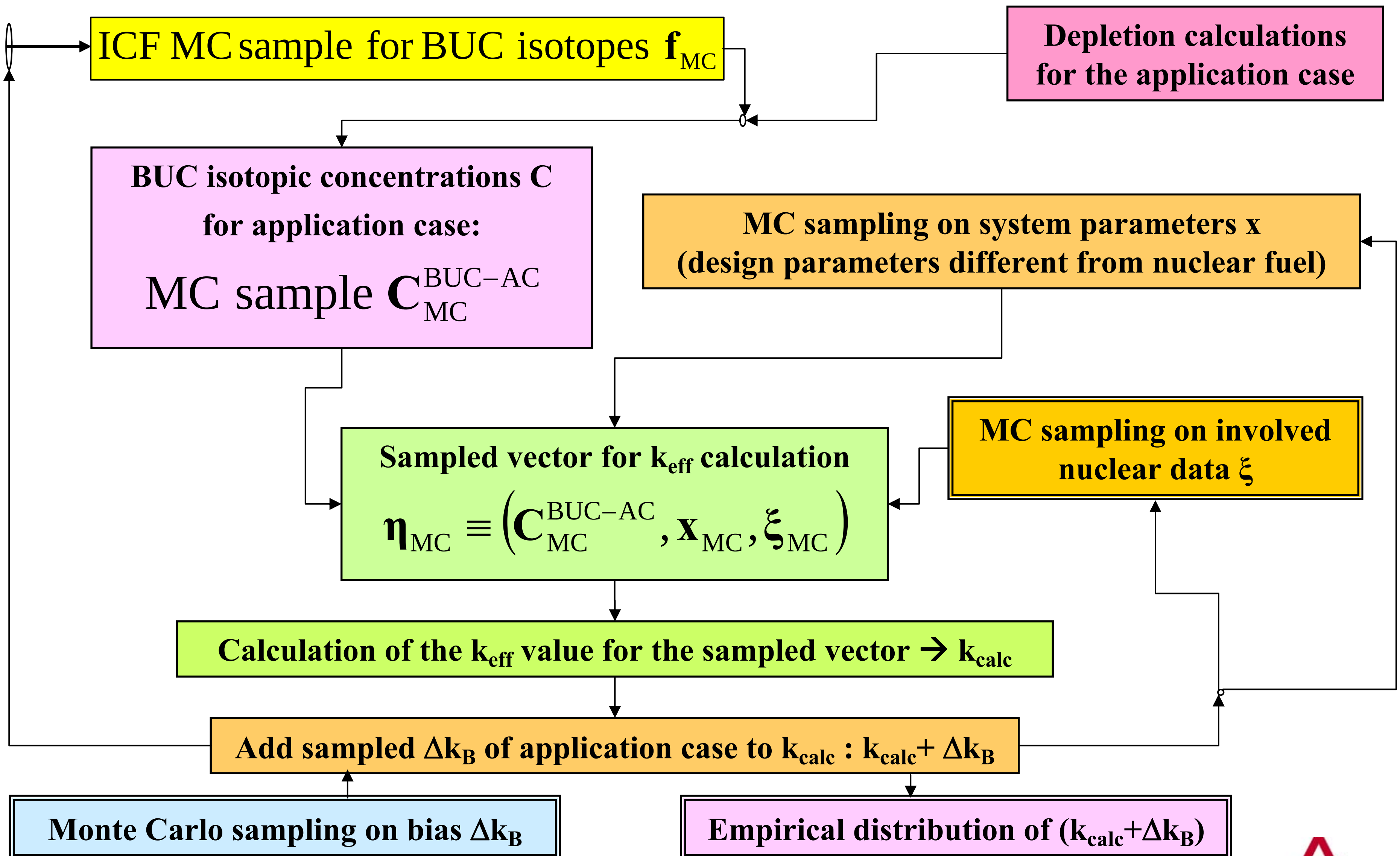
ICF MC sample for BUC isotopes $\mathbf{f}_{MC}$

Application to isotopic concentrations calculated for the application case

Depletion Calculation and Validation

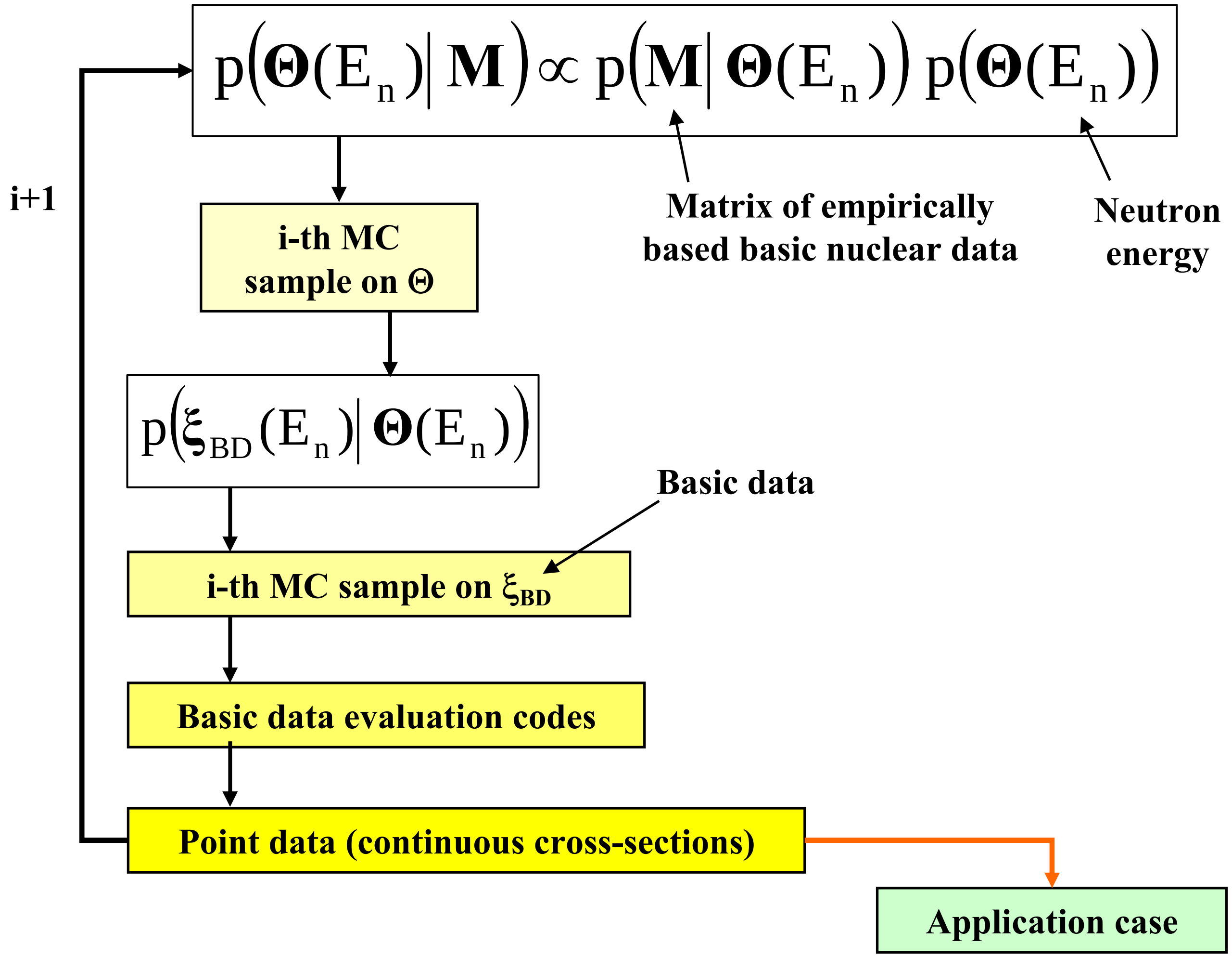


Criticality Analysis Application Case



Criticality Analysis Application Case

Uncertainty of nuclear data: Monte Carlo sampling on involved nuclear data ξ



Criticality Analysis Application Case

Uncertainty of Nuclear Data: Use of TSUNAMI

Perform n TSUNAMI calculations using different starting random numbers

Results $(\sigma_{ND})_1, \ldots, (\sigma_{ND})_n$

$$\overline{\sigma}_{ND} = \frac{1}{n}\sum_{i=1}^{n}(\sigma_{ND})_i$$

$$\hat{\tau}^2 = \frac{1}{n-1}\sum_{i=1}^{n}\left((\sigma_{ND})_i - \overline{\sigma}_{ND}\right)^2$$

$$\text{Inv}-\chi^2(n-1;\hat{\tau}^{-2}) \rightarrow \tau^2_{MC}$$

$$N(\overline{\sigma}_{ND}, \tau^2_{MC}/n) \rightarrow E[\sigma_{ND}]_{MC}$$

$$N(E[\sigma_{ND}]_{MC}, \tau^2_{MC}) \rightarrow (\sigma_{ND})_{MC}$$

$$N\left(0, (\sigma_{ND})^2_{MC}\right) \rightarrow \Delta k^{MC}_{ND}$$

Monte Carlo sampling on bias Δk_B

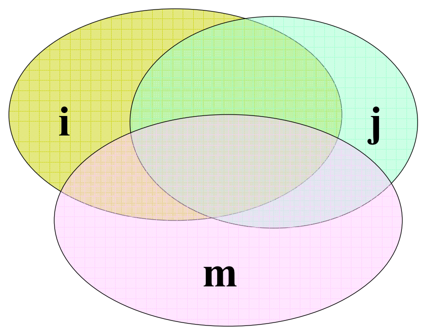
$$\text{Add to } k^{MC}_{calc} \text{ and } \Delta k^{MC}_{B} \rightarrow [k_{calc} + \Delta k_{ND} + \Delta k_B]^{MC}$$

AREVA

Criticality Analysis Validation

In many cases: "mutually dependent experiments"

Space of experimental parameters x of <u>all</u> the experiments



Monte Carlo sampling on entire x space

↓

For each sampled vector x_{MC} calculation of the k_{eff} values (k_1, k_2, …,k_N) for all the N experiments

↓

Bias vector (Δk_{B1}, Δk_{B2}, …,Δk_{Bn}) for all the N experiments

↓

Bayesian linear regression **with this bias vector using adequate explanatory variables**

↓

MC sample of the bias Δk_B for the application case

↓

Add to k_{calc} of application case: $(k_{calc}+\Delta k_{ND})+\Delta k_B$

(loop back to Monte Carlo sampling on entire x space)

MC sampling for application case → k_{calc}

MC sampling for application case on Δk_{ND} (TSUNAMI)

↓

Empirical distribution of $(k_{calc}+\Delta k_{ND}+\Delta k_B)$

J.C. Neuber, A. Hoefer, NCSD 2009 Topical Meeting, Sept. 13-17, 2009 Paper 33

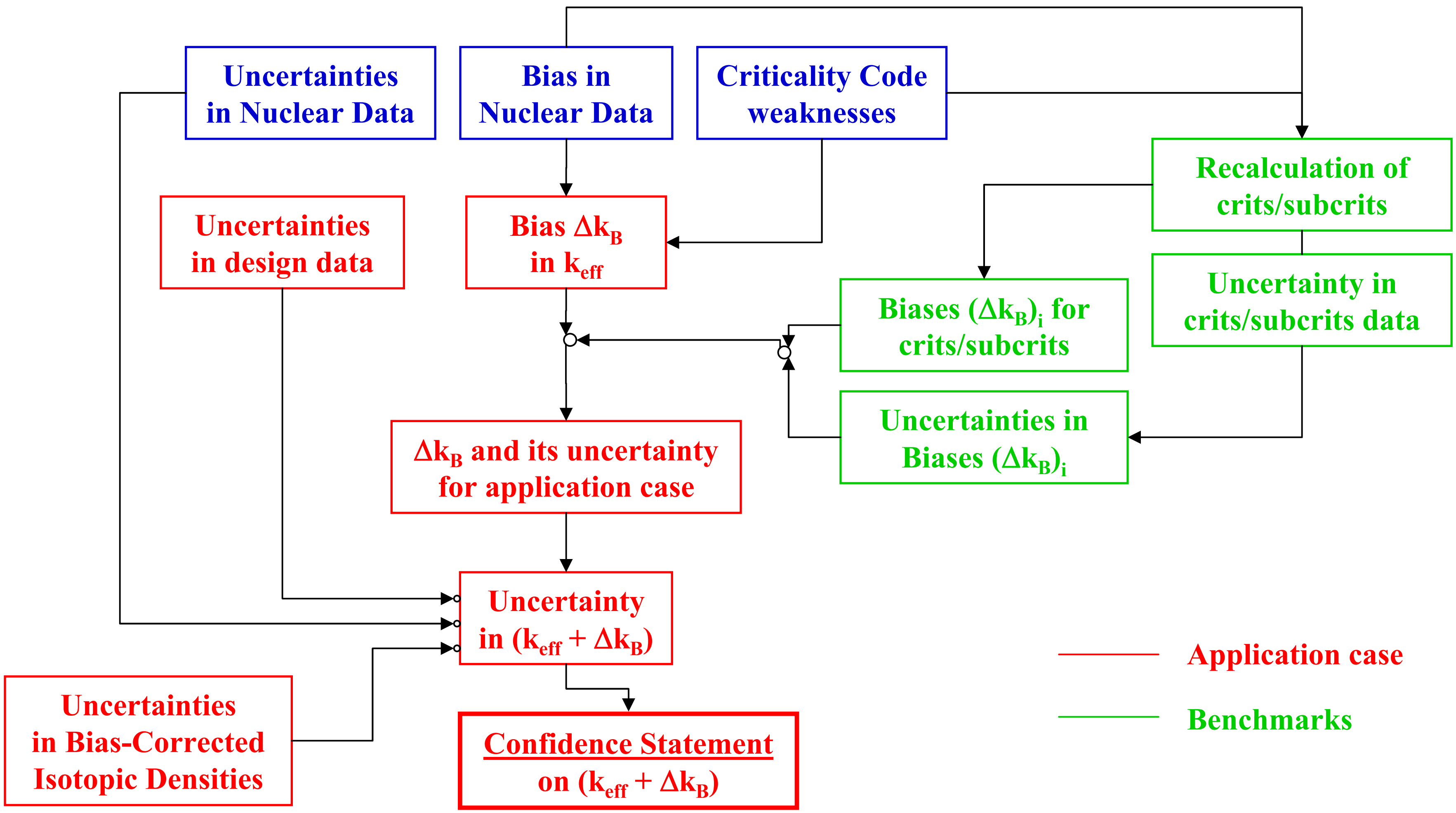
Criticality Analysis Validation

Explanatory variables

- **Isotopic sensitivity coefficients:** $\frac{N_I}{k_{eff}} \cdot \frac{\partial k_{eff}}{\partial N_I}$ or $\frac{N_I}{\rho} \cdot \frac{\partial \rho}{\partial N_I}$ **(N_I:= number density)**

- **Isotopic reactivity worths:** $\Delta\rho_I = \frac{1}{k(\text{without I})} - \frac{1}{k(\text{with I})}$

Criticality Calculation and Validation



Conclusions

What was the objective?:

- **We are using tools ⇔ Nuclear data, calculation codes**
- **<u>So, what is the bias in k_{eff} given these tools</u> (given code and given nuclear data)?**
- **→ Evaluation of experiments for estimating the bias**
- **Uncertainties in the experiments have to be considered**

Uncertainties in the nuclear data → have to be considered in the application case

Uncertainties in the design data of the application case

The MOCADATA procedure presented fullfill all the requirements and takes into account

- **all uncertainties due to experiments and application case**
- **all uncertainties due to**
  - empirical data required for performing the statistical analysis
  - the finite number of the data and
  - the possible incompleteness of the data
- **the fundamental variability due to the selection of probability distribution models required for evaluating empirical data.**