DE LA RECHERCHE À L'INDUSTRIE

Evaluation of Cross-Sections Uncertainties using Physical Constraints ^{238}U, ^{239}Pu and others…

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Presentation partly taken from NEMEA-7/CIELO

SG39, November 28-29, 2013, Issy-Les-Moulineaux(France)

CEA/CADARACHE GENERAL FRAMEWORK FOR NUCLEAR DATA ACTIVITIES

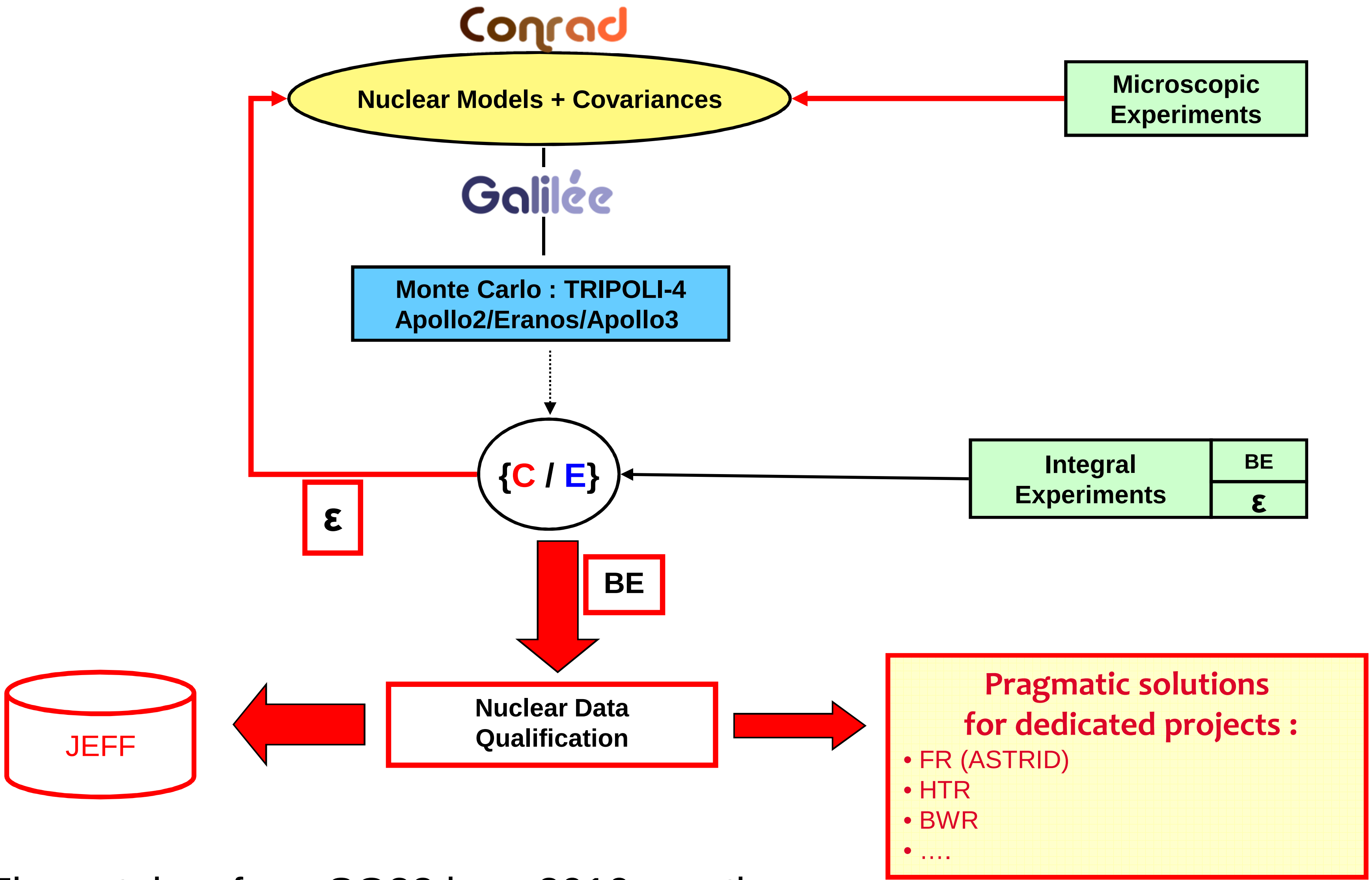

Figure taken from SG33 june 2010 meeting

CEA/CADARACHE WORK FOR SG39-SG40 RELATED TO THE BIG THREE

Best Knowledge coming from
- ❑Microscopic Measurements
- ❑Nuclear Reaction Models

"Public" Integral Experiments
- ❑Mini-Inca (ILL)
- ❑ICSBEP
- ❑…

Breakthrough
- ❑Covariances [0eV;20MeV]
- ❑Evaluation methodologies
- ❑Understanding of discrepancies
- ❑Covariance methodologies
- ❑Reduction of Uncertainties

CIELO-SG40

Breakthrough
- ❑ Choice of Integral experiments
- ❑ Experimental correlations
- ❑ Nuclear Model parameters and/or multigroup Cross sections
- ❑ Reduction of biases and uncertainties

SG39

Additional Integral Experiments
- ❑Minerve
- ❑PROFIL
- ❑…

CONSTRAINTS

- Physics :
  - Cross section is an observable
  - Isotopic lines (see CEA/DAM for JEFF3.2)
  - General laws : **"continuity" of cross sections, parameters**

- Experiments
  - Vector of constraints : shapes and uncertainties
  - Different type of experiments
    - Transmission, Capture yields, Fission, Inelastic
    - Integral experiments but in a validation framework
  - **Systematic uncertainties**
  - **Large domain experiments (decades) → several models**
  - **Integral experiment used during evaluation (Integral Data Assimilation)**

- Nuclear Reaction Models
  - Vector of Uncertainties : parameters
  - Different models / different energy domain
  - Unconstrained models
  - **Microscopic ingredients**
  - **Multi-model parameters**
  - **Model Defects**

Traditional

Additional

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Covariances Matrices evaluation on ^{238}U and ^{239}Pu

Determination of

Matrices

Bayesian inference (probability density):

$$p(\vec{x}\,|\,\vec{y},U) = \frac{p(\vec{x}\,|U)\cdot p(\vec{y}\,|\,\vec{x},U)}{\int d\vec{x}\cdot p(\vec{x}\,|U)\cdot p(\vec{y}\,|\,\vec{x},U)}$$

Model parameters

New measurements

a priori information

Formulation:

$$posterior[p(\vec{x}|\vec{y},U)] \propto prior[p(\vec{x}|U)]\cdot likelihood[p(\vec{y}|\vec{x},U)]$$

Estimation of the first two moments of the *a posteriori* distribution

Marginalization philosophy

$$\sigma = f(\vec{x}, \vec{\theta})$$

Model parameters

« **nuisance**» parameters

Nuisance parameters are **necessary** during comparisons with experiments (data reduction, normalization, background, detector efficiency…), but not for the final evaluation

$$\sigma = f(\vec{x}, \vec{\theta}) \Rightarrow \sigma = f(\vec{x})$$ + **Covariances**

Marginalization of the probability density:

$$p(\vec{x}, \vec{\theta} | \vec{y}, U) \Rightarrow p_{\vec{\theta}}(\vec{x} \mid \vec{y}, U) = \int d\vec{\theta} \cdot p(\vec{x}, \vec{\theta} \mid \vec{y}, U)$$

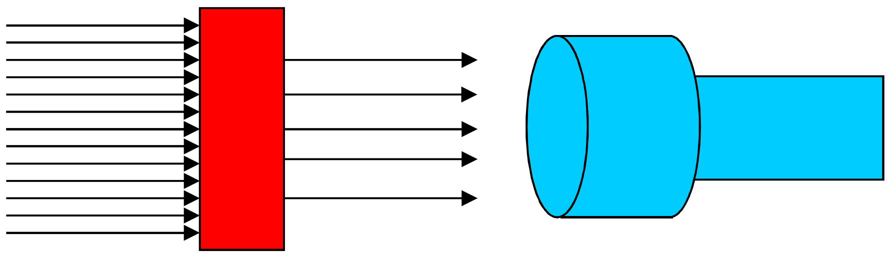
Marginalization :

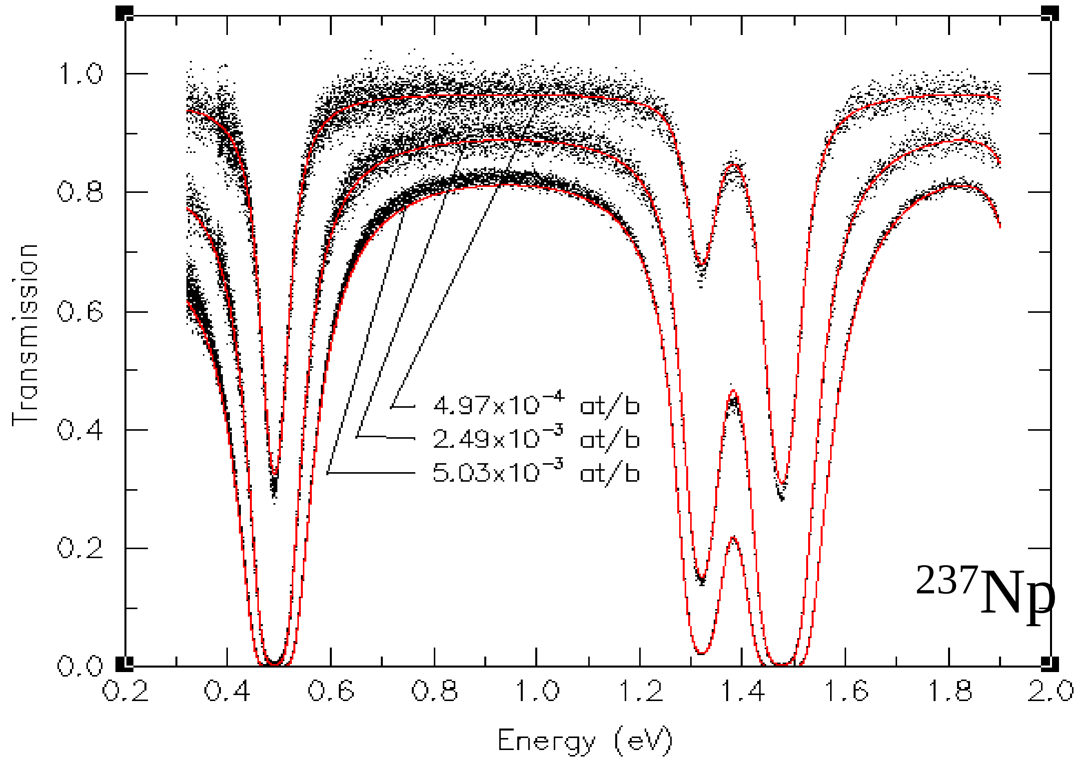
estimation of the first two moments of the marginal probability density

For further details see :
C. De Saint Jean et al., Nucl. Sci. Eng. 161, 363 (2009)
B. Habert et al., Nucl. Sci. Eng. 166, 276-287 (2010).

Transmission Measurement

@P. Schillebeeckx





Comparison

$$T_{th} = \vec{t}\,(\vec{\sigma}(\vec{x}),\vec{\theta}) \approx N_\theta e^{-n_\theta \sigma_t(\vec{x})} + B_\theta$$

and

$$T_{\exp} = N \frac{C'_{in} - B'_{in}}{C'_{out} - B'_{out}}$$

Data Assimilation

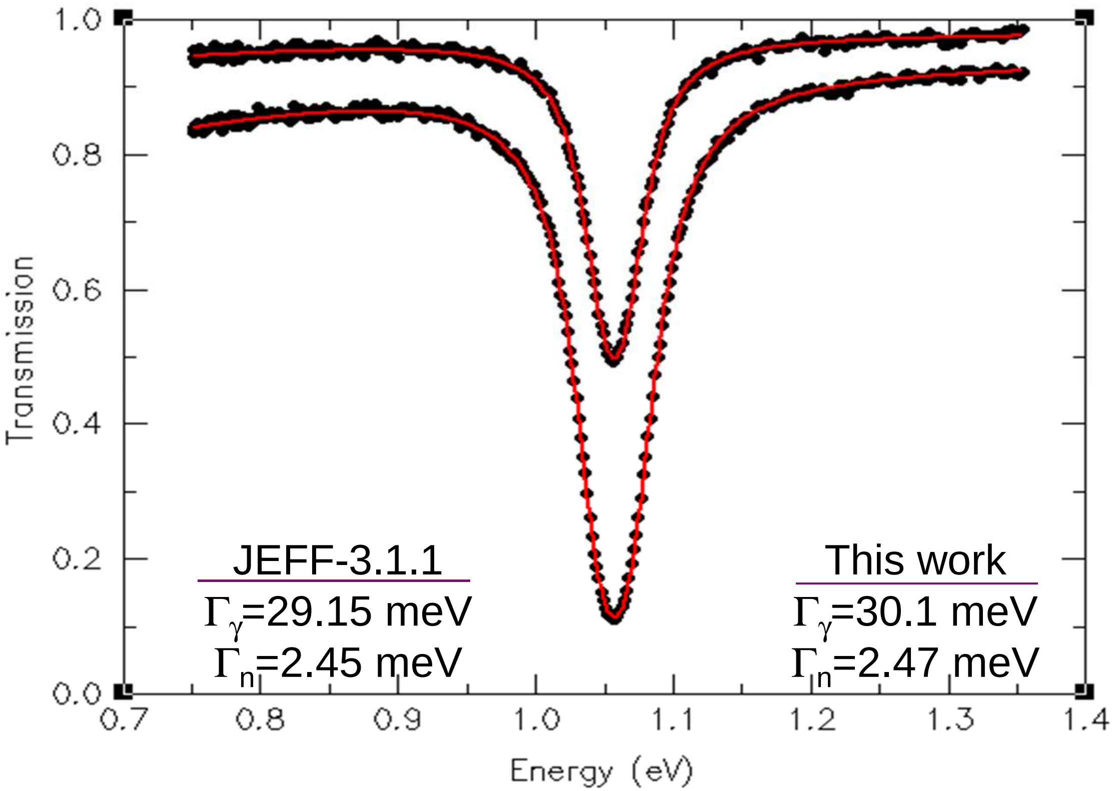
$$\vec{x} = \{\gamma_{a\lambda}, E_\lambda, a_c, R'\}$$

$$\vec{x} = \{\langle\Gamma_a\rangle, a_c, R^\infty, D_0, S_a\}$$

$$\vec{x} = \{\beta_2, a_c, d_c, V, W, \ldots\}$$

Transmission data measured by Harvey (T=77 K)

New Pu240 resonance parameters by using T_{eff} =91 K



Transmission data measured by Harvey (T=77 K)

Uncertainties on the resonance parameters calculated by Marginalization (Monte-Carlo)

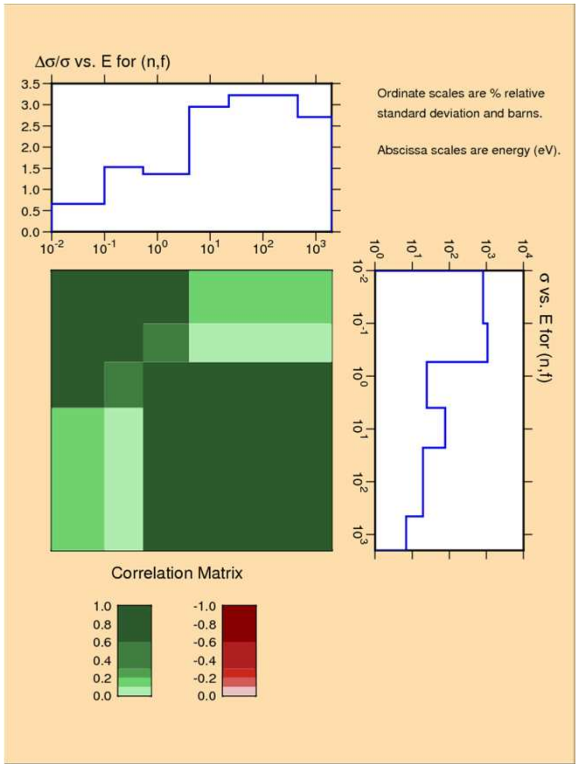
The uncertainty propagation takes into account the uncertainty on T_{eff} (±5K), sample composition (±1%), background, resolution function + Pu239 resonance parameters (Resonance Parameter Covariance Matrix from WPEC/SG34)

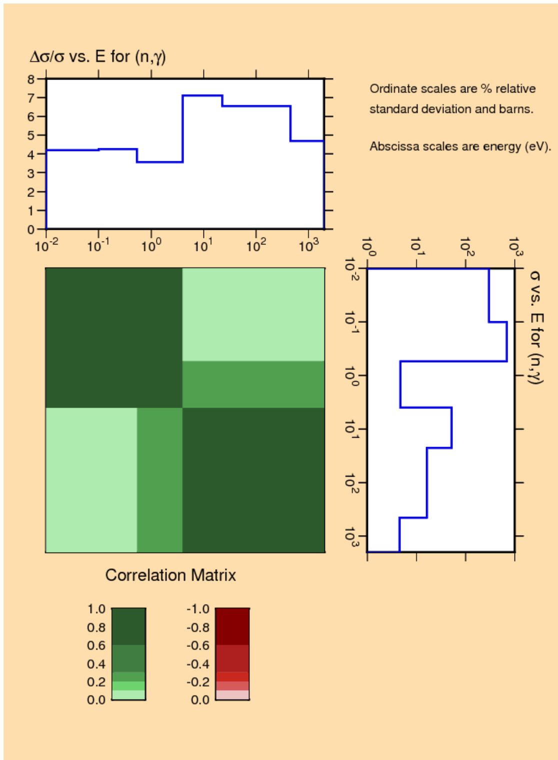
```
Statistical uncertainties :

 En = 0.1057E+01 +/-  0.3009E-04      0.003%   100
 Gg = 0.3008E-01 +/-  0.7848E-04      0.261%    -2 100
 Gn = 0.2468E-02 +/-  0.3249E-05      0.132%     5  40 100

Systematic uncertainties  :

 En = 0.1057E+01 +/-  0.2325E-02      0.220%   100
 Gg = 0.3008E-01 +/-  0.5220E-03      1.735%    19 100
 Gn = 0.2468E-02 +/-  0.5885E-04      2.384%    22  78 100

Total uncertainties       :

 En = 0.1057E+01 +/-  0.2325E-02      0.220%   100
 Gg = 0.3008E-01 +/-  0.5278E-03      1.755%    19 100
 Gn = 0.2468E-02 +/-  0.5893E-04      2.387%    22  77 100
 Gf = 0.8152E-05 +/-  0.1024E-05     12.556%    -3  -4  -4 100
```

^{239}PU COVARIANCE MATRICES

Resolved Resonance Range (SG34 and Jeff3.2)

- The RRR was divided in three energy ranges to account for the thermal cross section, the 1st resonance around 0.3 eV and the resonance integral (E>0.5 eV)
- Final uncertainties dominated by normalization accuracy introduced in the Marginalization procedure (0.5-3% for the fission cross section and 4-9% for the capture cross section)
- A neutron width selection based on the truncated Porter-Thomas integral distribution was performed to produce a "manageable" large covariance matrix

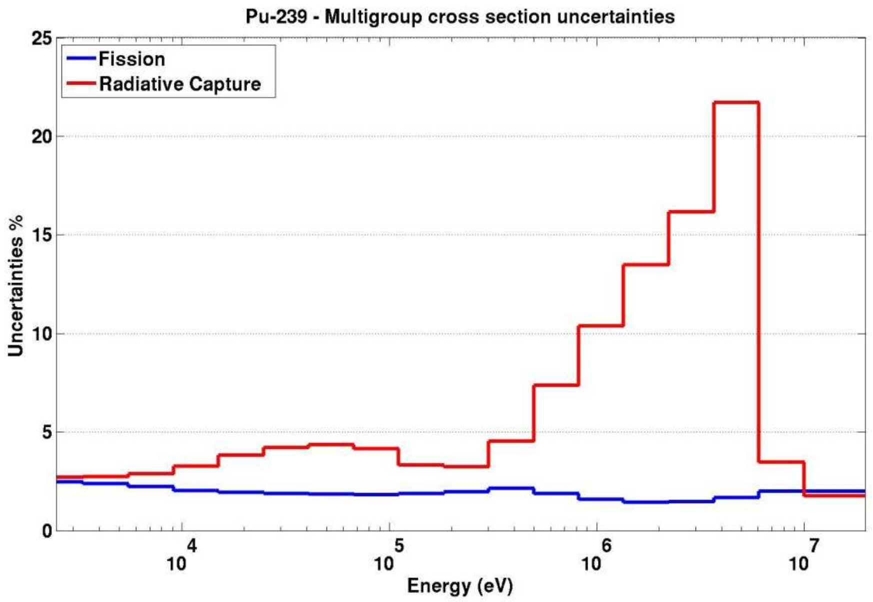


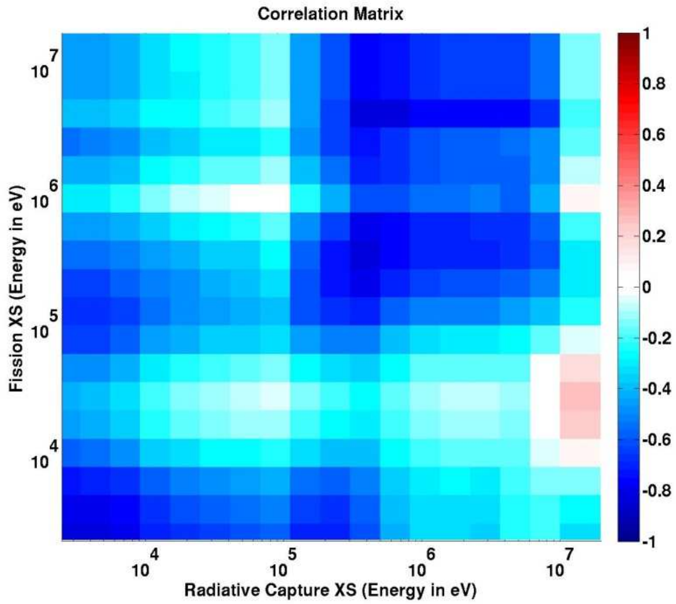


^{239}PU COVARIANCE MATRICES

Continuum Covariances (COMAC-V0.1)

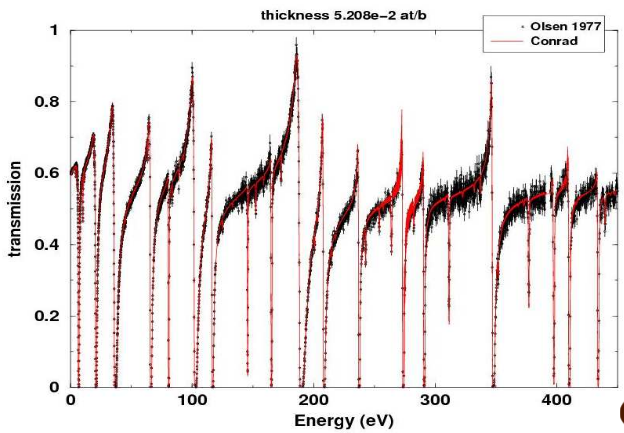
- Construction of an a-priori based on JEFF-3.2 cross sections
- Systematic uncertainties on fission and capture XS, based on "International Evaluation of Neutron Cross Section Standards" by Carlson *et al.* (CRP Report)

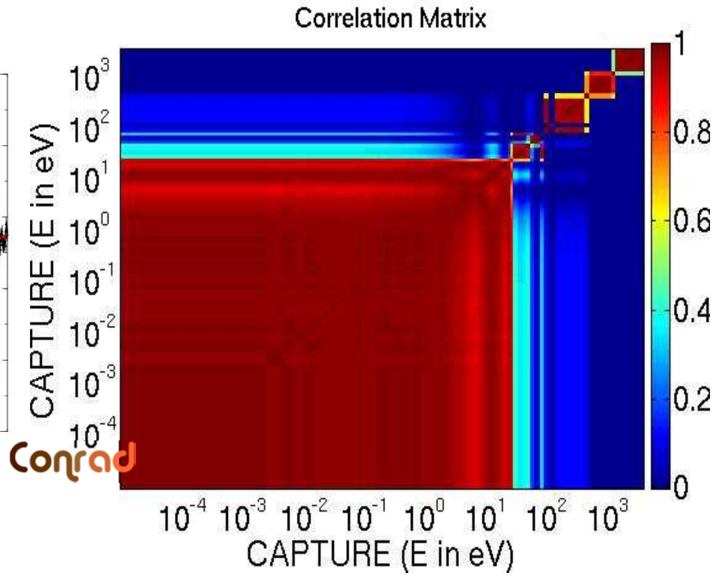


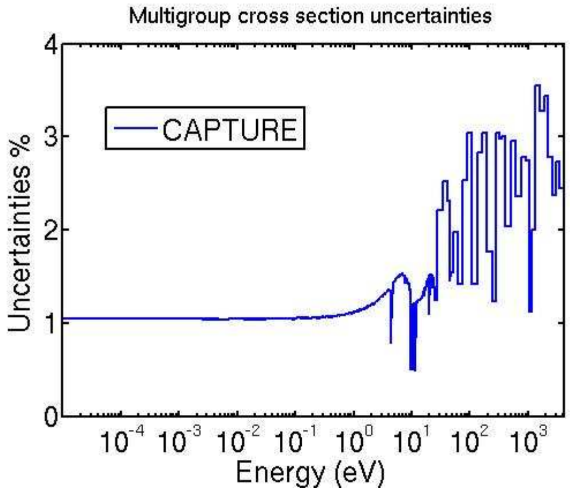


Resolved Resonance Range (Jeff3.2 and COMAC-V0.1)

- Proposed to Jeff3.2 (resonance parameters and cross sections)
- Based on Microscopic measurements + Systematic uncertainties taken into account
- Bayesian Framework + Marginalization for systematic exp. Uncertainties







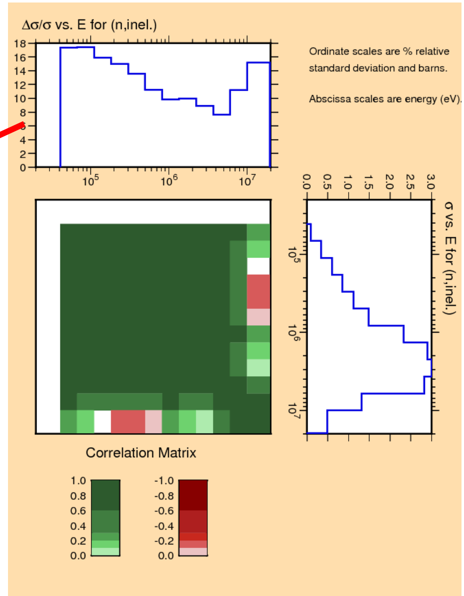
^{238}U COVARIANCE MATRICES

Continuum Covariances (COMAC-V0.1)

- Construction of an a-priori based on Jeff3.1.1
- “Simulated“ systematic uncertainties taken into account

Uncertainty Propagation of COMAC-V0 matrices on a SFR

Isotope	FISSION	CAPTURE	ELASTIC	INELASTIC	NXN	NU	TOTAL
B-10	—	11				—	**11**
C-0	—					—	**0**
O-16	—	34	29	2		—	**45**
Na-23	—	8	50	32		—	**60**
Cr-52	—	6	31	16		—	**35**
Fe-56	—	97	79	45		—	**135**
Ni-58	—	19	7	12		—	**24**
U-235	4	18	1	1		6	**19**
U-238	**367**	**533**	*i* 75	**452**	*i* 42	0	**784**
Pu-238	35	67	1	3		59	**94**
Pu-239	**992**	208	8	24		106	**1020**
Pu-240	49	77	13	52		65	**124**
Pu-241	58	91	1	5	1	28	**112**
Pu-242	21	32	2	7		12	**41**
Am-241	3	27	0	1		3	**27**
TOTAL	**1062**	**599**	**72**	**460**	***i* 42**	**142**	**1312**



COVARIANCE MATRICES CHALLENGES

- RRR/URR/OM Full treatment + Influential Model Parameters

- Importance of cross-correlations between reactions / energy ranges for reactor applications
- Inelastic XS for ^{238}U (new microscopic/integral experiment and new evaluation)
- ^{239}Pu Capture (low and high energy range and capture to fission ratio),
- ^{235}U Capture (intermediate energy range)
- Angular distributions, PFNS, nu-bar, O, Fe, $S\alpha\beta$
- New microscopic/integral experiments even on well-known isotopes
  (Normalization and background issues, URR, angular distributions,…)
- More microscopic ingredient (less “free” parameters)
- …..

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Additional Covariances Matrices evaluation methodologies used/to be used on ^{238}U and ^{239}Pu Determination of

Matrices

See C. De Saint Jean et al. ND2013 for Details

CROSS SECTIONS "KNOWLEDGE"

- **Experimentalist**
  Knowledge of cross section ⟺ finest microscopic experiments and smartest integral experiments ;
  Calibration; Syst. Uncertainties …

- **Theoretician**
  Knowledge of cross section ⟺ knowledge of models parameters and/or nuclear reaction models (resonance parameters, optical models, fission barrier, average width, ...) ; Systematics

⇓ ⇓ ⇓ ⇓

Evaluation work is done "***sometimes***" independently between :
- Resolved resonance range / unresolved resonance range / continuum
- International Experts (that is what CIELO is all about right ??)

As a result, one may ended with several inconsistencies :
- **mismatches** and larger uncertainties at the boundaries for punctual cross section
- **no cross correlation between high energy domain and resonance range.**
- Good overall integral behavior with deviations among Evaluations (B. Morillon et al. JEFDOC) → compensating effects

Uncertainties must reflect the lack of knowledge, inconsistencies as well as advances

Add physical constraints to find the most physical values

One Model / Several Experiments

Marginalization philosophy

$$\sigma = f(\vec{x}, \vec{\theta})$$

Model parameters

« n... ...rs

Nuisance parameters are **necessary** durin... ...isons with experiments (data reduction, normalization,…) ... ...or the final evaluation

$$\sigma = f(\vec{x}, \vec{\theta}) \quad \Rightarrow \quad \sigma = f(\vec{x})$$ + **Covariances**

Marginalization of the ... density:

$$p(\vec{x}, \vec{\theta}|\vec{y}, U) \quad \Rightarrow \quad p_{\vec{\theta}}(\vec{x} \mid \vec{y}, U) = \int d\vec{\theta} \cdot p(\vec{x}, \vec{\theta} \mid \vec{y}, U)$$

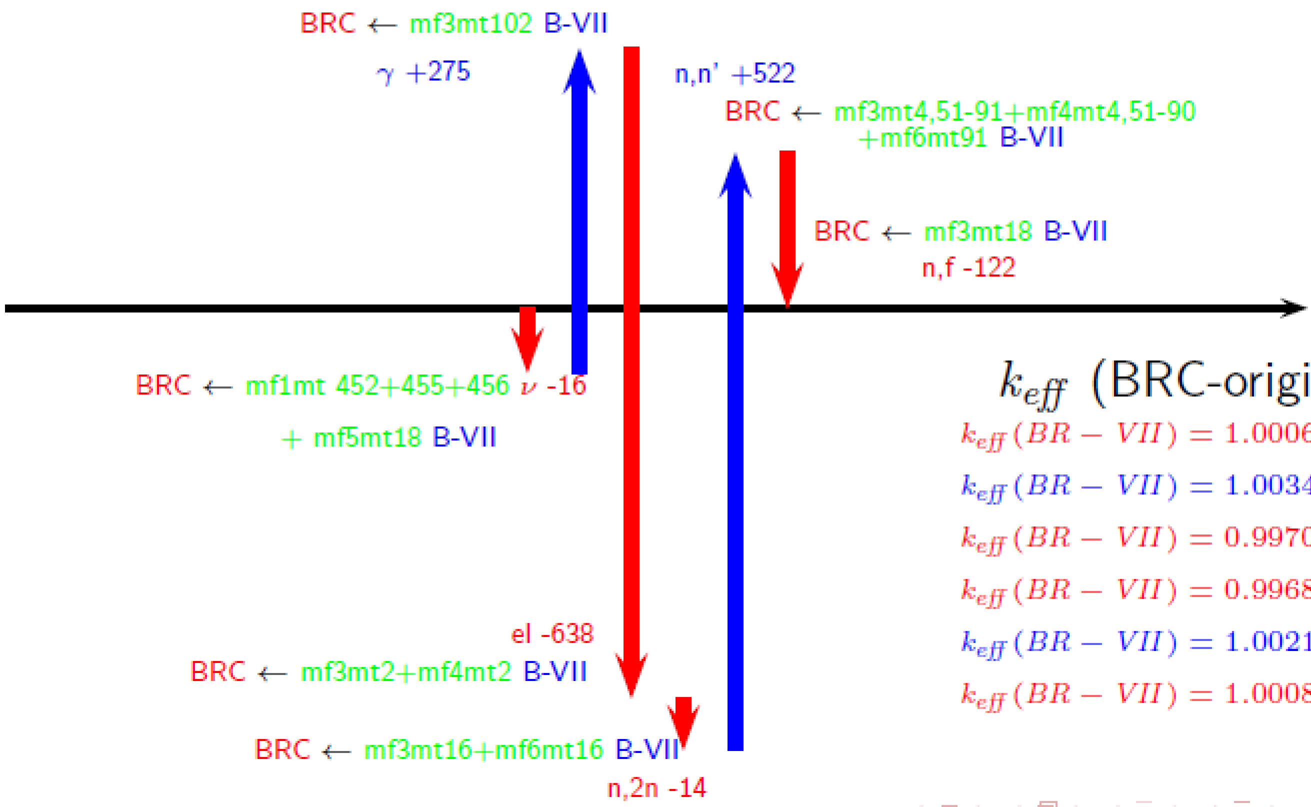
Marginalization :

estimation... ...rst two moments of the marginal probability density

Fresnel Representation - ^{239}Pu

MCNP study of the JEZEBEL critical benchmark

$k_{eff}(BRC) = 1.00082(11)$ $k_{eff}(B\text{-}VII) = 1.00060(12)$



k_{eff} (BRC-origin)

$k_{eff}(BR - VII) = 1.00066(12)$

$k_{eff}(BR - VII) = 1.00341(12)$

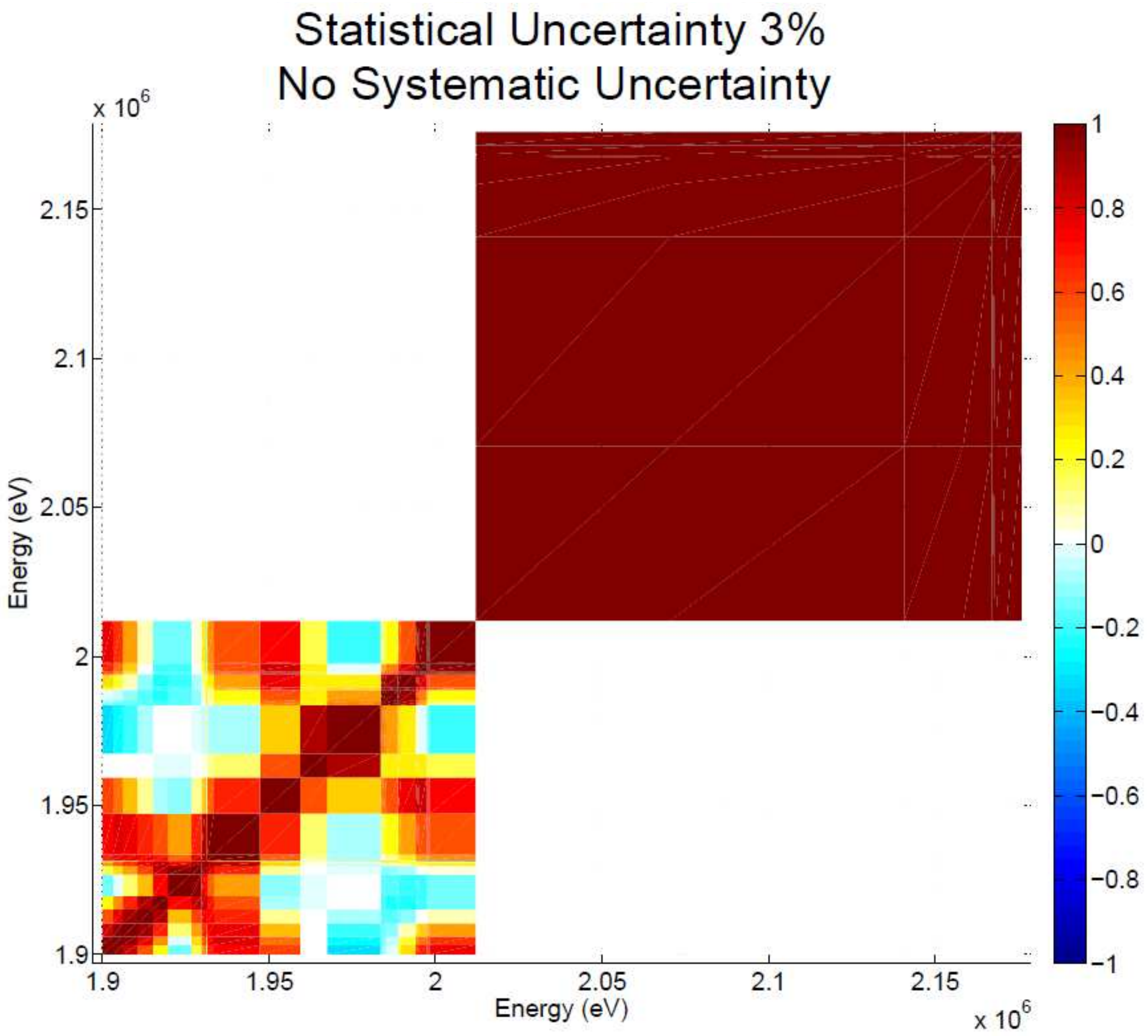
$k_{eff}(BR - VII) = 0.99703(12)$

$k_{eff}(BR - VII) = 0.99689(12)$

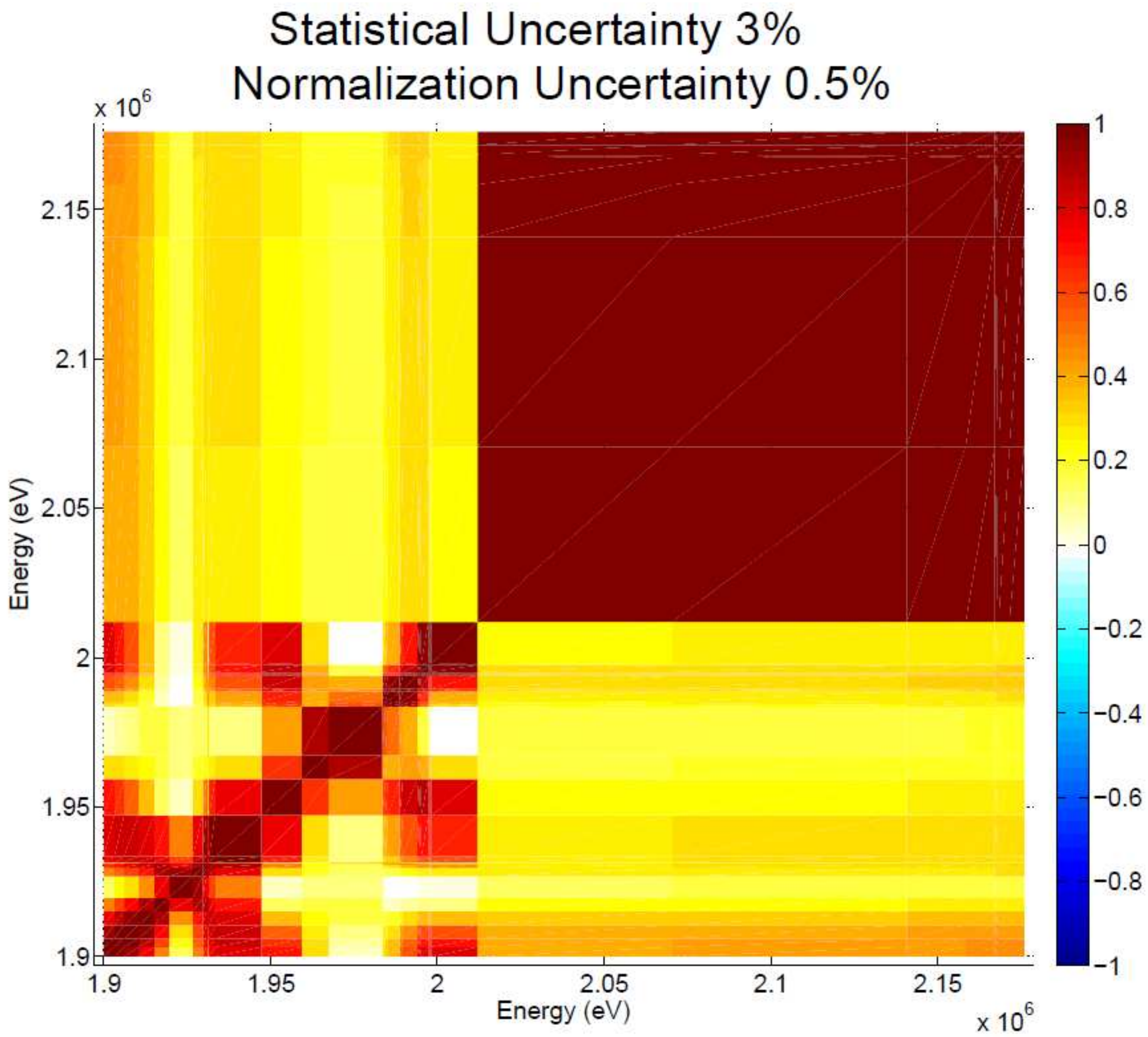
$k_{eff}(BR - VII) = 1.00211(12)$

$k_{eff}(BR - VII) = 1.00089(1$

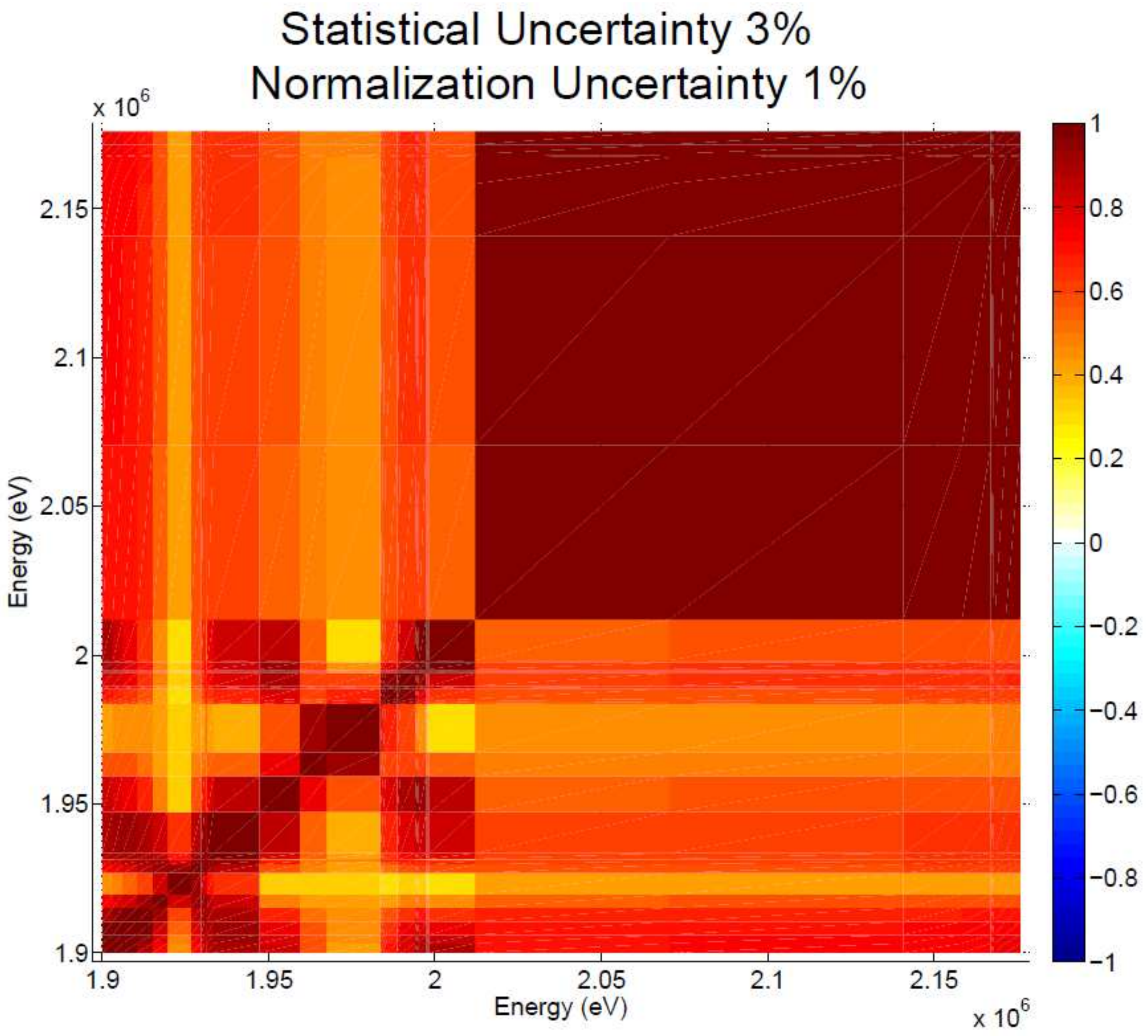
IMPOSING CONSTRAINTS ON SEVERAL MODELS SYST. EXP; UNCERTAINTIES; ^{23}NA EXAMPLE



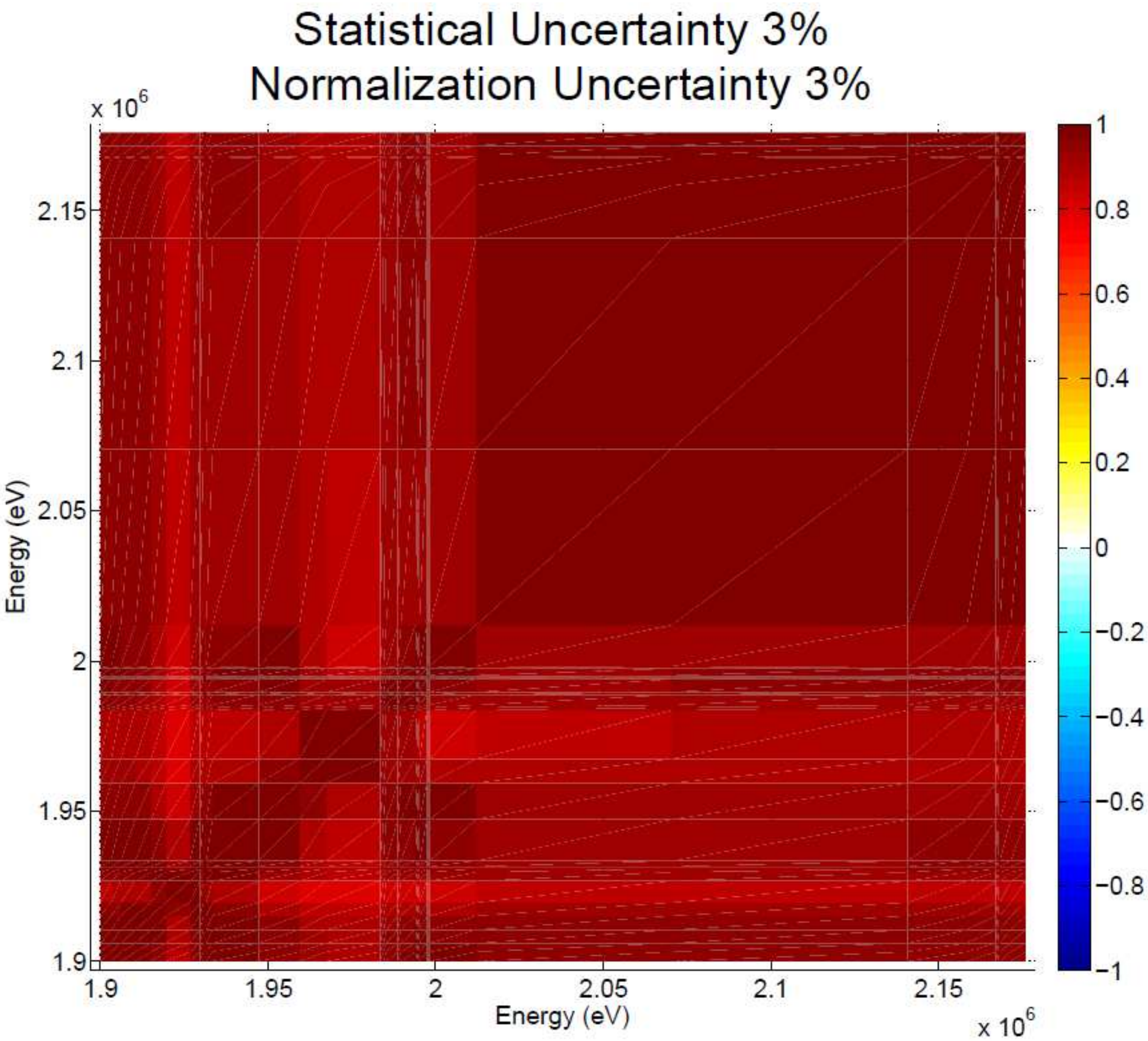
IMPOSING CONSTRAINTS ON SEVERAL MODELS SYST. EXP; UNCERTAINTIES; ^{23}NA EXAMPLE



IMPOSING CONSTRAINTS ON SEVERAL MODELS
SYST. EXP; UNCERTAINTIES; ^{23}NA EXAMPLE



IMPOSING CONSTRAINTS ON SEVERAL MODELS SYST. EXP; UNCERTAINTIES; ^{23}NA EXAMPLE



IMPOSING CONSTRAINTS ON SEVERAL MODELS
LAGRANGE MULTIPLIERS

$$\chi^2_{GSL} = (\vec{x} - \vec{x}_m)^T M_x^{-1} (\vec{x} - \vec{x}_m) + \left(\vec{y} - \vec{t}(\vec{x})\right)^T M_y^{-1} \left(\vec{y} - \vec{t}(\vec{x})\right)$$

$$\chi^2_{GLS+C} = (\vec{x} - \vec{x}_m)^T M_x^{-1} (\vec{x} - \vec{x}_m) + (\vec{y} - \vec{t})^T M_y^{-1} (\vec{y} - \vec{t}) + 2[C^T(\vec{x})] \cdot \lambda$$

Constraints

Lagrange Multipliers

Linearization

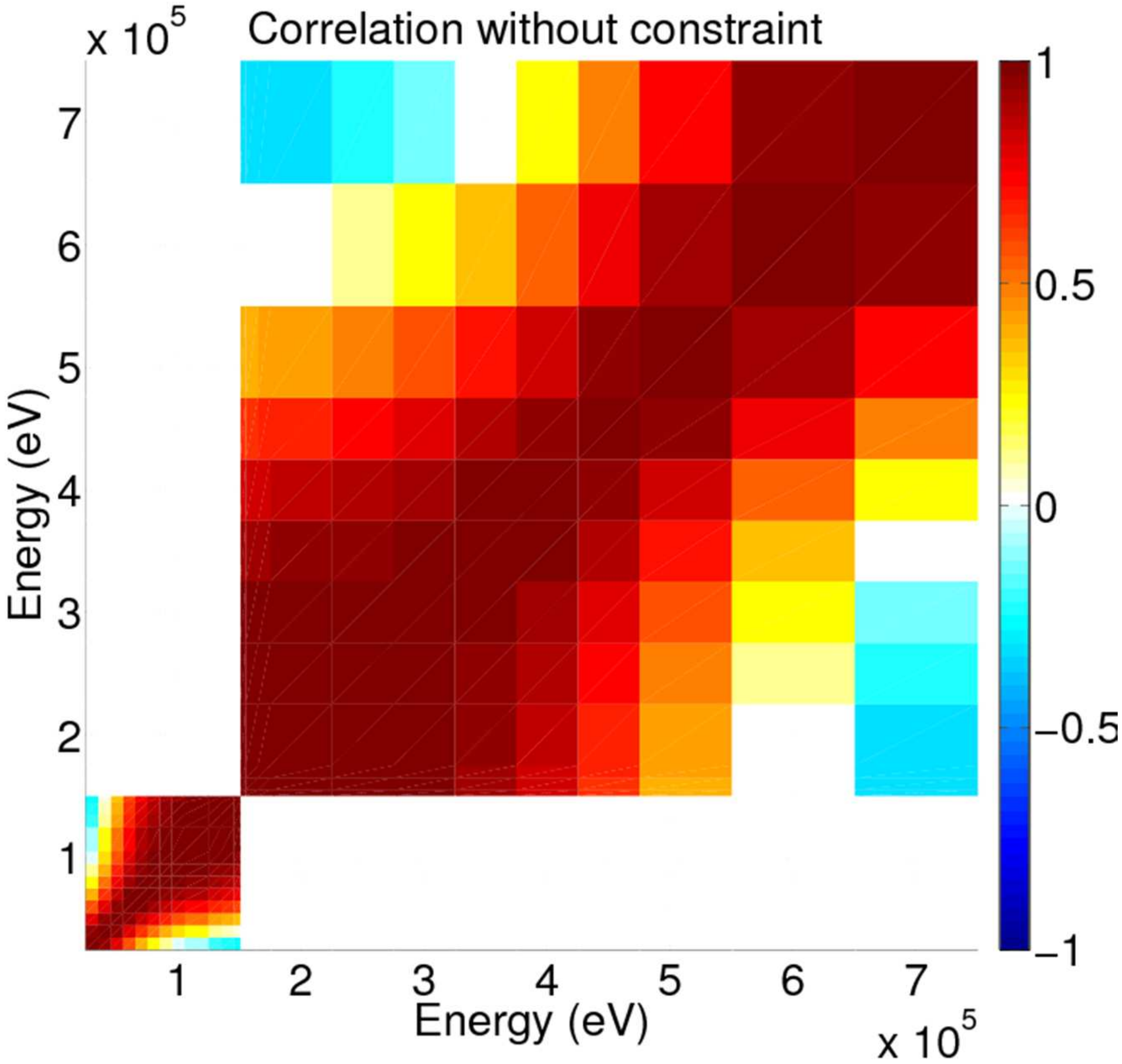
$$\begin{pmatrix} A(\tilde{x}) & S_c^T(\tilde{x}) \\ S_c(\tilde{x}) & 0 \end{pmatrix} \begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} A(\tilde{x})\tilde{x} - S_t^T(\tilde{x}) M_y^{-1} (y(\tilde{x}) - t) \\ S_c(\tilde{x})\tilde{x} - C(\tilde{x}) \end{pmatrix}$$

with $A(x) = M_{\tilde{x}}^{-1} + S_t^T(x) M_y^{-1} S_t(x)$

@ Conrad

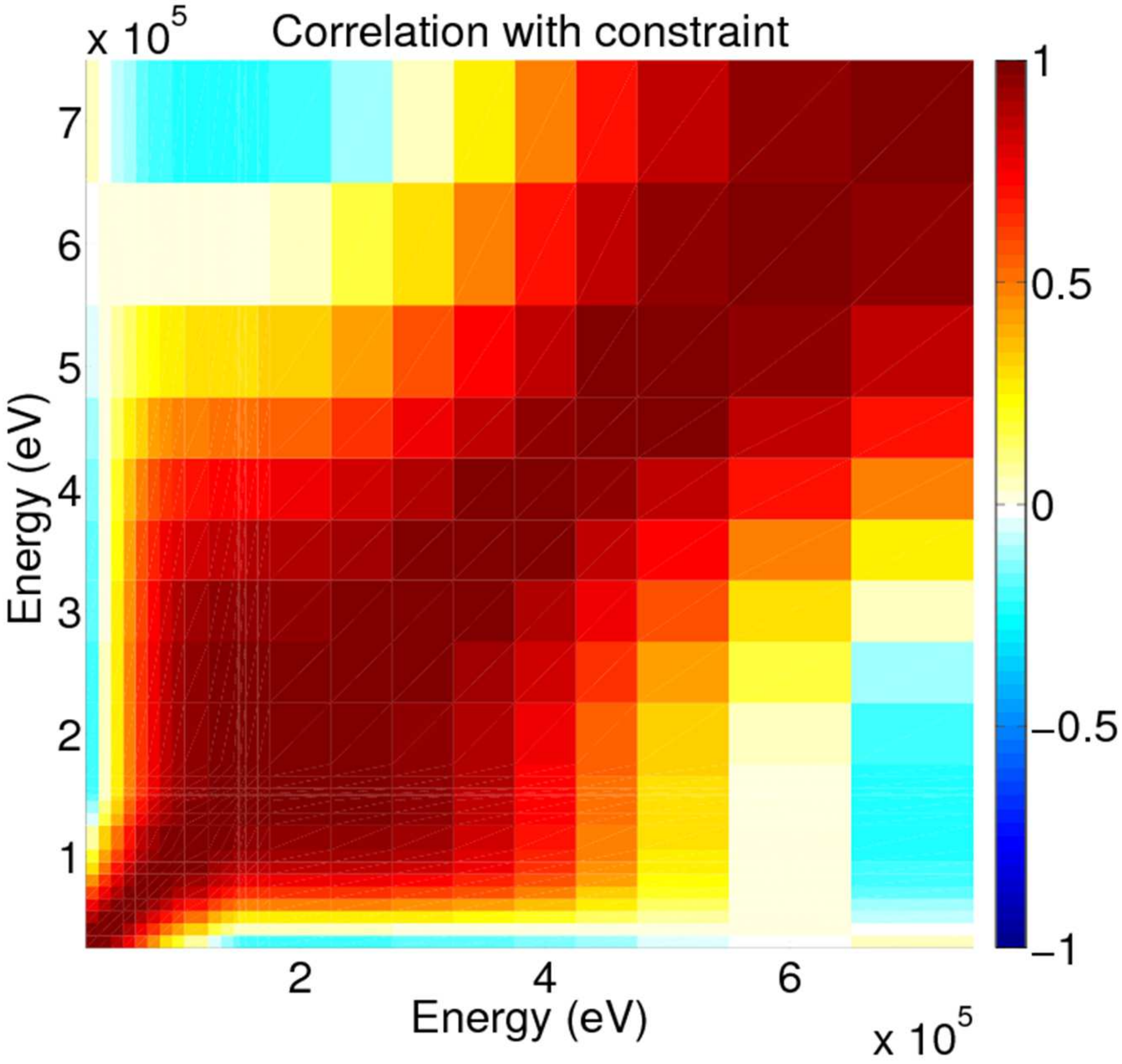
IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS ; ^{238}U EXAMPLE

- Toy Model URR/URR



IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS ; ^{238}U EXAMPLE

- Toy Model URR/URR

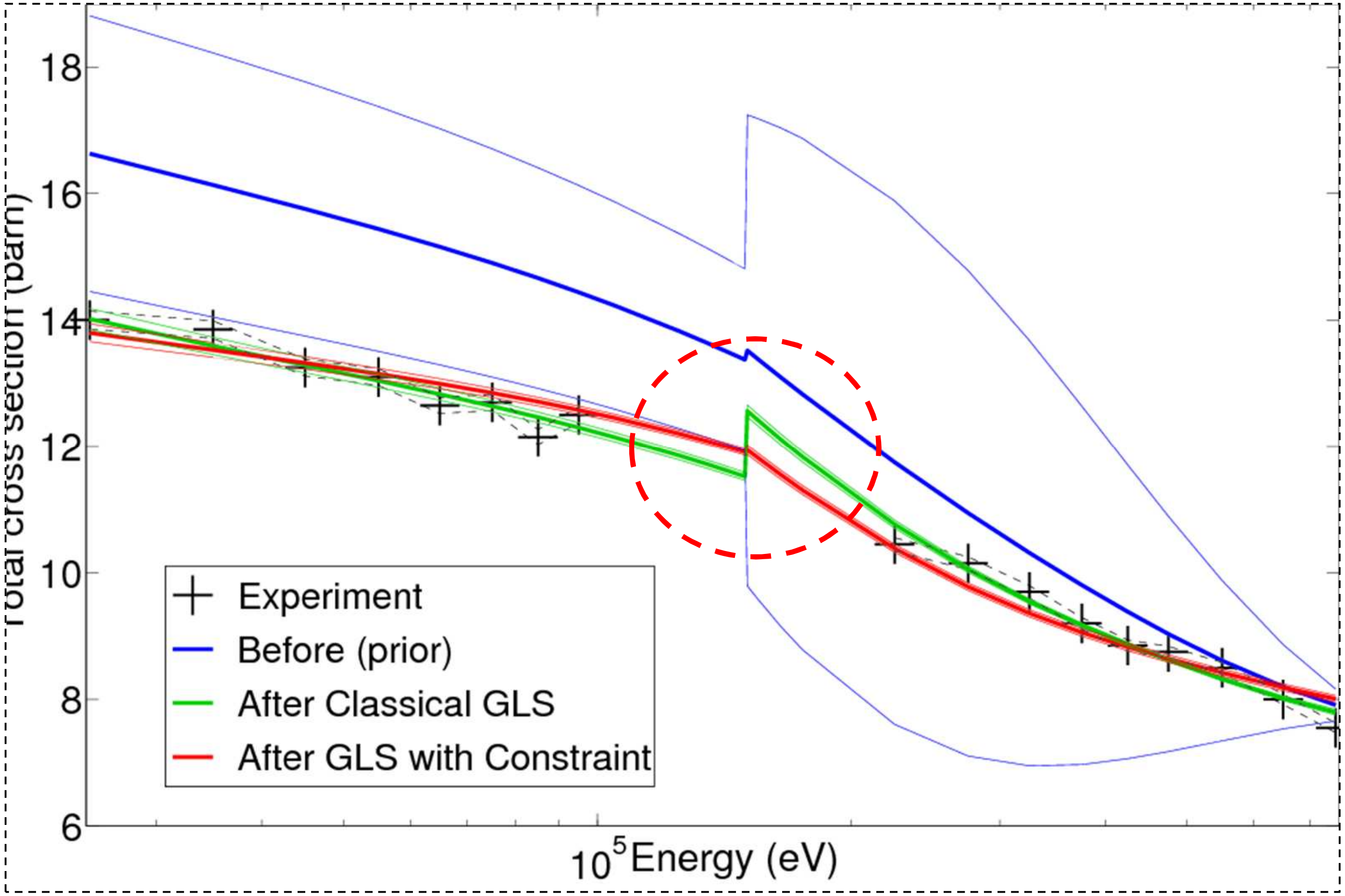


$\rho \leq \pm 0.9$

IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS ; ^{238}U EXAMPLE

- Realistic Application URR/OM

- Parameters used :
  - Strength function (l=0,1) ; Distant level (l=0,1) ; Effective Radius
  - Reduce radius ; Diffusiveness



IMPOSING CONSTRAINTS ON SEVERAL MODELS

- Promising methods (Lagrange multipliers + Syst. Uncertainties on several models)

Correlations between energy ranges appear in cross section covariances : no more block diagonal matrices → could enhanced final uncertainties on applications …

- Syst. Uncertainty
  - Tends to ensure cross section continuity…if no gap in experiment in energies
  - 1st attempt with normalization → Generalize to other experimental parameters creating systematic uncertainties (backround, resolution parameters., isotopic concentration)

- Lagrange multipliers →1st constraint chosen is continuity between two models calculated cross sections ; Other ideas are underway on nuclear model parameters, average cross sections, …

- Both method are not straightforward → choice of parameters to be included very important
- Difficulty arises if :
  - Parameters are not well chosen
  - Boundary is not well chosen : too high or too low making one model outside its scope
  - There are Model defects

- Use of this approach in a “true” evaluation :1st true evaluation made on ^{23}Na (Jeff3.2)

Major Isotopes : Big 3 + Additional

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Covariances Matrices evaluation methodologies using integral experiments on ^{238}U and ^{239}Pu Determination of

and

Matrices

CONTRAINTS : INTEGRAL EXPERIMENTS

Data Assimilation framework for evaluation using integral experiments

$$\chi^2_{GSL} = (\vec{x}-\vec{x}_m)^T M_x^{-1}(\vec{x}-\vec{x}_m) + (\vec{E}-\vec{C}(\sigma(\vec{x})))^T M_E^{-1}(\vec{E}-\vec{C}(\sigma(\vec{x})))$$

$\boxed{\vec{y} \longrightarrow \vec{E}}$ → Intégrales Exp. $\boxed{\vec{x} \longrightarrow}$

$\boxed{\vec{x} = \{\gamma_{a\lambda}, E_\lambda, a_c, R'\}}$

$\boxed{\vec{x} = \{\langle\Gamma_a\rangle, a_c, R^\infty, D_0, S_a\}}$

$\boxed{\vec{x} = \{\beta_2, a_c, d_c, V, W, \ldots\}}$

$$\boxed{\vec{G} = \partial\vec{C}/\partial\vec{x} = \partial\vec{C}/\partial\vec{\sigma} \otimes \partial\vec{\sigma}/\partial\vec{x}}$$

Conrad

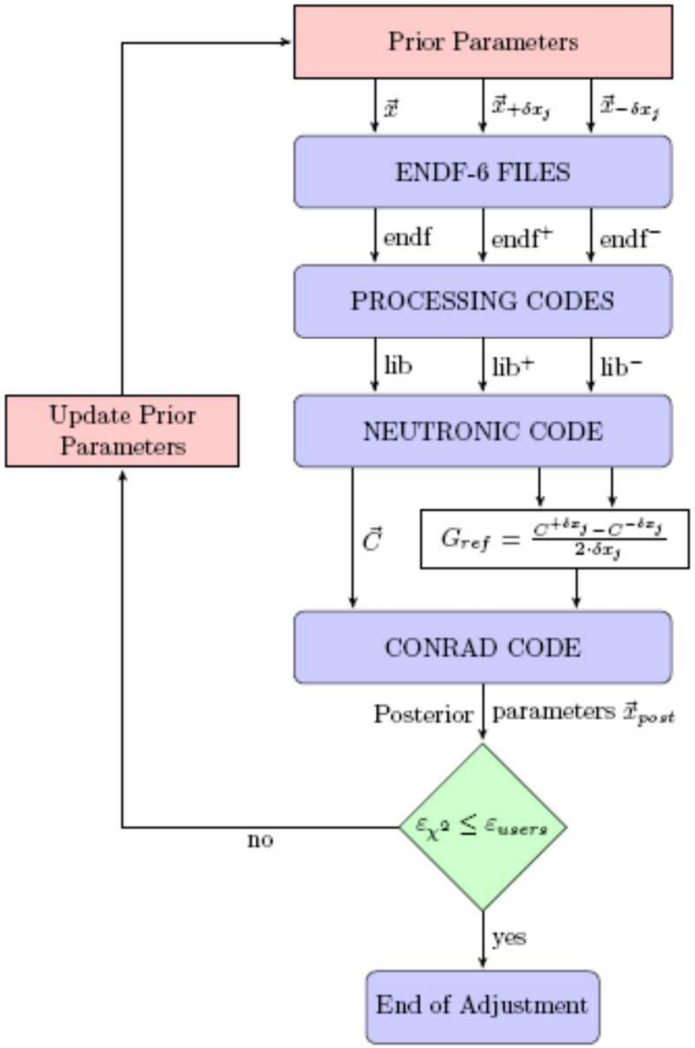
Sammy,
Refit,
TALYS,

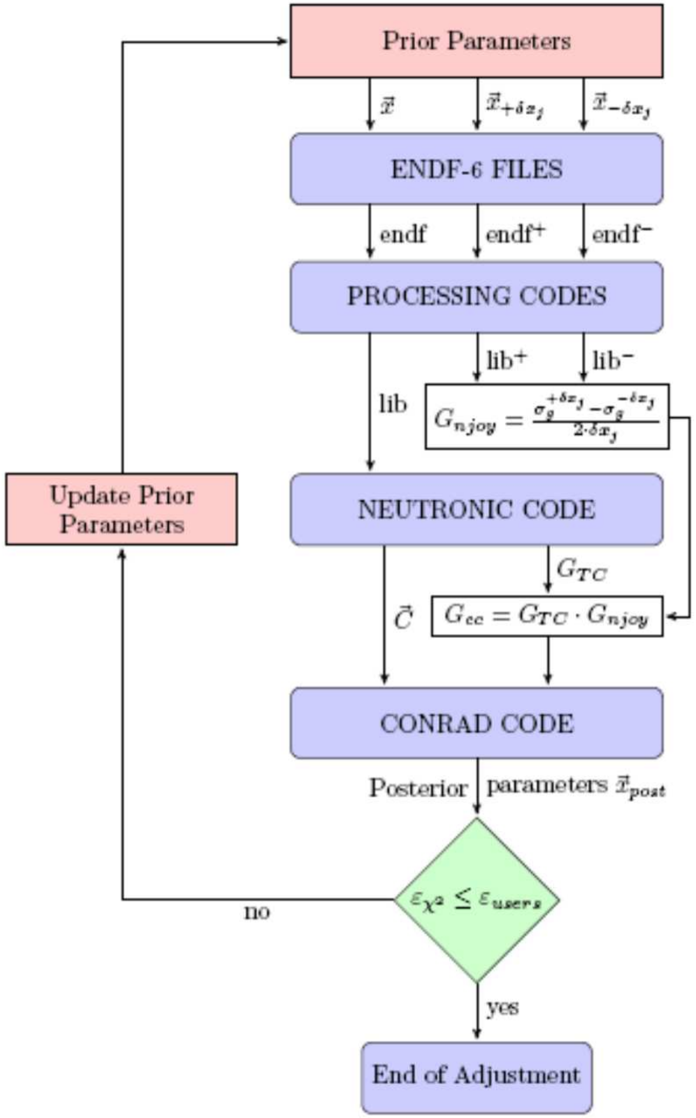
AP2/CRONOS2, ERANOS/PARIS, APOLLO3
MCNP, Tripoli-4

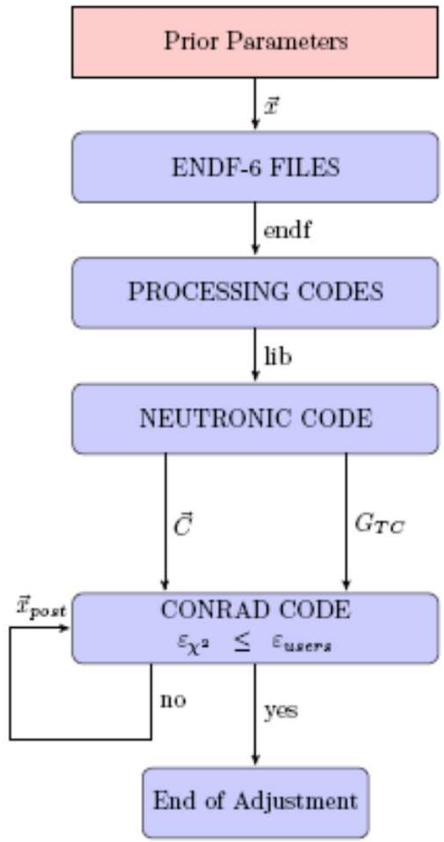
ND Treatment

CONTRAINTS :
INTEGRAL EXPERIMENTS

Data Assimilation framework for evaluation using integral experiments







INTEGRAL EXPERIMENTS

Validation and/or DataAssimilation → $\vec{x} = \{\gamma_{a\lambda}, E_\lambda, a_c, R', OMP, ...\}$ +BIASES and/or σ_g^r and χ_g, υ... + TRENDS

"Public" Integral Experiments

- ❑Mini-Inca (ILL)
- ❑ICSBEP/IRPHe
- ❑...

Used as validation for evaluation →C/E ~1

Using benchmark in relative (see ND2013) to focus on some reaction (^{238}U (n,n'))

Take care of experimental correlation between ICSBEP series

Additional Integral Experiments

- ❑Irradiation Exp. PROFIL/MANTRA
- ❑Oscillation Exp. MINERVE/DIMPLE
- ❑...

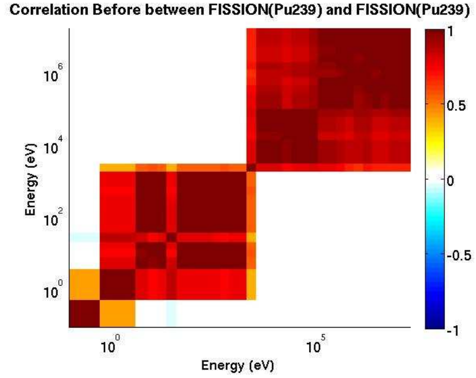
High Precision (Oscillation : 1-3% ; PROFIL : ~2%)

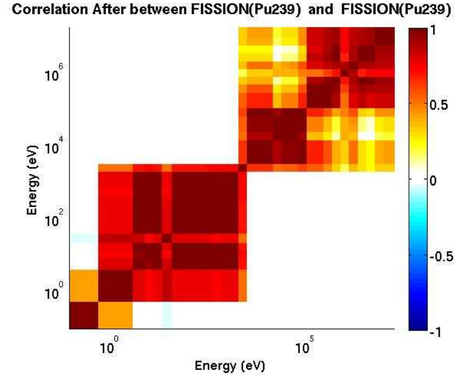
Flexibility in terms of neutronic spectrum

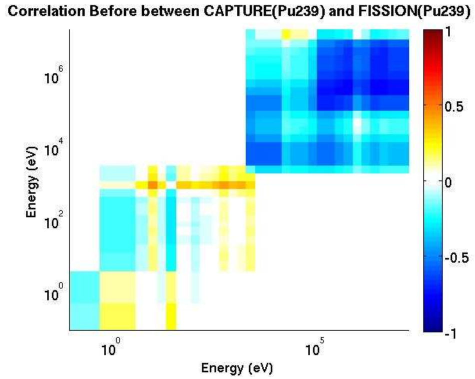
→Deconvolution of energy domain

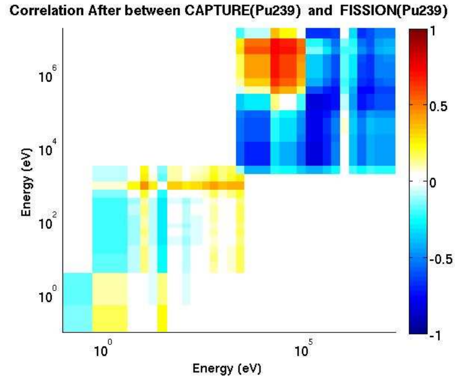
SG39 ↔ SG40

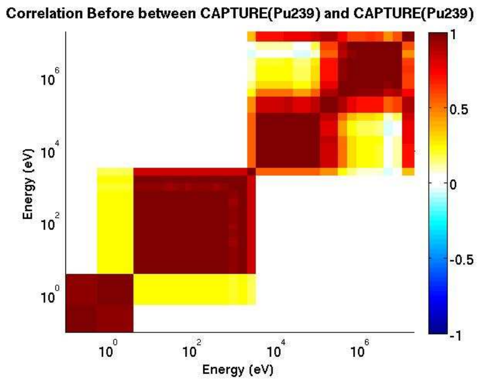
^{239}PU COVARIANCE MATRICES

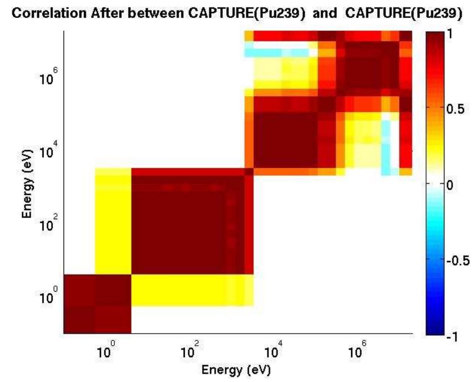


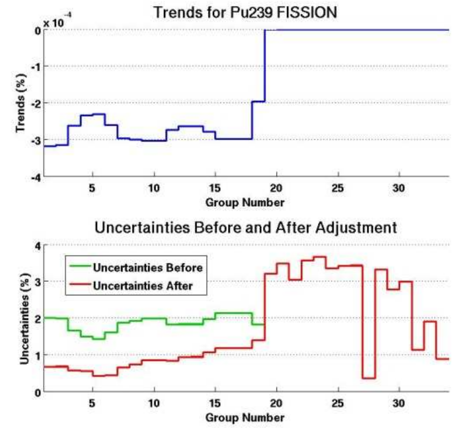






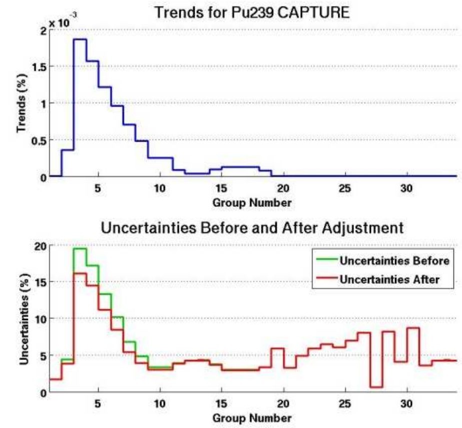






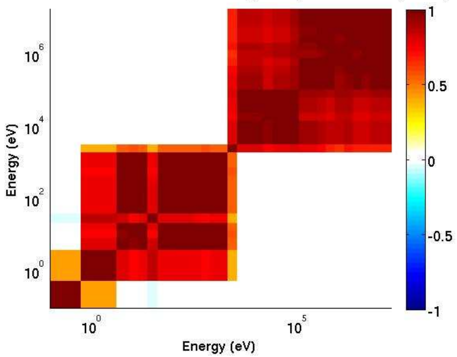
“Public” Integral Experiments

- **ICSBEP (JEZEBEL)**

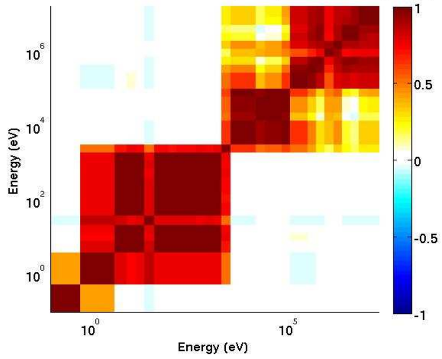


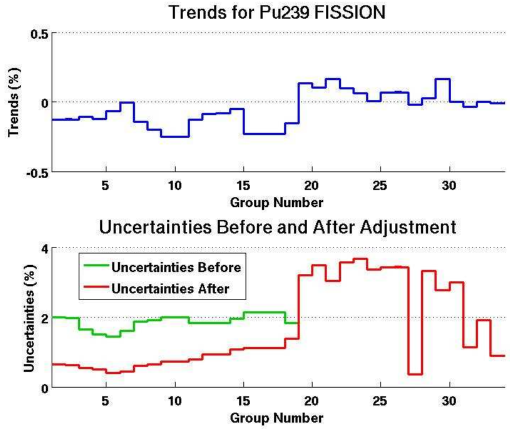
^{239}PU COVARIANCE MATRICES

Correlation Before between FISSION(Pu239) and FISSION(Pu239)

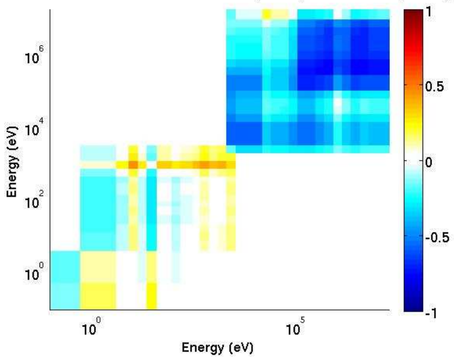


Correlation After between FISSION(Pu239) and FISSION(Pu239)

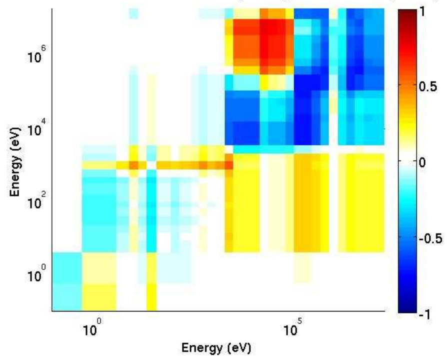




Correlation Before between CAPTURE(Pu239) and FISSION(Pu239)



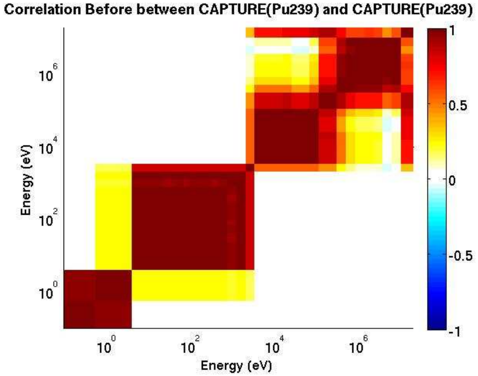
Correlation After between CAPTURE(Pu239) and FISSION(Pu239)



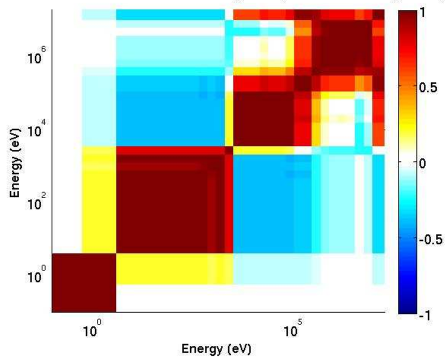
Additional Integral Experiments

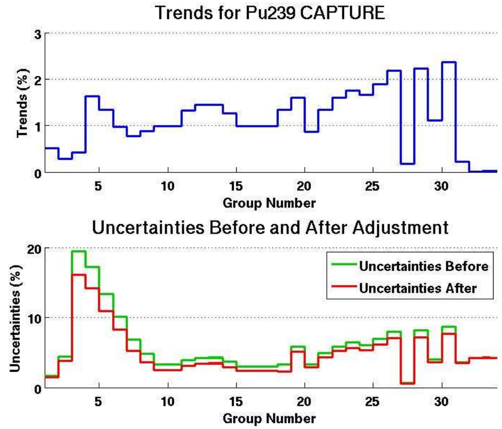
- PROFIL

Correlation Before between CAPTURE(Pu239) and CAPTURE(Pu239)



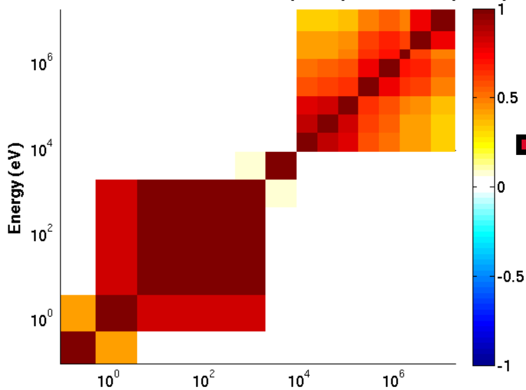
Correlation After between CAPTURE(Pu239) and CAPTURE(Pu239)



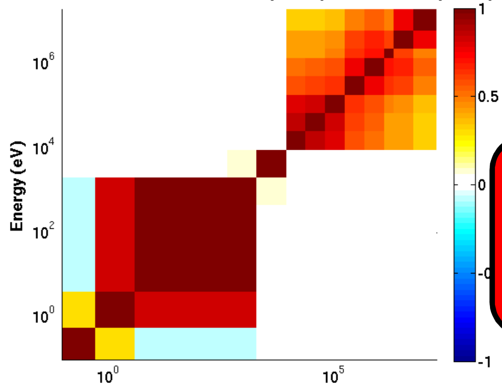


^{239}PU COVARIANCE MATRICES

Correlation Before between FISSION(Pu239) and FISSION(Pu239)

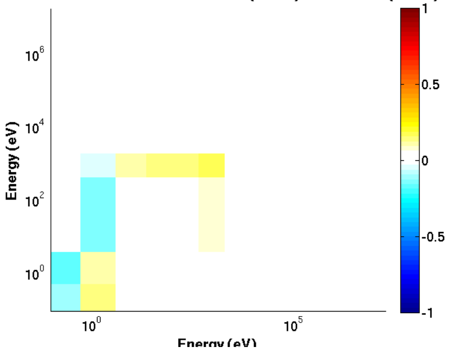


Correlation After between FISSION(Pu239) and FISSION(Pu239)

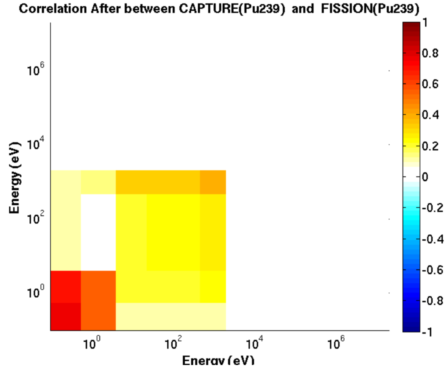


Additional Integral Experiments
❑CERES Program in MINERVE/DIMPLE

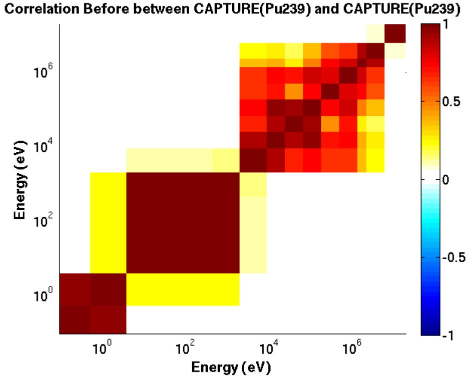
Correlation Before between CAPTURE(Pu239) and FISSION(Pu239)



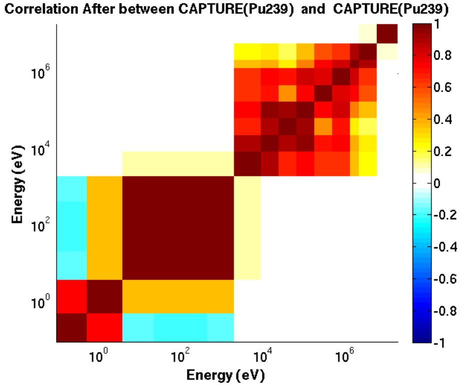
Correlation After between CAPTURE(Pu239) and FISSION(Pu239)



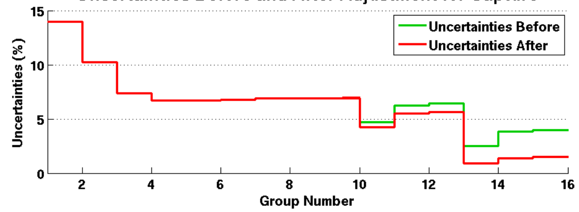
Correlation Before between CAPTURE(Pu239) and CAPTURE(Pu239)



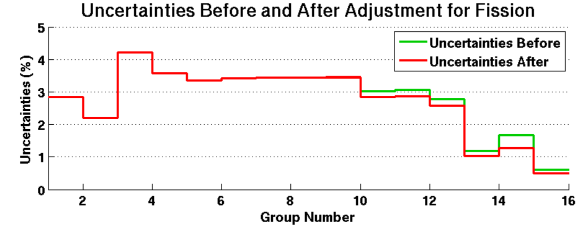
Correlation After between CAPTURE(Pu239) and CAPTURE(Pu239)



Uncertainties Before and After Adjustment for Capture



Uncertainties Before and After Adjustment for Fission



IMPOSING CONSTRAINTS ON SEVERAL MODELS INTEGRAL EXPERIMENTS

- Reduction of Uncertainties with dedicated integral experiments is major (Factor 5-10)

- Work presented here on multigroup Cross sections,but
  - nuclear parameters assimilation of integral experiments
  - on going work on PROFIL/JEZEBEL for parameters as well

see C. De Saint Jean et al. in NEMEA-5, ND2010 proceedings

- Choice of integral experiments is crucial to disentangle nuclear data sensitivities

  - Use integral experiments sensitive to different reactions or parameters
  - Relative integral experiments (reflector effect instead reactivity,
  - Experimental correlation may permit to focus on less influential isotopes

see D. Bernard et al. , ND2013)

- Difficulty arises if :
  - Parameters are not well chosen or forgotten (PFNS, angular distributions …etc…)
  - Spurious Integral experiment (as for microscopic ones) with hidden error
  - Correlation between experiments are neglected (ICSBEP series …)

- Traditional questions arises → “old” experiments, effect is diluted on several ND,.. etc

→ **Sometimes true but**
CIELO and SG39 could give answers

CONCLUSIONS

- ❑ Several kind of Nuclear Data
- ❑ Several kind of Nuclear Reaction Models
- ❑ Several kind of Experiments
- ❑ Several kind of Covariance Matrices
- ❑ Several kind of International experts (☺)

- ❑ CIELO and SG39 could allow progress on methodologies related to :
  - o *Data assimilation for traditional evaluation*
  - o *Data assimilation for evaluation using specific integral experiments (IDA)*
  - o Data assimilation for evaluation with physical constraints
    - ▪ Systematic uncertainty constraints effect on several models
    - ▪ Lagrange multipliers in the cost function
    - ▪ ……
  - o Link between evaluation and integral experiment beyond validation issues