DE LA RECHERCHE À L'INDUSTRIE



Evaluation of Cross-Sections Uncertainties using Physical Constraints ²³⁸U, ²³⁹Pu and others...

Cyrille DE SAINT JEAN, Edwin PRIVAS, Pascal ARCHIER, Gilles NOGUÈRE, Olivier LITAIZE, Pierre LECONTE, David BERNARD

CEA, DEN-Cadarache, F-13108 Saint-Paul-lez-Durance, France

www.cea.fr

NEMEA-7, November 5-8, 2013, Geel (Belgium)



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. JEFDO and P. Romain talk) → compensating effects

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

Add physical constraints to find the most physical values



CONSTRAINTS

- Physics :
 - Cross section is an observable
 - Isotopic lines (see CEA/DAM Romain talk)
 - 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



CONSTRAINTS

- Physics :
 - Cross section is an observable
 - Isotopic lines (see CEA/DAM Romain talk)
 - 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



CIELO INITIATIVE BIG THREE: WHAT SHOULD/COULD BE SHARED?

Ideal world

■ Utopic view → Everything should be shared for Nuclear Physics advances

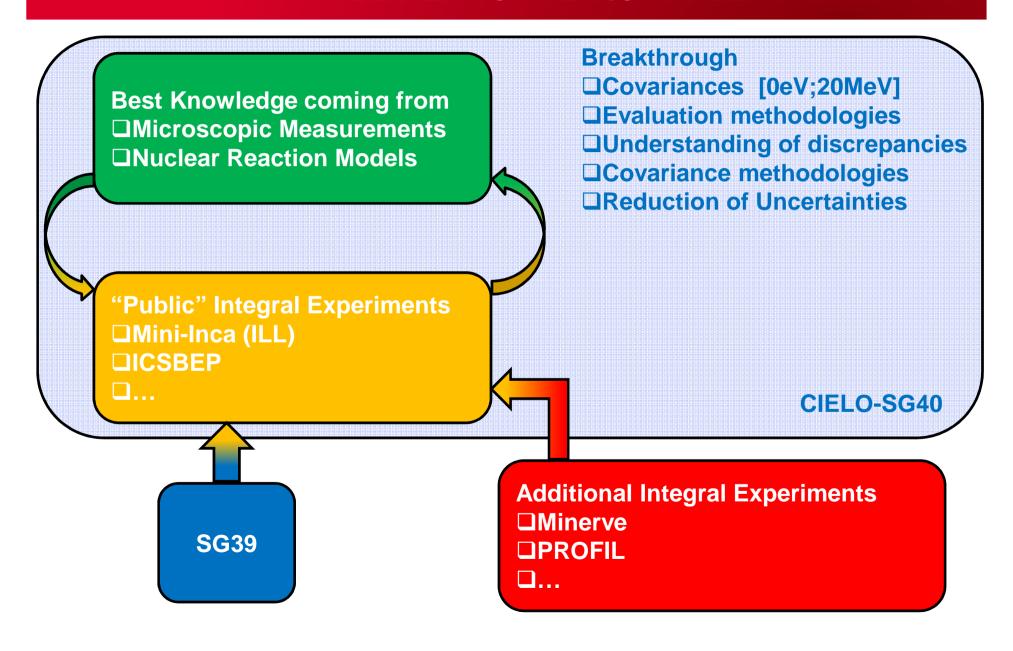
Real world

- Resolved and unresolved resonance range:
 - Various past SG (²³⁸U, ²³⁹Pu, etc, ...) :
 - sharing among participant of resonance **parameters**, microscopic measurements, some integral experiments ("public") + experimental knowledge
 - Test of advances on additional integral experiments ("proprietary")
 - Covariances evaluation on the shared information could be performed and compared
- Continuum:
 - What about nuclear models?
 - Do we share Physics ? Or Parameters (both ?)
 - Microscopic and "public" integral experiments + experimental knowledge
 - "Confidential experiments"

For Uncertainty evaluation the shared part is crucial CIELO should allow a step forward



CEA/CADARACHE STRATEGY FOR JEFF IN CIELO RELATED TO THE BIG THREE



DE LA RECHERCHE À L'INDUSTRIE



Covariances Matrices evaluation on ²³⁸U and ²³⁹Pu Determination of



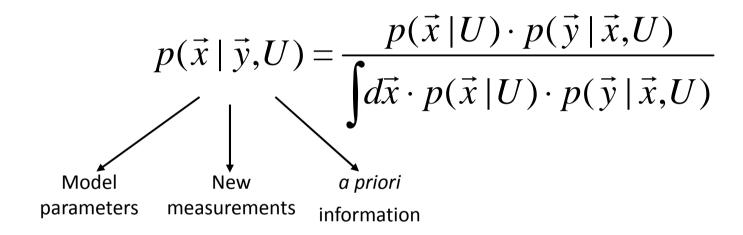
Matrices

www.cea.fr



EVALUATIONS AND UNCERTAINTIES GENERAL MATHEMATICAL FRAMEWORK

Bayesian inference (probability density):



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



SYSTEMATIC EXPERIMENTAL UNCERTAINTIES → AGS/RETROACTIVE/MARGINALIZATION

Marginalization philosophy

$$\sigma = f(\vec{x}, \vec{\theta})$$
Model "nuisance" parameters parameters

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

Marginalization of the probability density:

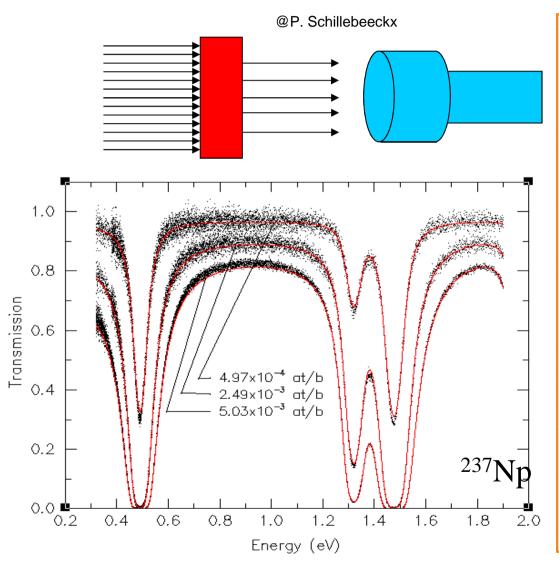
$$p(\vec{x}, \vec{\theta} | \vec{y}, U) \longrightarrow p_{\vec{\theta}}(\vec{x} | \vec{y}, U) = \int d\vec{\theta} \cdot p(\vec{x}, \vec{\theta} | \vec{y}, U)$$

Marginalization:

estimation of the first two moments of the marginal probability density

MICROSCOPIC EXPERIMENTS (IRMM, CERN...)

Transmission Measurement



Comparison

$$T_{th} = \vec{t} (\vec{\sigma}(\vec{x}), \vec{\theta})$$
 and $T_{\text{exp}} = N \frac{C_{in} - B_{in}}{C_{out} - B_{out}}$ $\approx N_{\theta} e^{-n_{\theta} \sigma_{t}(\vec{x})} + B_{\theta}$



Data Assimilation



$$\vec{x} = \left\{ \gamma_{a\lambda}, E_{\lambda}, a_{c}, R' \right\}$$

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

$$\vec{x} = \left\{ \beta_2, a_c, d_c, V, W, \dots \right\}$$

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

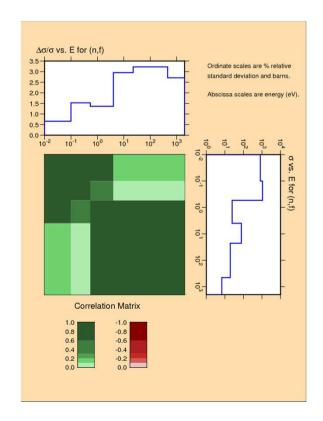


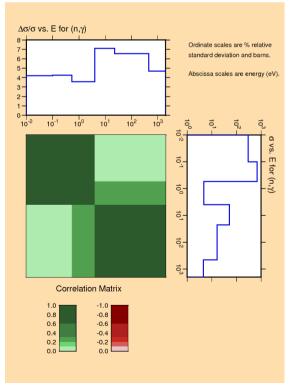


²³⁹PU COVARIANCE MATRICES

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





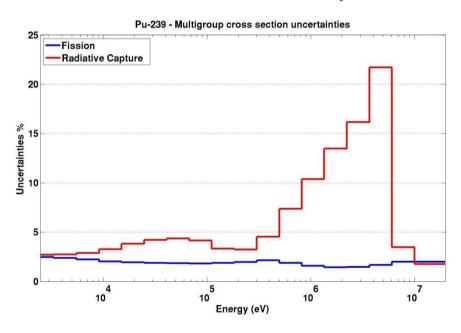


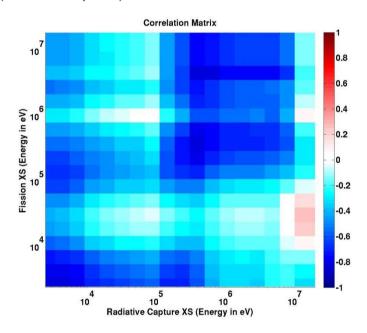


²³⁹PU COVARIANCE MATRICES

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)





- Improvements / On going work :
- Use microscopic experiments
- Add "public" integral nuclear data oriented experiment
- Add CEA integral nuclear data oriented experiment

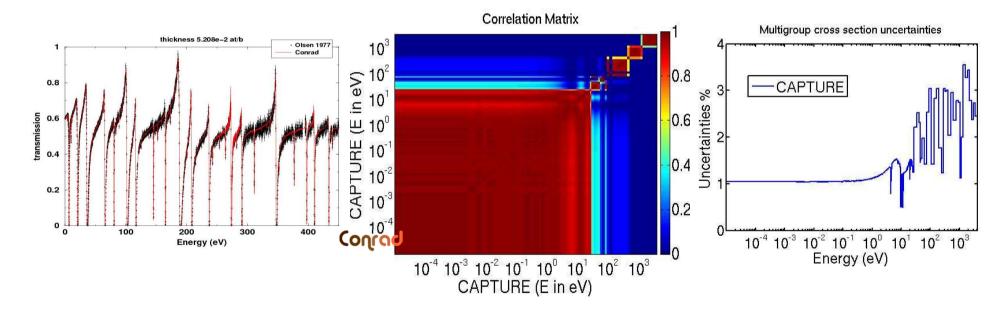




²³⁸U COVARIANCE MATRICES

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



- Improvements / On going work:
 - Add additional microscopic experiments (Ex : Macklin 88 Capture data)
 - Add "public" integral nuclear data oriented experiment
 - Add CEA integral nuclear data oriented experiment





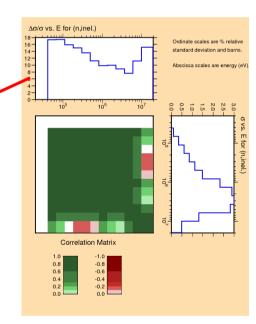
²³⁸U COVARIANCE MATRICES

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			Ş
Na-23	_	8	50	32			60
Cr-52	_	6	31	16		-	35
Fe-56	_	97	79	45		_	135
Ni-58	_	19	7	1		_	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



- Improvements / On going work :
 - Add additional microscopic experiments + "Stick" to Jeff3.2 evaluation
 - Add "public" integral nuclear data oriented experiment
 - Add CEA integral nuclear data oriented experiment

COVARIANCE MATRICES CHALLENGES FOR CIELO

- RRR/URR/OM Full treatment + Influential Model Parameters
- Define "wrapping" benchmark for Covariance estimation in RRR/Continuum and RRR+Continuum
- Importance of cross-correlations between reactions / energy ranges for reactor applications
- Inelastic XS for ²³⁸U (new microscopic/integral experiment and new evaluation)
- ²³⁹Pu Capture (low and high energy range and capture to fission ratio),
- 235U Capture (intermediate energy range)
- **Angular distributions, PFNS, nu-bar, O, Fe, S** α β
- New microscopic/integral experiments even on well-known isotopes (Normalization and background issues, URR, angular distributions,...)
- More microscopic ingredient (less "free" parameters)



DE LA RECHERCHE À L'INDUSTRIE



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



Matrices

www.cea.fr

IMPOSING CONSTRAINTS ON SEVERAL MODELS SYST. EXP; UNCERTAINTIES

Marginalization philosophy

$$\sigma = f(\vec{x}, \vec{\theta})$$
Model «r
parameters

Nuisance parameters are **necessary** during sons with experiments (data reduction, normalization,...) or the final evaluation

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

 $\sigma = f(ec{x})$ + Covariances

Marginalization of the r density:

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

Marginalization:

estimation st two moments of the marginal probability density



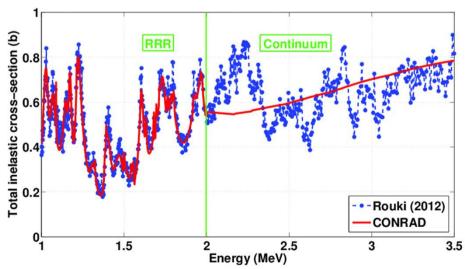
Unified model on an energy domain

[E_L, E_R] + Boundary at E_C:
$$\vec{t} = \vec{t}_L(x_\mu) \text{ if } E_L \ge E \ge E_c$$

$$\vec{t} = \vec{t}_R(x_\mu) \text{ if } E_R \le E \le E_c$$

- Didactic example : Sodium inelastic cross sections
 - Energy Range studied [1.9 2.1 MeV]; Boundary at 2 MeV.
 - Below 2 MeV : Resolved resonance range (Jeff3.2Beta)
 - Above 2 MeV : Jeff3.2Beta (Optical Potential + Partial models)

- "Simulated" experimental Data :
 - Based on theoretical points (red)
 - 3% statistical uncertainties
 - No/0.5/1/3% systematic uncertainties



- Considered parameters :
 - Resonance Range
 Neutron and inelastic Width (Γ_{n} , Γ_{n} ,)

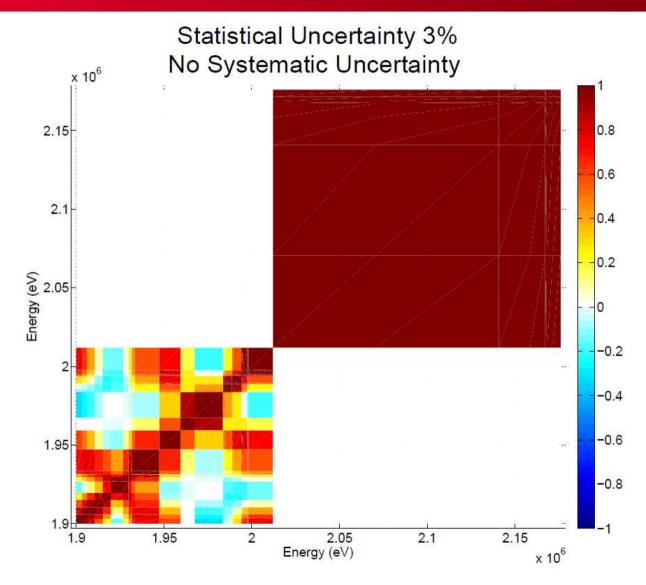
E(MeV)	Jπ
1.9215	3-
1.9625	2+
1.9723	1+

Optical Model

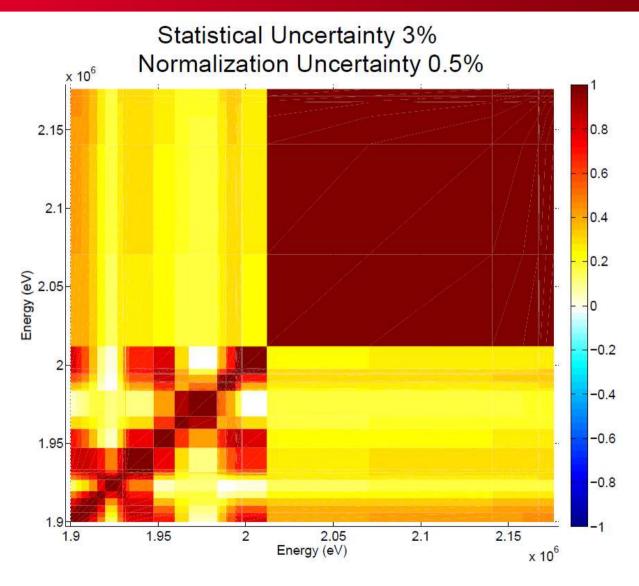
Reduced Scattering Radius ($^{\Gamma}_{0}$)
Diffusiveness ($^{a}_{0}$)



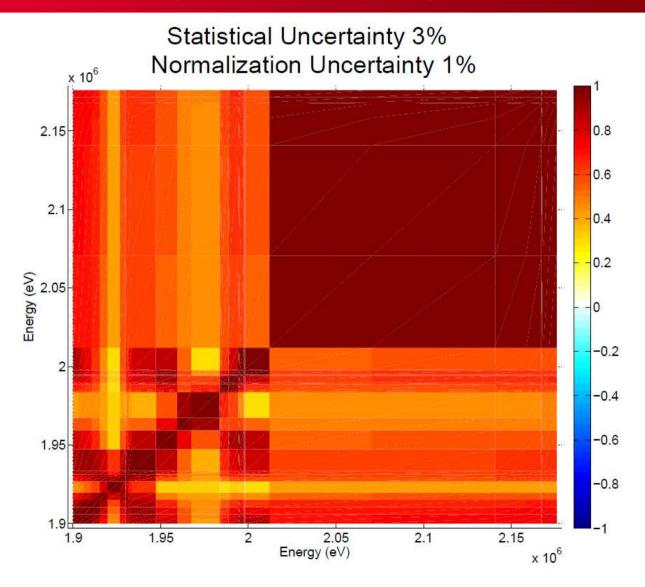




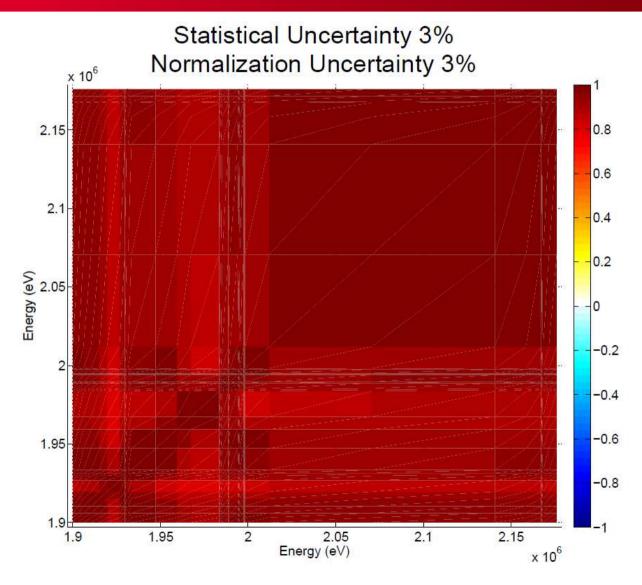














Correlations obtained on parameters as well (3% normalization case)

	Γ_n^{3-}	$\Gamma_{n'1}^{3-}$	Γ_n^{2+}	$\Gamma_{n'1}^{2+}$	Γ_n^{1+}	$\Gamma_{n'1}^{1+}$	R_0
Γ_n^{3-}	1	0.83	-0.39	0.74	-0.11	0.41	0.83
$\Gamma_{n',1}^{3}$		1	-0.37	0.89	0.03	0.56	0.98
$\Gamma_{n_1}^{2^+}$			1	-0.36	-0.05	-0.32	-0.38
$\Gamma_{n',1}^{2^+}$				1	-0.09	0.42	0.90
Γ_{n}^{1+}					1	-0.37	0.03
$\Gamma_{n'1}^{1+}$						1	0.58
\ddot{R}_0							1

- Parameters driving the cross section "level" end up correlated
- Correlation created between two different models : Γ_n , Γ_n and r0



IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS

$$\chi_{GSL}^{2} = (\vec{x} - \vec{x}_{m})^{T} M_{x}^{-1} (\vec{x} - \vec{x}_{m}) + (\vec{y} - \vec{t} (\vec{x}))^{T} M_{y}^{-1} (\vec{y} - \vec{t} (\vec{x}))$$

$$\chi_{GLS+C}^{2} = (\vec{x} - \vec{x}_{m})^{T} M_{x}^{-1} (\vec{x} - \vec{x}_{m})$$

$$+ (\vec{y} - \vec{t})^{T} M_{y}^{-1} (\vec{y} - \vec{t})$$

$$+ 2C^{T}(\vec{x}) \lambda \qquad \text{Lagrange Multipliers}$$



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

DE LA RECHERCHE À L'INDUSTRIE

IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS; 238U EXAMPLE

Unified model on an energy domain

$$[E_L, E_R]$$
 + Boundary at E_{C^1}

$$\vec{t} = \vec{t}_L(x_\mu) \text{ if } E_L \ge E \ge E_c$$

$$\vec{t} = \vec{t}_R(x_\mu)$$
 if $E_R \leq E \leq E_c$

■ Didactic example : Uranium Total cross section

- Energy Range studied [25 750 keV]; Boundary at 150 keV.
- Below 150 keV : Average R matrix
- Above 150 keV : Average R matrix or Optical Potential

Constraint on Cross sections at E_C

$$C(x) = <\sigma_t^R>_{E_c} - <\sigma_t^L>_{E_c} = 0$$

- "Real" experimental Data:
 - Based on C.A.Uttley et al., 1966
 - 1% statistical uncertainties
 - No systematic uncertainties

Considered parameters:

<u>Unresolved Resonance Range</u>

Effective Radius, Strenght, Distant level

$$R', S_{l=0,1}, R^{\infty}_{l=0,1}$$

Optical Model
Reduced Scattering Radius (a)
Diffusiveness (a)



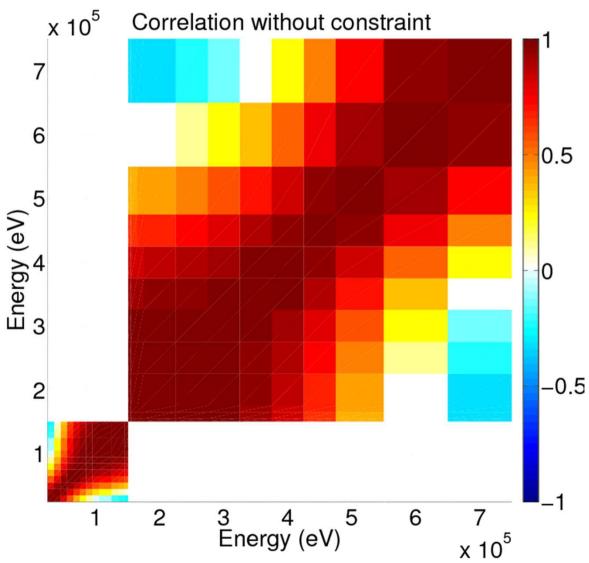
Two cases studied:

- 1. URR/URR : Toy model → act as if they were 2 ≠ models
- 2. URR/Continuum: "Realistic application"



IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS; 238U EXAMPLE

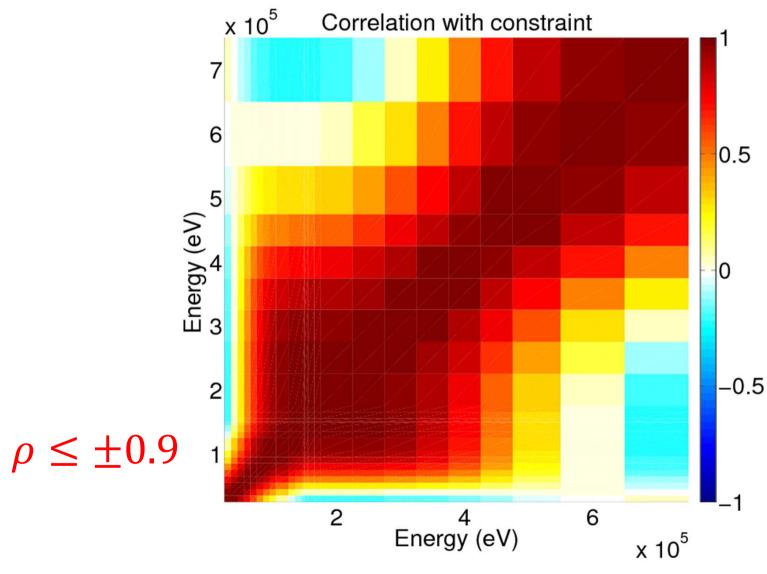
■ Toy Model URR/URR





IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS; ²³⁸U EXAMPLE

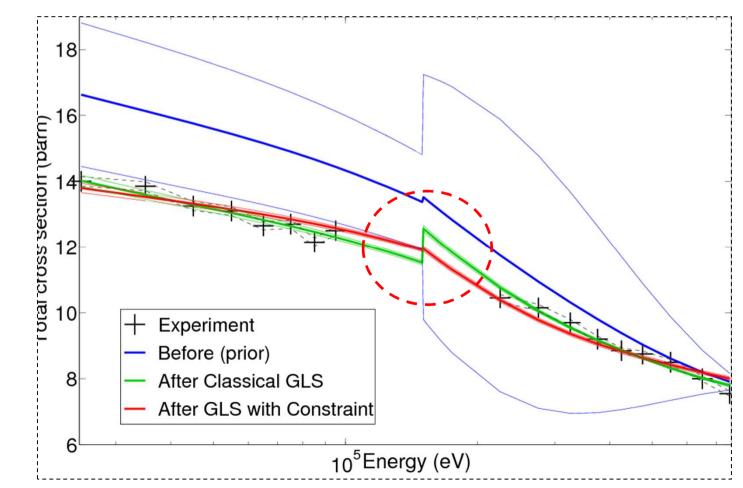
■ Toy Model URR/URR





IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS; 238U EXAMPLE

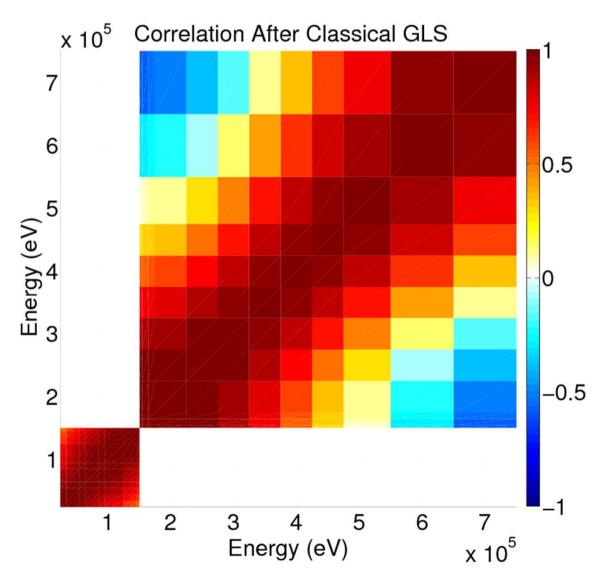
- Realistic Application URR/OM
- Parameters used :
 - Strength function (I=0,1); Distant level (I=0,1); Effective Radius
 - Reduce radius ; Diffusiveness





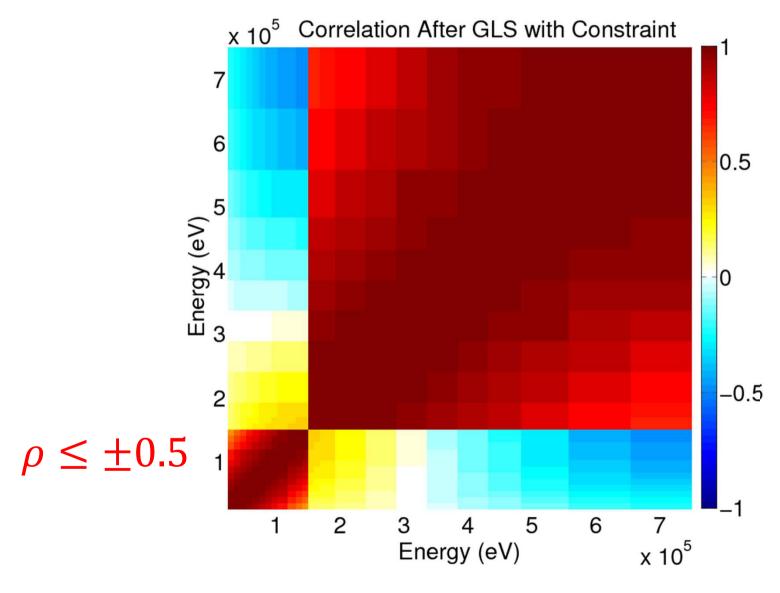
IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS; ²³⁸U EXAMPLE

Realistic Model URR/OM



IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS; 238U EXAMPLE

Realistic Model URR/OM





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 23Na (Jeff3.2)



DE LA RECHERCHE À L'INDUSTRIE



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



Matrices

www.cea.fr



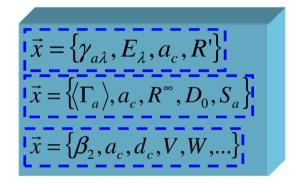
CONTRAINTS: INTEGRAL EXPERIMENTS

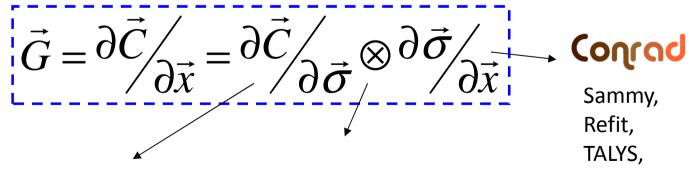
Data Assimilation framework for evaluation using integral experiments

$$\chi_{GSL}^{2} = (\vec{x} - \vec{x}_{m})^{T} M_{x}^{-1} (\vec{x} - \vec{x}_{m}) + (\vec{E} - \vec{C}(\sigma(\vec{x})))^{T} M_{E}^{-1} (\vec{E} - \vec{C}(\sigma(\vec{x})))$$

$$ec{y}
ightarrow ec{E}
ightarrow$$
 Intégrales Exp. $ec{\mathcal{X}}
ightarrow$

$$\vec{x} \rightarrow$$





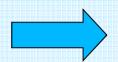
AP2/CRONOS2, ERANOS/PARIS, APOLLO3 MCNP, Tripoli-4

ND Treatment



INTEGRAL EXPERIMENTS

Validation and/or **DataAssimilation**



$$\vec{x} = \left\{ \gamma_{a\lambda}, E_{\lambda}, a_{c}, R', OMP, \ldots \right\}$$
 +BIASES

and/or
$$\sigma_g^r$$
 and $\chi_g, v...$ + 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 ($^{238}U(n,n')$)

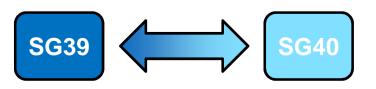
Take care of experimental correlation between ICSBEP series

Additional Integral Experiments □Irradiation Exp. PROFIL/MANTRA **□Oscillation Exp.** MINERVE/DIMPLE □....

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

Flexibility in terms of neutronic spectrum

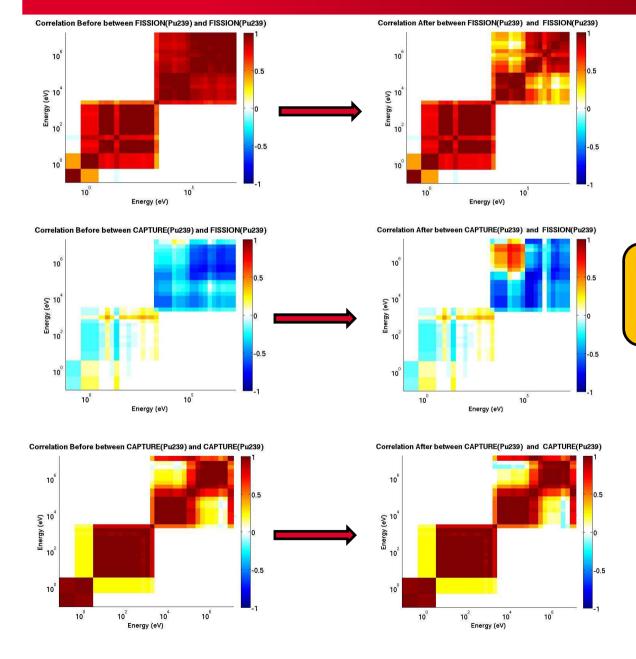
→ Deconvolution of energy domain

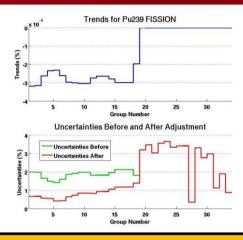






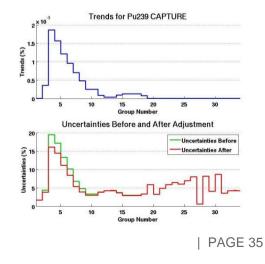
²³⁹PU COVARIANCE MATRICES





"Public" Integral Experiments

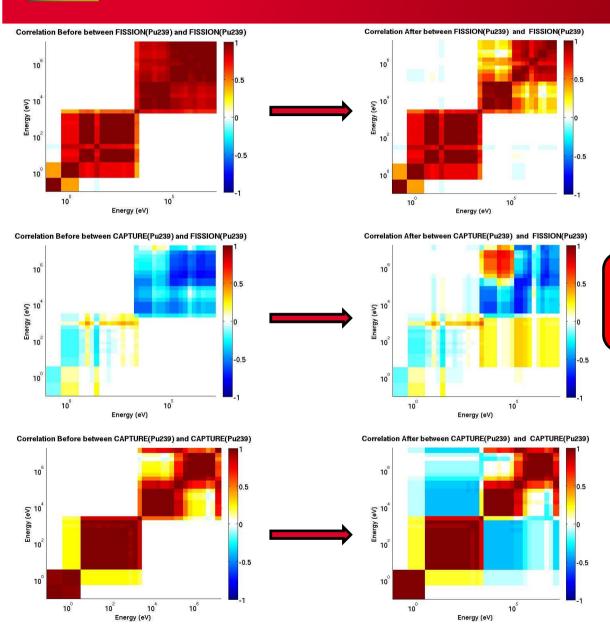
□ICSBEP (JEZEBEL)

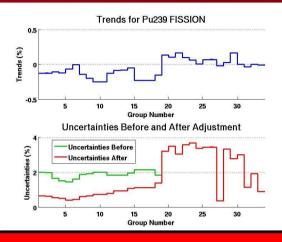




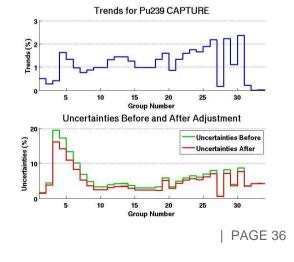


²³⁹PU COVARIANCE MATRICES



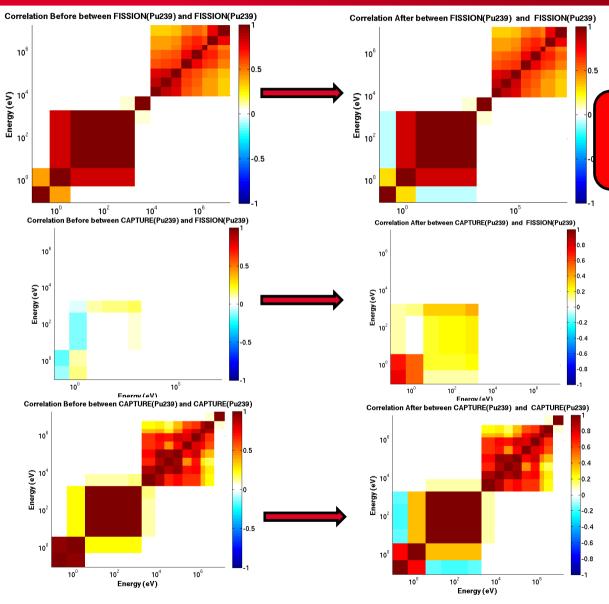


Additional Integral Experiments □PROFIL

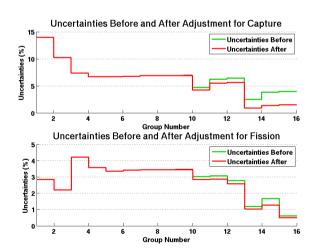








Additional Integral Experiments CERES Program in MINERVE/DIMPLE





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 →nuclear parameters are also be in the game (especially for thermal benchmarks; see NEMEA-5, C. De Saint Jean et al.) + on going work on PROFIL);
- 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 of reactivity, 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 \rightarrow "old" experiments, effect is diluted on several ND,.. etc



Sometimes true but CIELO and SG39 could give answers

□ 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 could allow progress on methodologies related to :
 - o Data assimilation for traditional evaluation
 - o Data assimilation for evaluation using specific integral experiments (IDA)
 - Data assimilation for evaluation with physical constraints
 - Systematic uncertainty constraints effect on several models
 - Lagrange multipliers in the cost function
 - •
 - 0

- \Box To understand discrepancies \rightarrow BENCHMARKS with sensitivity calculations
- □ To understand covariances methodologies → List a limited set of ingredients (exp., syst. Unce.,...) and do benchmarking (same inputs → compare results)
- □ To obtain first whole energy range covariances → list a less limited set of experiments (micro + integral) + model parameters + "new" methods +Codes?
- ☐ For CEA/Cadarache, files are not the finality; methods and understanding of discrepancies on evaluation and related covariances is the major interest
- Work on evaluation and covariances for Big 3 and Fe, O,