DE LA RECHERCHE À L'INDUSTRIE

# *From low to high energy nuclear data evaluations Issues and perspectives on nuclear reaction models and covariances*

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*With contributions of :*
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# State of the art of methodologies for Cross Section evaluation in the resonance range

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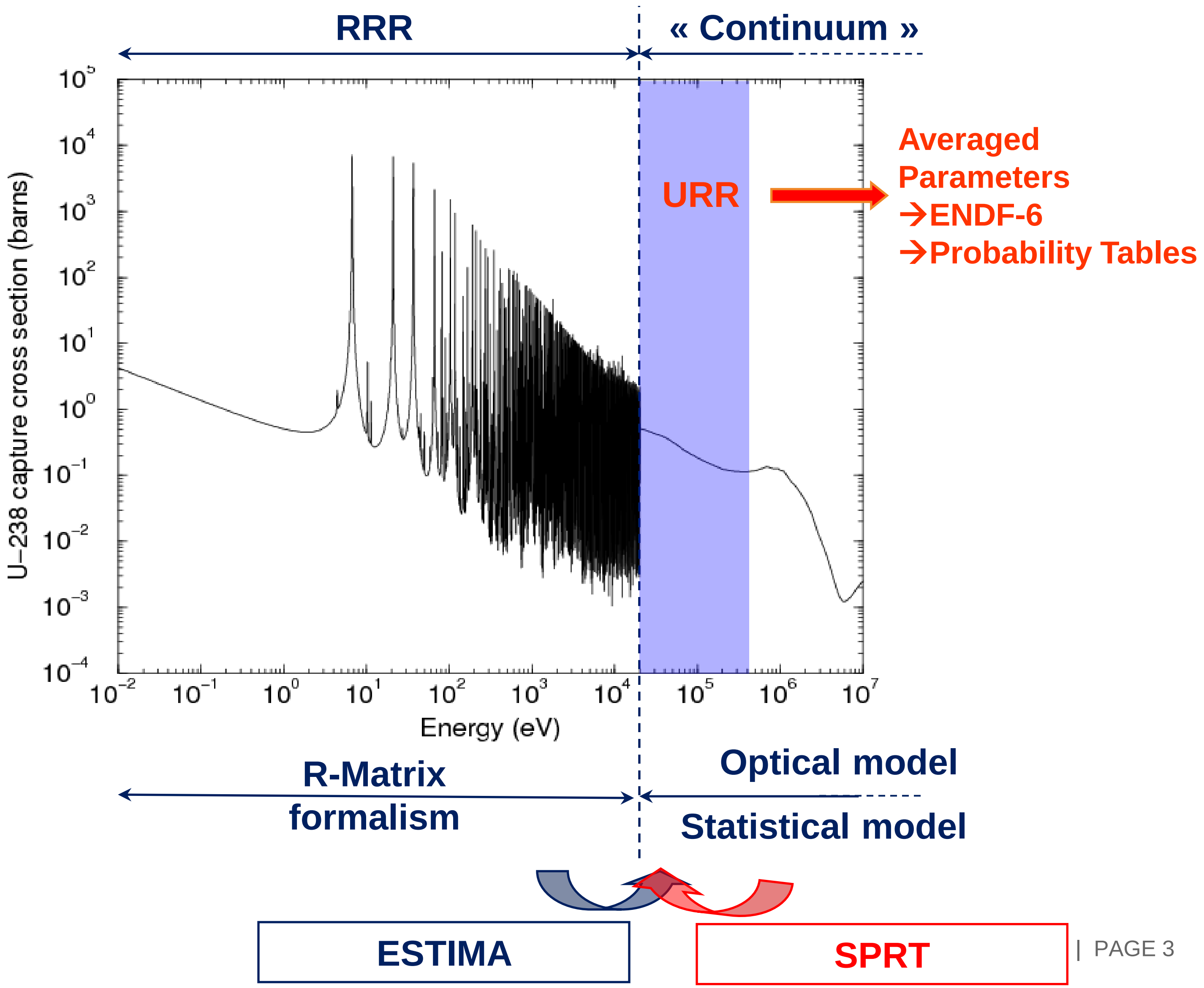
# General Actual Framework



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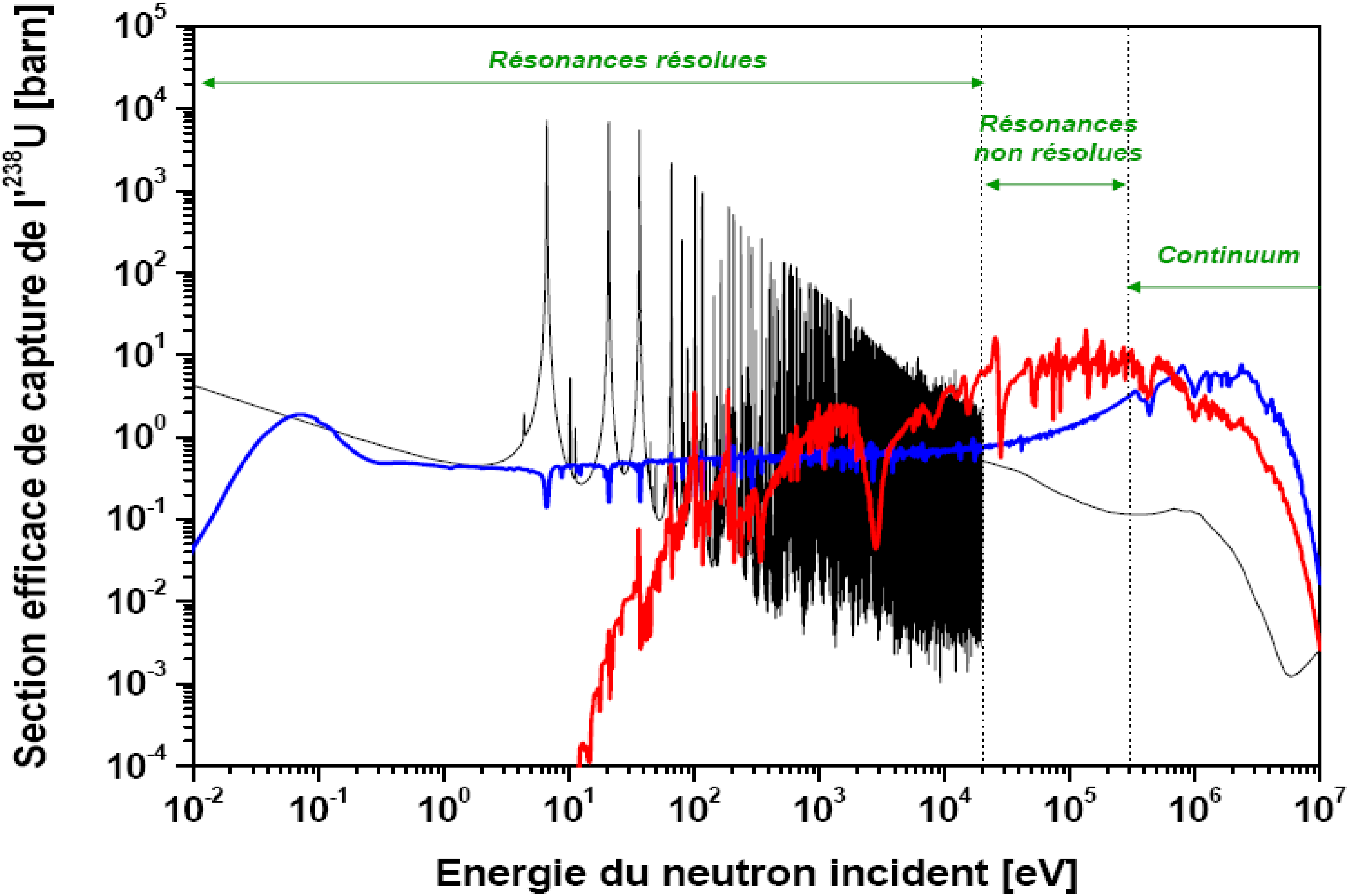
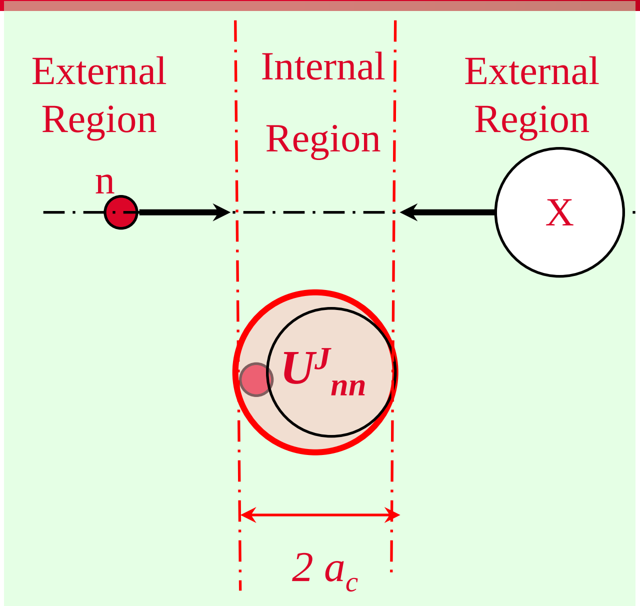


# General Actual Framework

- Reactor context :
  - PWR, BWR ; thermal and epithermal energy range
  - FR ; epithermal and fast range
  - Needs of reliable Uncertainties (not too optimistic/ not too pessimistic)

- Objectives/perspectives
  - Proper link between Resonance range and continuum
  - Take benefit of nuclear reaction models progress in high energy range
  - Increase physical contents of resonance parameters
  - Get rid of some “free” parameters
  - Find guidelines for new evaluation
  - Avoid compensations (Fresnel representation of Morillon)




## General Hypothesis

I. Non-relativistic Quantum Mechanics
II. Only process with two product nuclei
III. No processes of creation/destruction
IV. Channel c = $\{J^{\pi}, \alpha_1\alpha_2, \{q_i\}\}$
V. For r>$a_c$ (in configuration space) : V=V(r)

## Additional Considerations in RRR

A. Compound nucleus
B. Potential square well (Hard sphere)
C. Level Approximations (Breit-Wigner, Reich-Moore)
D. Fission ; Capture
E. Averaged R-Matrix →URR

## R-Matrix

$$R_{ab} = \sum_{\lambda} \frac{\gamma_{a\lambda} \times \gamma_{b\lambda}}{E - E_{\lambda}}$$

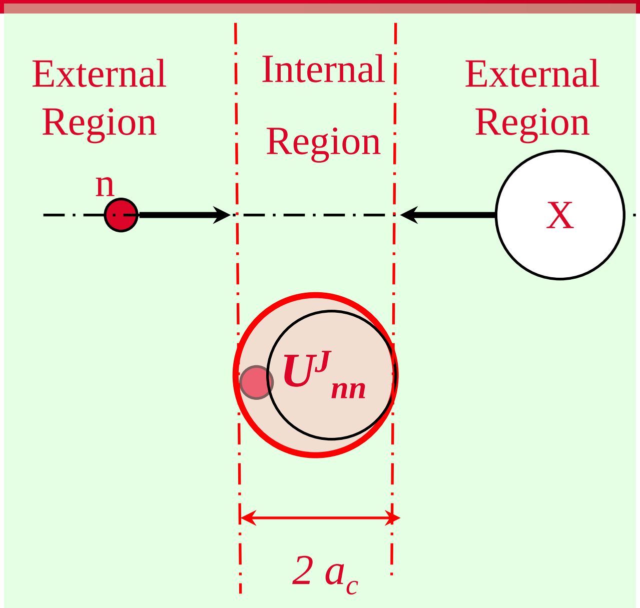
## Collision Matrix *

$$U_{ab} = e^{i(\Omega_a+\Omega_b)}(\delta_{ab}(1-2iP_a/L_a) + 2i\sqrt{P_a}(I-RL)^{-1}_{ab}\sqrt{P_b}/L_b)$$
$$= e^{i(\Omega_a+\Omega_b)}(\delta_{ab} + i\sum_{\lambda\lambda'}\Gamma^{1/2}_{\lambda a}\Gamma^{1/2}_{\lambda' b}A_{\lambda\lambda'})$$

where $\Gamma^{1/2}_{\lambda a} = (2P_a)^{1/2}\gamma_{a\lambda}$

and $(A_{\lambda\lambda'})^{-1} = (E_\lambda - E)\delta_{\lambda\lambda'} - \sum_a \gamma_{\lambda a} L^0_a \gamma_{\lambda' a}$

* Lane and Thomas for details : Rev. Mod. Phys. **30** (2) p.275 (1958)

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- ⊕ $\gamma$'s / $E_\lambda$ are real numbers independent of E + Physical Meaning of $\Gamma$'s
- ⊕ VERY SUCCESSFUL : $^{233\rightarrow 238}$U, $^{238\rightarrow 242}$Pu; $^{56}$Fe, $^{16}$O, $^{23}$Na, Fission products …etc
- ? ac is framing the resonance parameters ; Boundary Conditions ;
- ? RRR/URR/Continuum ; Averaged Parameters ; Link to Optical Model
- ? Modelling of Fission
- ? Uncertainties
- ? ……

We will present a few perspective that could be achieved in the future

- (+) $\gamma$'s / $E_\lambda$ are real numbers independent of E + Physical Meaning of $\Gamma$'s
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- (?) Modelling of Fission — 2 3
- (?) Uncertainties — 4 5 6
- (?) ……

We will present a few perspective that could be achieved in the future

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# Step Forwards for Cross Section evaluation in the resonance range

1

# What about Optical Potential in the Resonance range ?

## Collision Matrix

$$U_{ab} = e^{i(\Omega_a+\Omega_b)}(\delta_{ab} + i\sum_{\lambda\lambda'}\Gamma^{1/2}_{\lambda a}\Gamma^{1/2}_{\lambda' b}A_{\lambda\lambda'})$$ where $$\Gamma^{1/2}_{\lambda a} = (2P_a)^{1/2}\gamma_{a\lambda}$$

Penetrability is calculated via a potential square well for entrance channel (neutron most of the time) +Coulomb barrier for charged particles

→ Arbitrary choice of ac and several Boundary cond.

Effect of a **diffuse edge optical potential** ?*

→

$$\Gamma^{1/2}_{\lambda a} = (2P^{OM}_a)^{1/2}\gamma_{a\lambda}$$ Calculate Penetrability with Optical Potential

$$\Gamma^{1/2}_{\lambda a} = (2P^{SW}_a)^{1/2}\gamma_{a\lambda} f$$ Correction factor keeping Square Well*

$$\Gamma^{1/2}_{\lambda a} = (2P^{ESW}_a)^{1/2}\gamma_{a\lambda}$$ Equivalent Square Well →choice of proper ac

* Vogt for details : Rev. Mod. Phys. **34** (4) p.723 (1962)

# R-MATRIX WITH AVERAGE PHENOMENOLOGICAL POTENTIAL

## Collision Matrix

$$U_{ab} = e^{i(\Omega_a+\Omega_b)}(\delta_{ab} + i\sum_{\lambda\lambda'}\Gamma_{\lambda a}^{1/2}\Gamma_{\lambda' b}^{1/2}A_{\lambda\lambda'})$$ where $$\Gamma_{\lambda a}^{1/2} = (2P_a)^{1/2}\gamma_{a\lambda}$$

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1st Perspective

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## Averaged Collision Matrix (over a limited energy domain)

**Phase Shift**
**depends on $a_c$**

$$\overline{U}_c = e^{2i\phi_c} \frac{1 + iP_L \overline{R}_c^{\infty} - \dfrac{\pi S_c \sqrt{E} P_L}{2P_0}}{1 - iP_L \overline{R}_c^{\infty} + \dfrac{\pi S_c \sqrt{E} P_L}{2P_0}}$$

**Penetrability**
**depends on $a_c$**

**No direct reaction contributions considered here (absorption)**

In R-Matrix ; ac is arbitrary
Choose to give ac a proper physical interpretation using models coming from high energy

# Choice of channel radius $a_c$

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## Forward : from OM to R-Matrix

Choose $a_c$ using phase shift $\phi_c$ coming from optical model calculations

# Choice of channel radius $a_c$

## Forward : from OM to R-Matrix

**Choose $a_c$ using phase shift $\phi_c$ coming from optical model calculations**

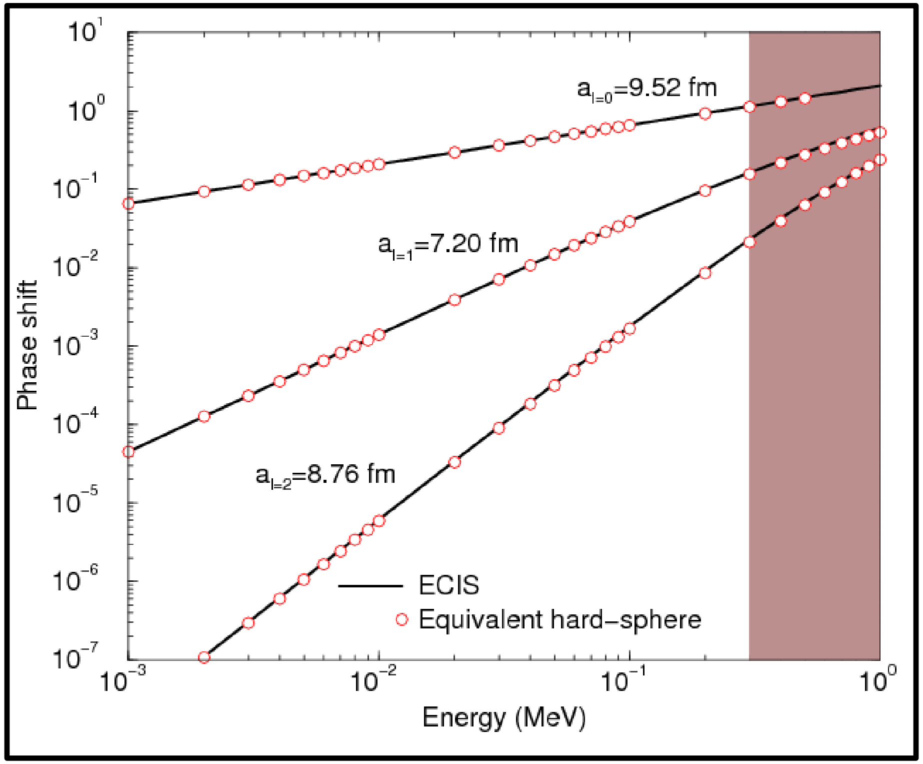
$$\begin{cases} \phi_0(\rho) = \rho \\ \phi_1(\rho) = \rho - \tan^{-1}(\rho) \\ \phi_2(\rho) = \rho - \tan^{-1}\left(\dfrac{3\rho}{3-\rho^2}\right) \end{cases}$$

$$\rho = k a_c$$

# Choice of channel radius $a_c$

## Forward : from OM to R-Matrix

**Choose $a_c$ using phase shift $\phi_c$ coming from optical model calculations**



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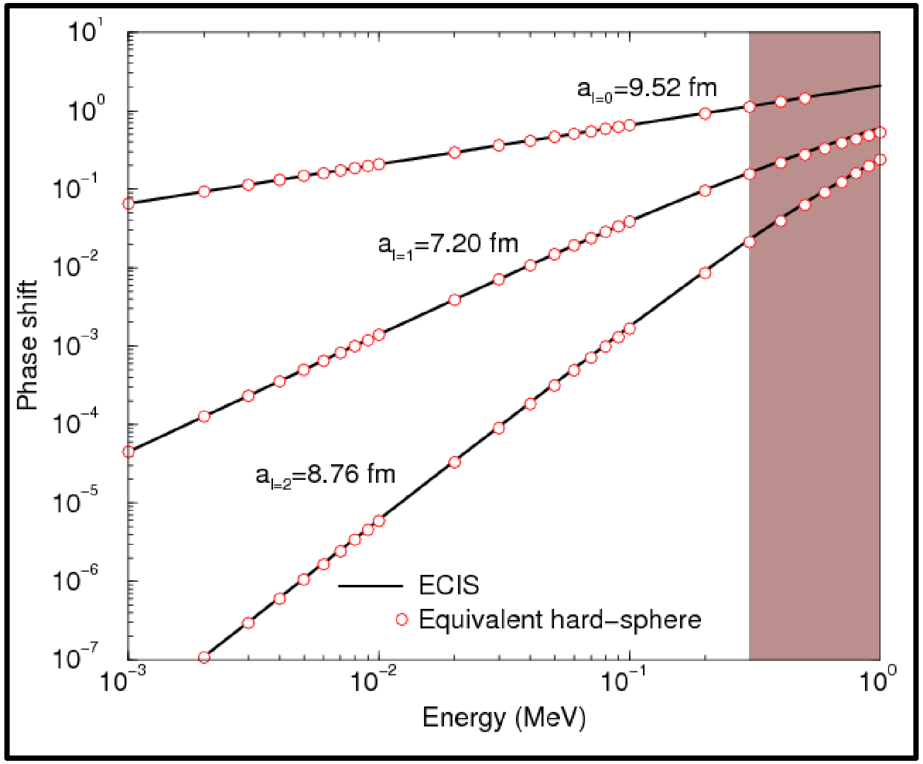


**Backward →Verify ac choice with transmission factor $T_c$**

$$T_c = 1 - \left|\overline{U}_c\right|^2 \longrightarrow T_c \approx 4\pi P_L s_c$$

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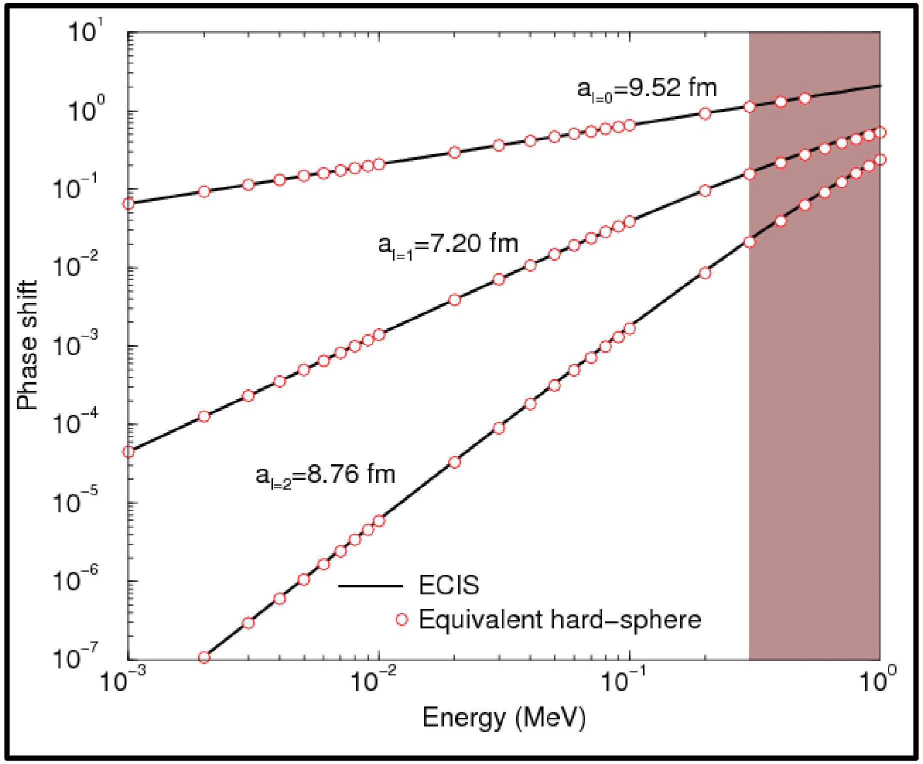


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$$\begin{cases} P_0(\rho) = \rho \\ P_1(\rho) = \dfrac{\rho^3}{1+\rho^2} \\ P_2(\rho) = \dfrac{\rho^5}{9+3\rho^2+\rho^4} \end{cases}$$

$$\rho = k a_c$$

$$P \Rightarrow P^{ESW}$$

# Choice of channel radius $a_c$

$^{241}Am+n$

**Forward : from OM to R-Matrix**

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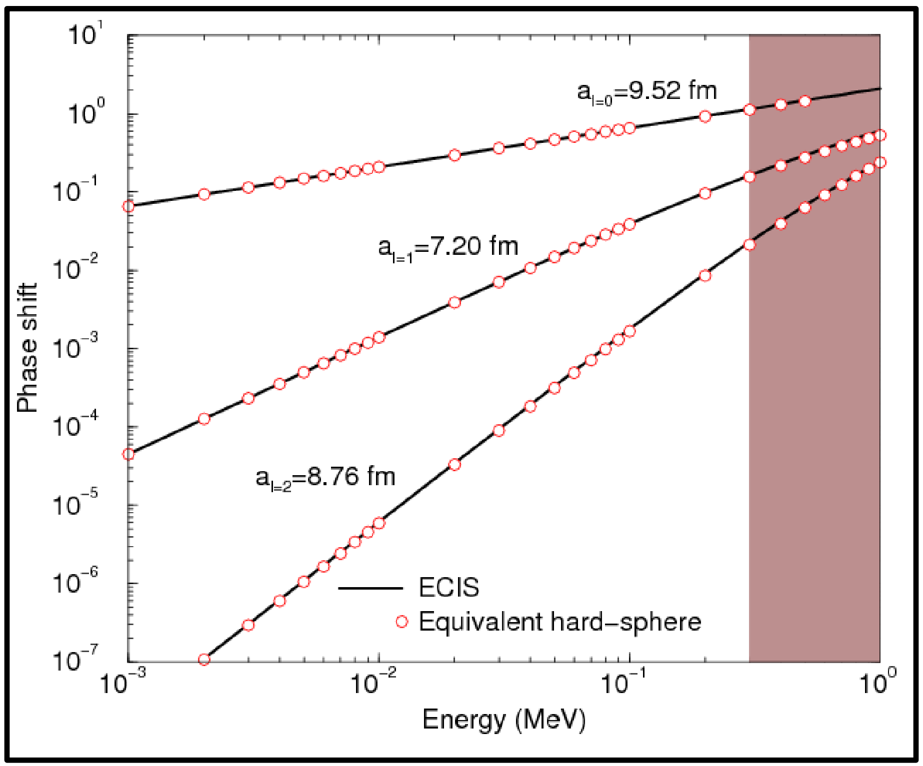


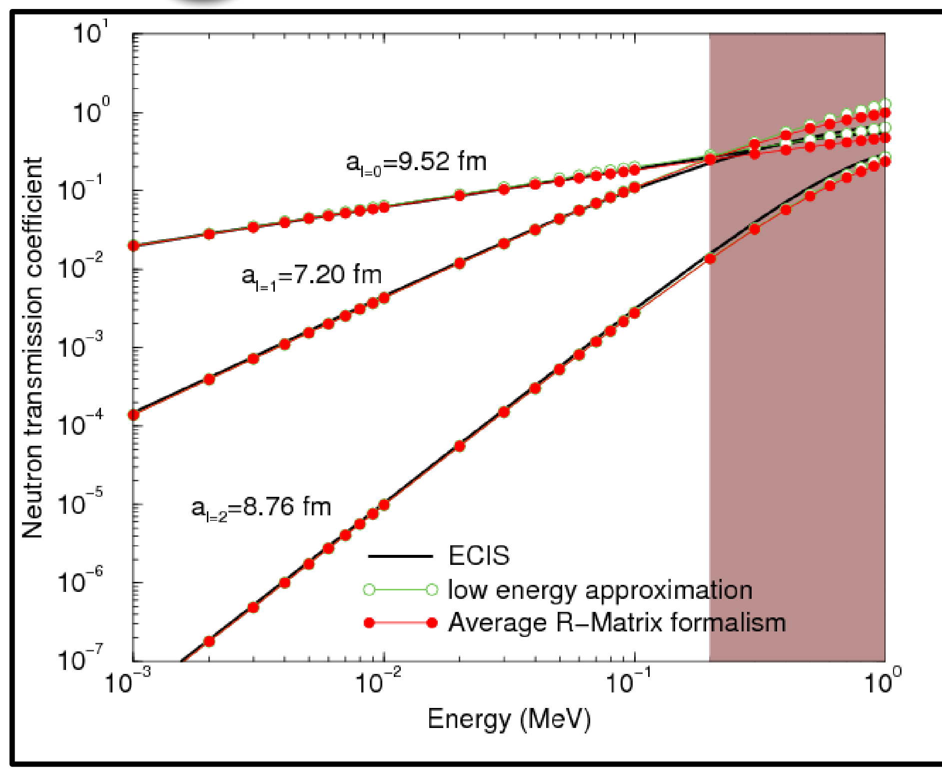

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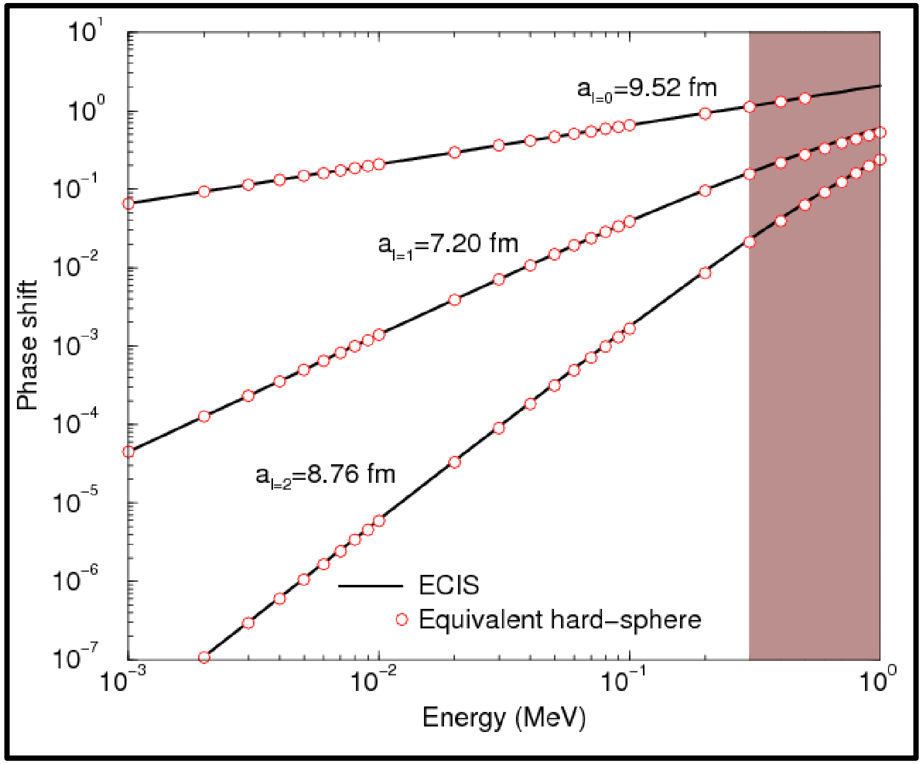
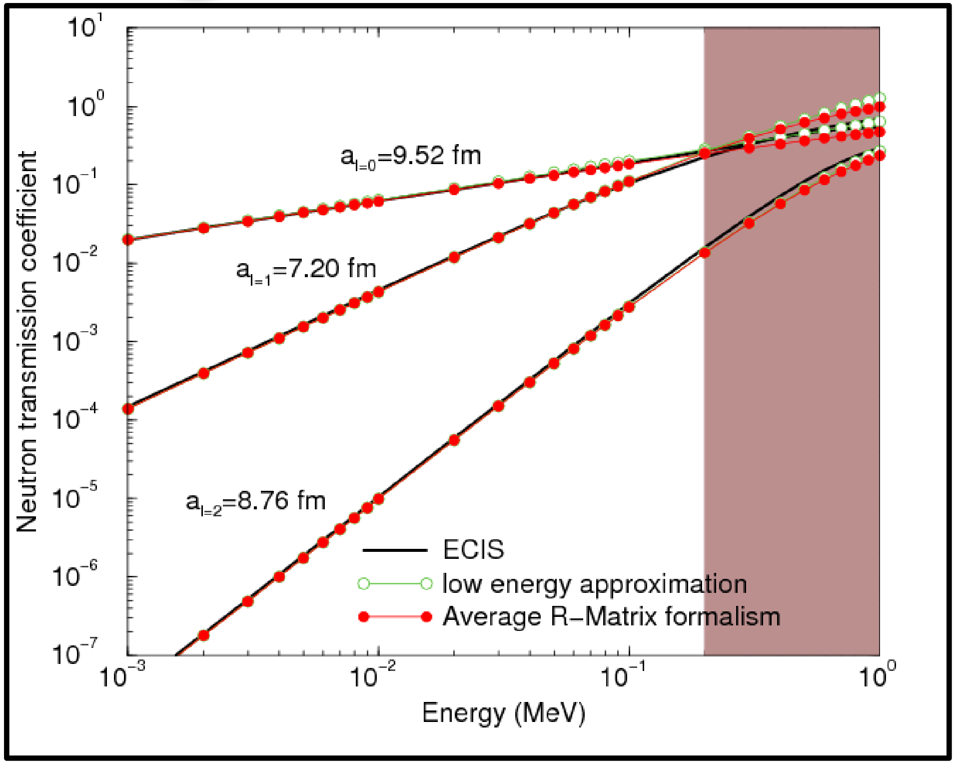



⇒ **Very good agreement between ECIS and « hard sphere » up to 200-300 keV**

⇒ **Different ac for different orbital momenta**

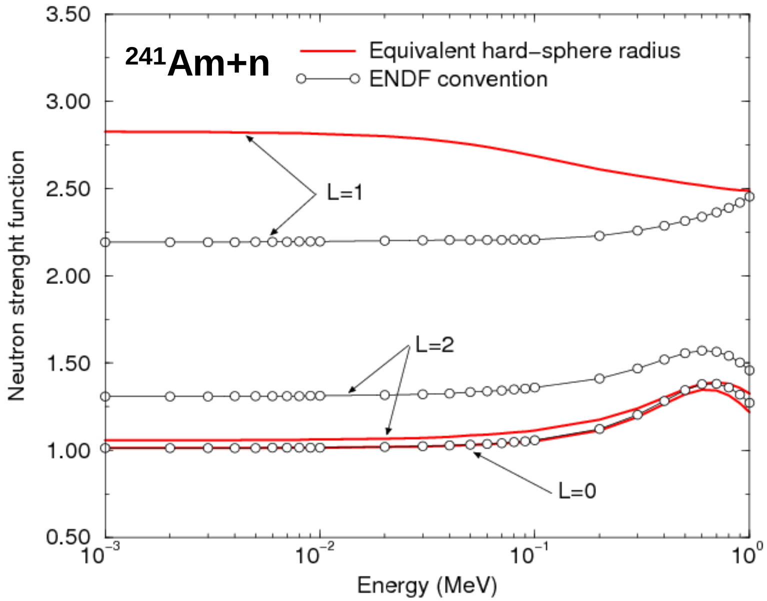
# Find Strenght functions and $R^\infty$ with SPRT*

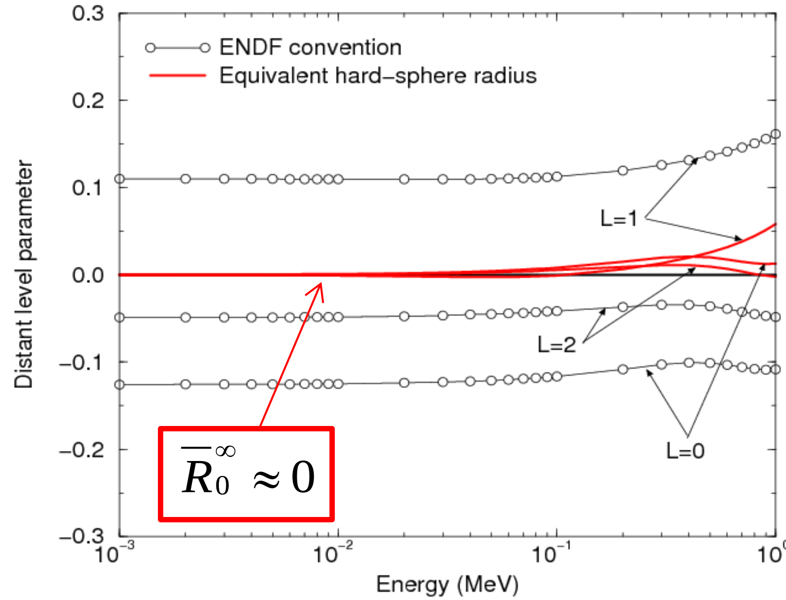
Equivalent hard-sphere radius ac comming from $\phi_c$

$a_0$=9.52 fm
$a_1$=7.20 fm
$a_2$=8.76 fm

$a_0$=8.46 fm
$a_1$=8.46 fm
$a_2$=8.46 fm

Convention ENDF-6




Confirmation of empirical rule (F. Frohner, O. Bouland, NSE, 2001) **$S_0 \approx S_2 \approx$cst**

$\overline{R}_0^\infty \approx 0$ $\Rightarrow$ **Effective Radius R' equal to channel radius (Averaged R-Matrix formalism)**

$$\sigma_p = \lim_{E \to 0} \sigma_{e_c}(E) = 4\pi R'^2 \qquad R' = a_0(1 - \overline{R}_0^\infty) \Rightarrow R' \approx a_0$$

*Delaroche et Lagrange (IAEA-190, 1976)
*E.Rich et al. NSE, **162** (2009) 76-86

# Apply equivalent methods to Resolved Resonance range

**Phase Shift** **depends on $a_c$**

$$U_{ab} = e^{i(\Omega_a+\Omega_b)}(\delta_{ab} + i\sum_{\lambda\lambda'}\Gamma_{\lambda a}^{1/2}\Gamma_{\lambda' b}^{1/2}A_{\lambda\lambda'})$$

$$\Gamma_{\lambda a}^{1/2} = (2P_a)^{1/2}\gamma_{a\lambda}$$

**Penetrability** **depends on $a_c$**

1st Perspective
Benefit from any phenomenological or microscopic models

In R-Matrix ; ac is arbitrary
Choose to give ac a proper physical interpretation using models coming from high energy

Allow a coherent treatment from 0eV to 20 MeV for penetrability and various radius
Amplitude with more physics →Statistics

Fertile nuclei ok ; What about fissile nuclei ?

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# Step Forwards for Cross Section evaluation in the resonance range

2 3

## What about Fission in the Resonance Range?

# FISSION

In the Unresolved resonance range and Continuum

Fission Barriers calculations used for

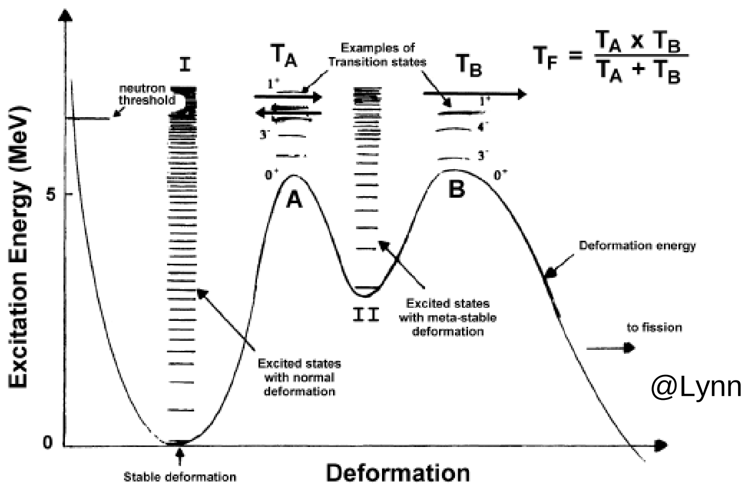
Transmission coefficient

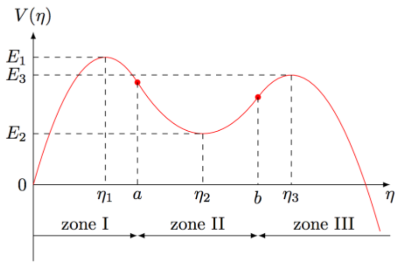
$$\sigma_{n,f} = \frac{\pi}{k^2}\frac{T_n \cdot T_f}{T}W_{nf}$$

+ Fission ingredients

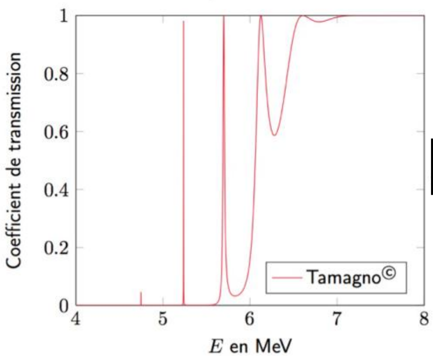
(J,K, Rotational band, class II, etc …)

**Fission barriers calculation in the Resolved Resonance Range ?**

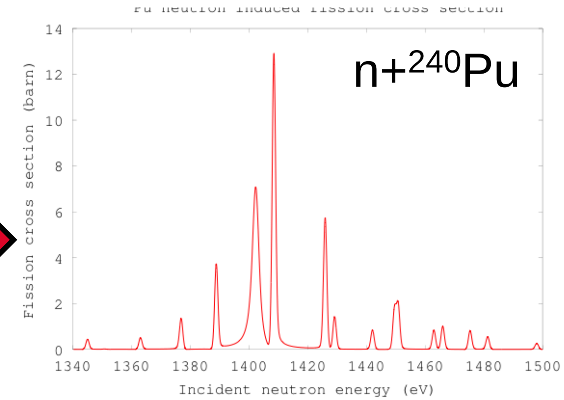


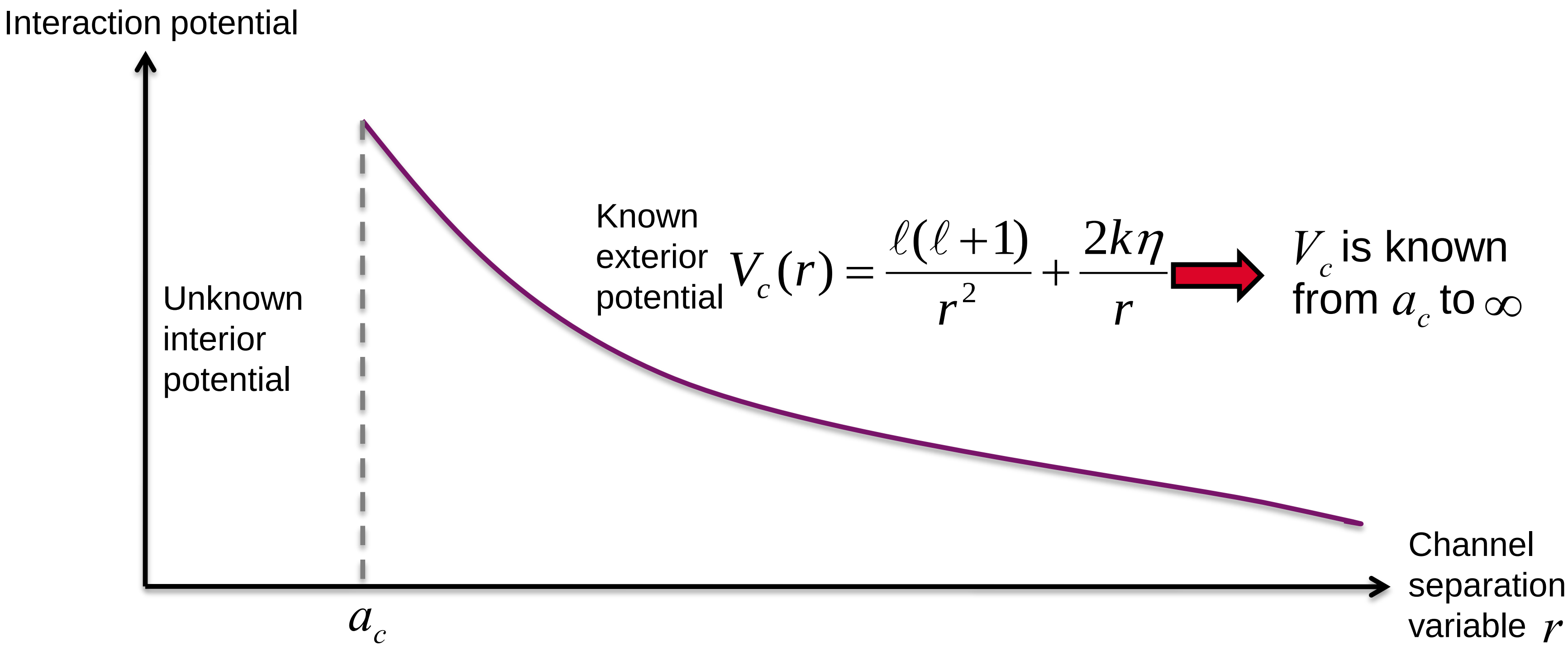

Simple Cramer-Nix Barrier




?



# R-MATRIX WAS IS MAINLY DEDICATED TO PARTICLE CHANNEL




The exterior Schrödinger equation $\left[\hat{T}_c + \hat{V}_c\right]\varphi_c = E\varphi_c$ is solved $\varphi_c = \left(G_c + F_c\right)e^{i\omega_c}$

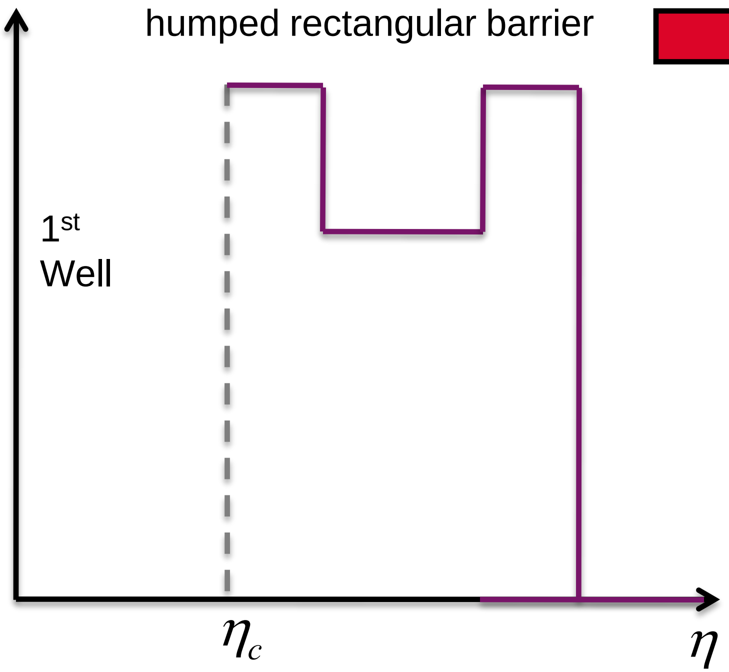
$P_c$ and $S_c$ are defined from $\varphi_c$ and evaluated at $r = a_c$, statistics can be done on $E_\lambda, \gamma_{\lambda c}$

$$S_c + iP_c = \left[\frac{r_c}{\varphi_c}\frac{\partial \varphi_c}{\partial r_c}\right]_{r_c = a_c}$$

Is a similar approach possible for fission?

$V^{(\mu)}(\eta)$ ; $\eta$ characterizes a collective fission coordinate (e.g. $Q_2$, $ß_2$, …)

Parameterized double-humped rectangular barrier




Numerical solution of $\varphi_\mu$ two information can be extracted:

•Probability current and transmission coefficient

$$\vec{j} = \frac{\hbar}{2iB(\mu)}\left[\varphi_\mu^* \vec{\nabla} \varphi_\mu - \varphi_\mu \vec{\nabla} \varphi_\mu^*\right]$$

$$T(E) = \left|\frac{\vec{j}_{\text{right}}}{\vec{j}_{\text{left}}}\right|^2$$

High energy (Hauser-Feshbach)

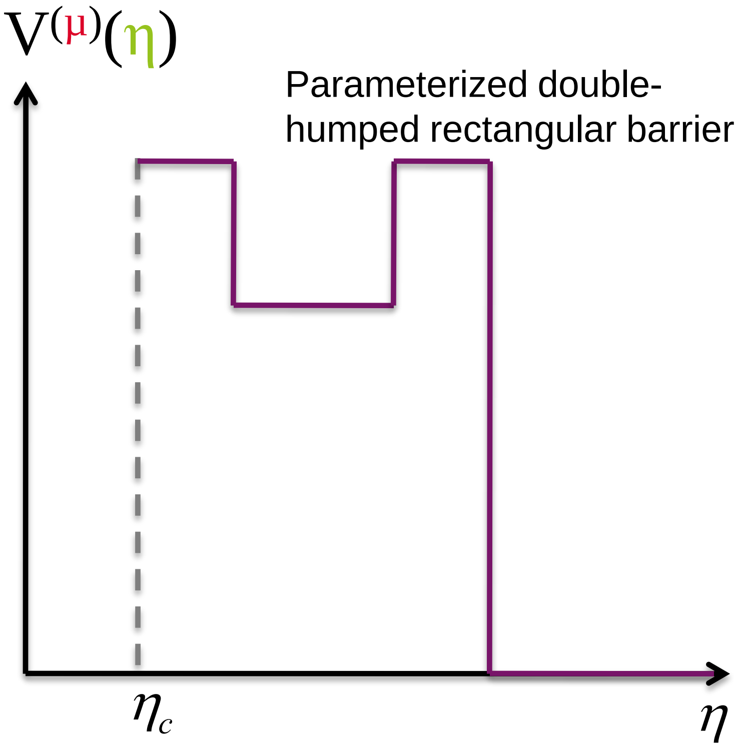
Low energy (R-Matrix)

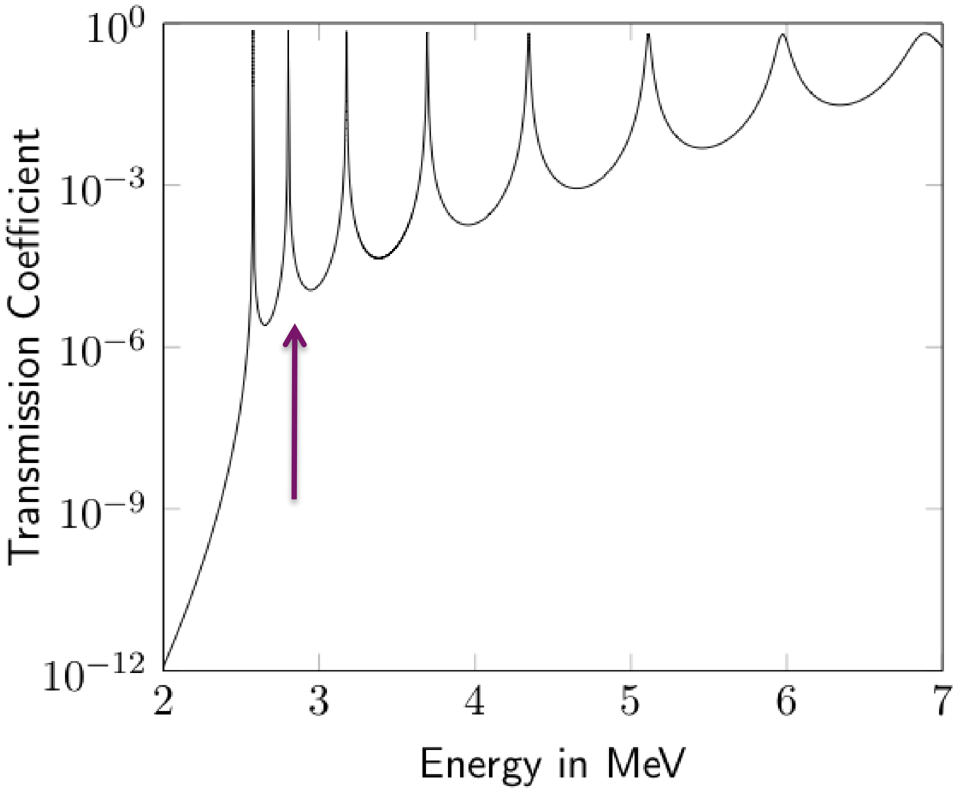
•Shift and penetration factors

$$S^{(\mu)} + iP^{(\mu)} = \left[\frac{1}{f\varphi_\mu}\frac{\partial(f\varphi_\mu)}{\partial\eta}\right]_{\eta=\eta_c}$$

* Lynn for details : J. Phys. A. : Math. Nucl. Gen. **6** p.542 (1973)

# EXAMPLE OF EXPLICIT TREATMENT OF THE FISSION BARRIER



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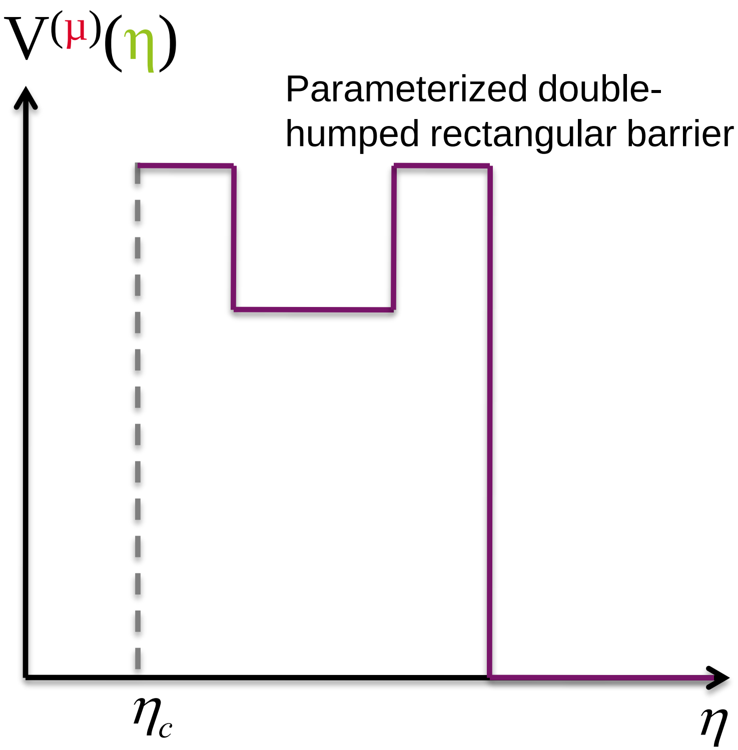


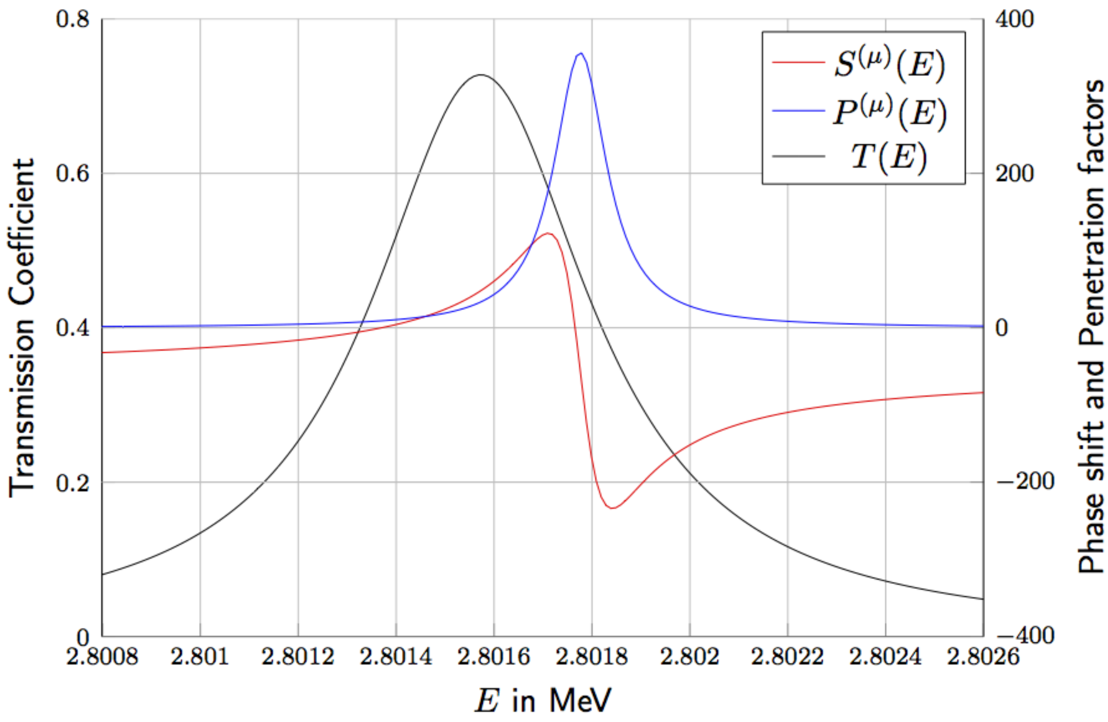

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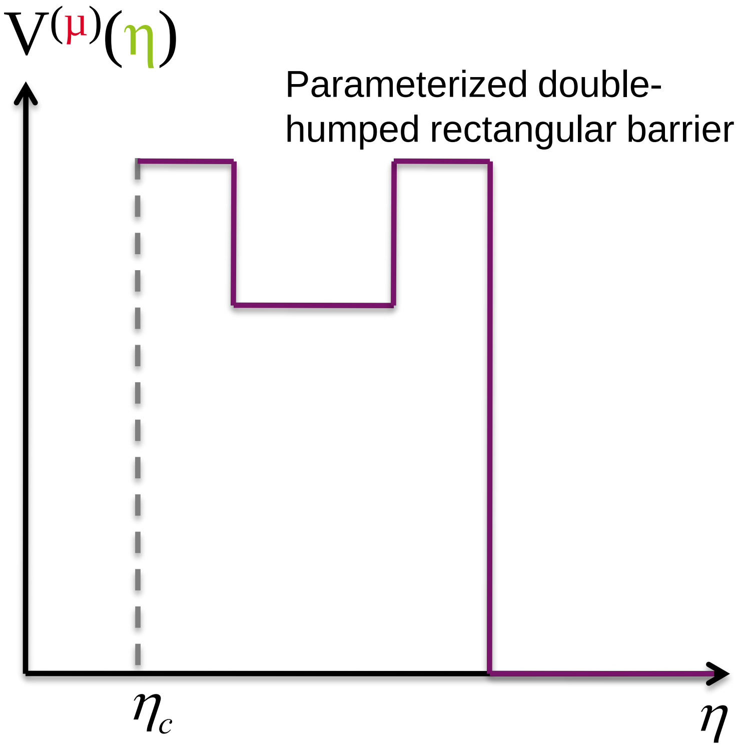
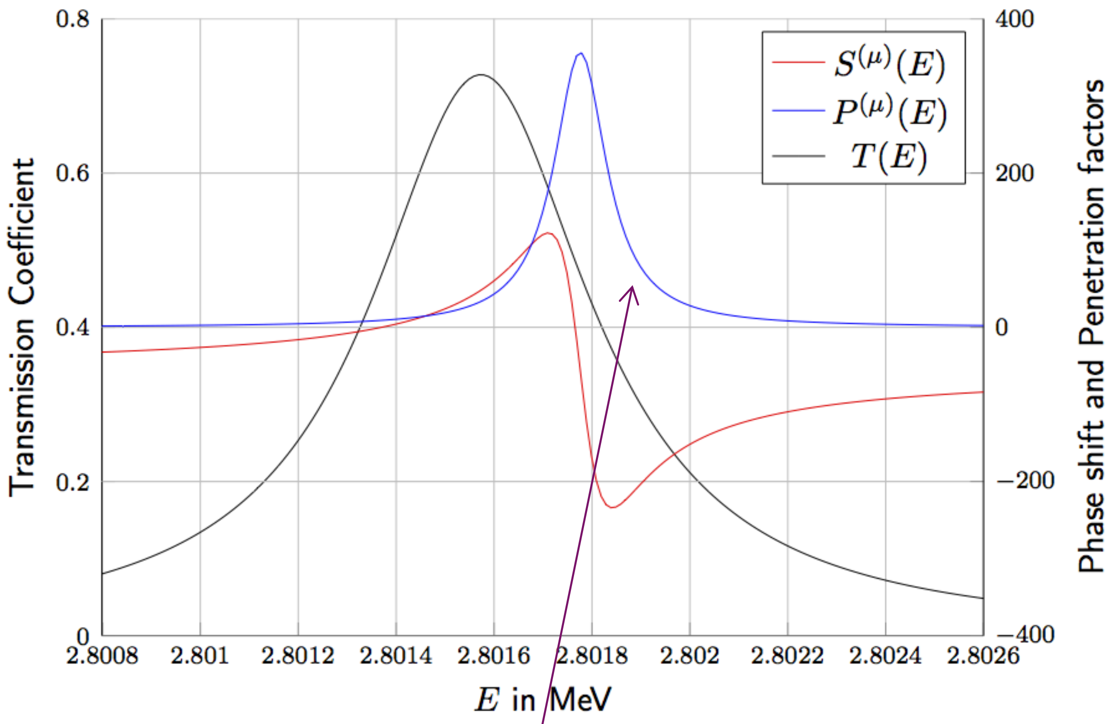
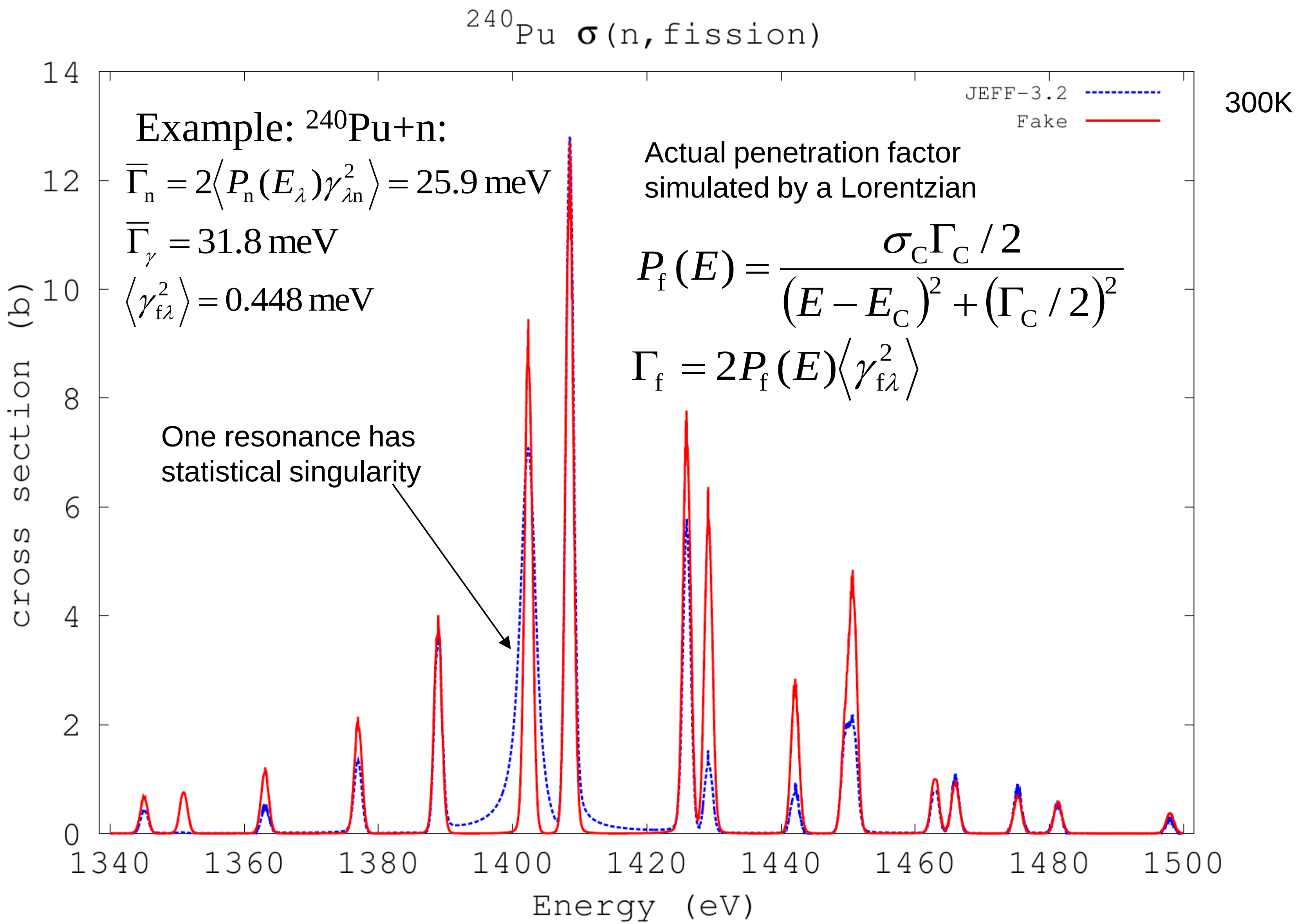



2nd Perspective ⇒

$$\Gamma_{\lambda a}^{1/2} = \left(2P_a\right)^{1/2} \gamma_{a\lambda}$$

# EXAMPLE OF EXPLICIT TREATMENT OF THE FISSION BARRIER




$$\overline{\Gamma}_n = 2\langle P_n(E_\lambda)\gamma^2_{\lambda n}\rangle = 25.9\,\text{meV}$$

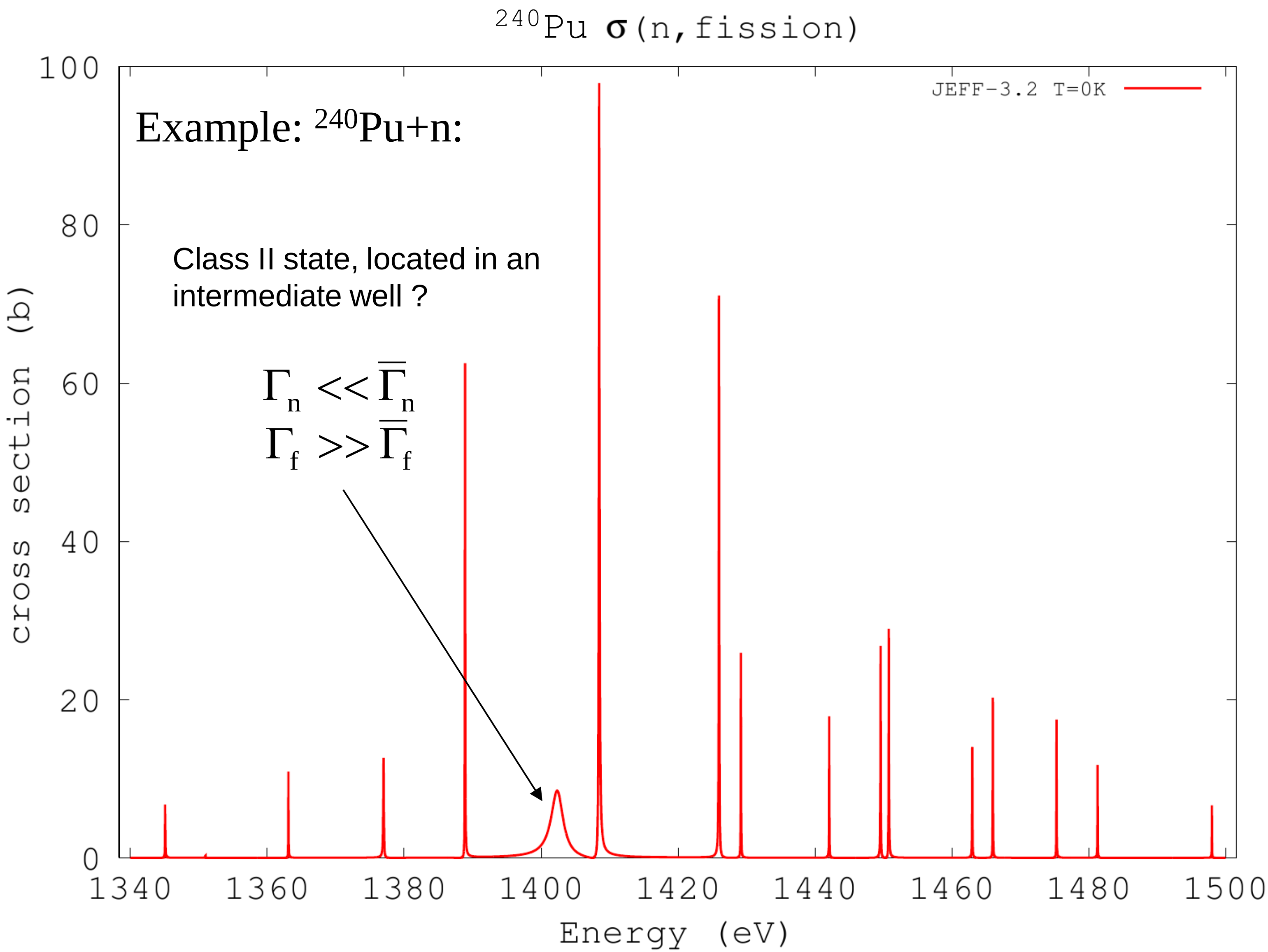
$$\overline{\Gamma}_\gamma = 31.8\,\text{meV}$$

$$\langle \gamma^2_{f\lambda}\rangle = 0.448\,\text{meV}$$

$$P_f(E) = \frac{\sigma_C \Gamma_C / 2}{(E - E_C)^2 + (\Gamma_C/2)^2}$$

$$\Gamma_f = 2P_f(E)\langle \gamma^2_{f\lambda}\rangle$$

# EXAMPLE OF EXPLICIT TREATMENT OF THE FISSION BARRIER



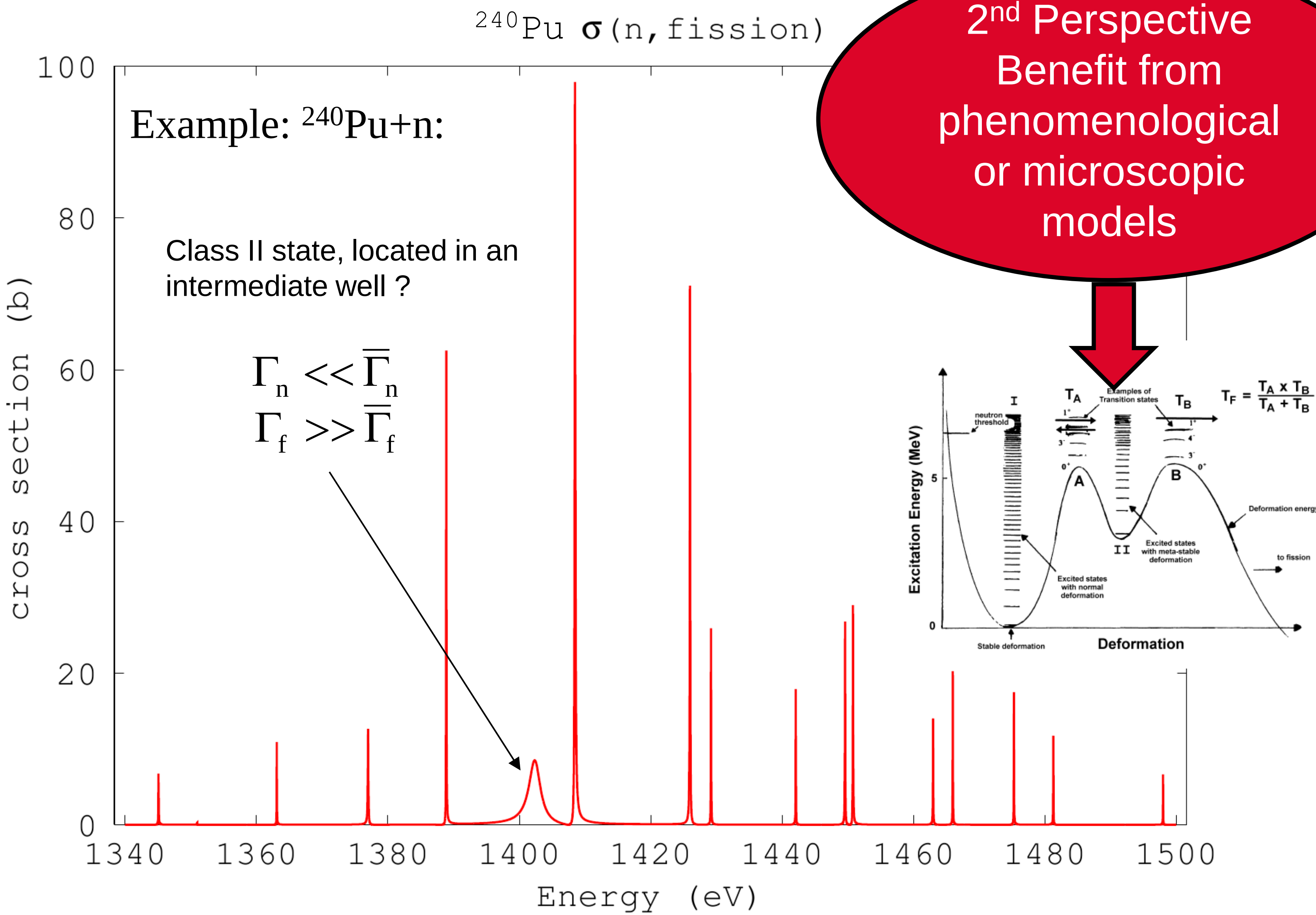
# EXAMPLE OF EXPLICIT TREATMENT OF THE FISSION BARRIER

2nd Perspective
Benefit from phenomenological or microscopic models

Example: $^{240}$Pu+n:

Class II state, located in an intermediate well ?

$$\Gamma_n << \overline{\Gamma}_n$$
$$\Gamma_f >> \overline{\Gamma}_f$$



# FISSION ANALYSIS IN RESOLVED RESONANCE RANGE TOWARDS BETTER EVALUATION OF FISSION WIDTHS

Generic issues for defining fission channels:
Reich-Moore allows a good description of fission
→For Heavy Nuclei ; 1 radiative capture channel with $\Gamma_\gamma$~constant
Hypothesis: many photons interferences cancel out

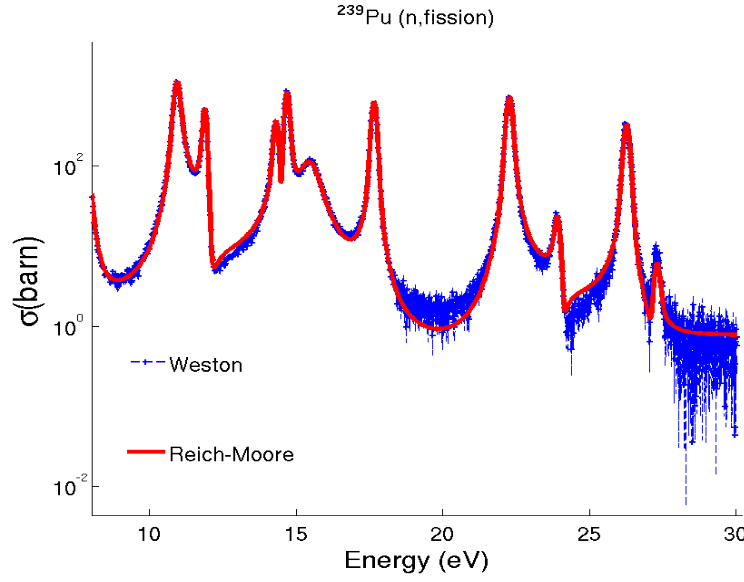
$$\left(A_{\lambda\lambda'}\right)^{-1} = \left(E_\lambda - E\right)\delta_{\lambda\lambda'} - \sum_a \gamma_{\lambda a} L_a^0 \gamma_{\lambda' a} \xrightarrow{\text{Reich-Moore}} \left(A_{\lambda\lambda'}\right)^{-1} = \left(E_\lambda - E - i\Gamma_{\lambda,\gamma tot}/2\right)\delta_{\lambda\lambda'} - \sum_{a\neq\gamma} \gamma_{\lambda a} L_a^0 \gamma_{\lambda' a}$$

$$R_{ab} = \sum_\lambda \frac{\gamma_{a\lambda} \times \gamma_{b\lambda}}{E - E_\lambda} \rightarrow R_{ab} = \sum_\lambda \frac{\gamma_{a\lambda} \times \gamma_{b\lambda}}{E - E_\lambda - i\Gamma_{\lambda,\gamma tot}/2}$$

→Fission channels allow fission interference
→No fundamental physical meaning
→$^{239}$Pu

$0^+$→ 2 Fission channels
$1^+$→ 1 Fission channel

→Statistics ? ; $\nu_{eff}$ ??? ; (n,γf) process ?



# FISSION ANALYSIS IN RESOLVED RESONANCE RANGE TOWARDS BETTER EVALUATION OF FISSION WIDTHS

Use an additional quantum number* → K (proj. of J on the fission axis)

Fission channels defined by $c_{f,K} = \{J^\pi, \text{fission}, \{K\}\}$ → $\Gamma_{cf,K}$

$$\sigma_{n,f}(E) = \sum_{J^\pi} \sigma_{n,f}^{J^\pi}(E) = \sum_{J^\pi,K} \sigma_{n,f}^{J^\pi,K}(E)$$

**Need of new experiments:**

- Polarized neutron/target
- Angular Distribution of F.F.

**Development in Analysis codes:**

- Polarized neutron/target
- K contributions
- Angular Distribution of fission fragments

**For $^{235}U$ :**

**some experiments**

N.J. Pattenden et al.; Nucl. Phys. A **167** (1971)

G.A. Keyworth et al.;Conf. On nuclear cross section and technology, Washington D.C., USA, NBS Special Publication 425 (1975) p.576

**few evaluations**

M.S. Moore, L.C. Leal, et al., Nulc. Phys. A **502** (1989)

**Evaluation in Resonance Range**

Disentangle fission channels

Evaluation of J, K and $\Gamma_{cf,K}$

* W.I. Furman: FJ/OH Spring Session'99, Neutron data measurements & evaluation May 17 **1999**, Geel

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3rd Perspective : 3.1

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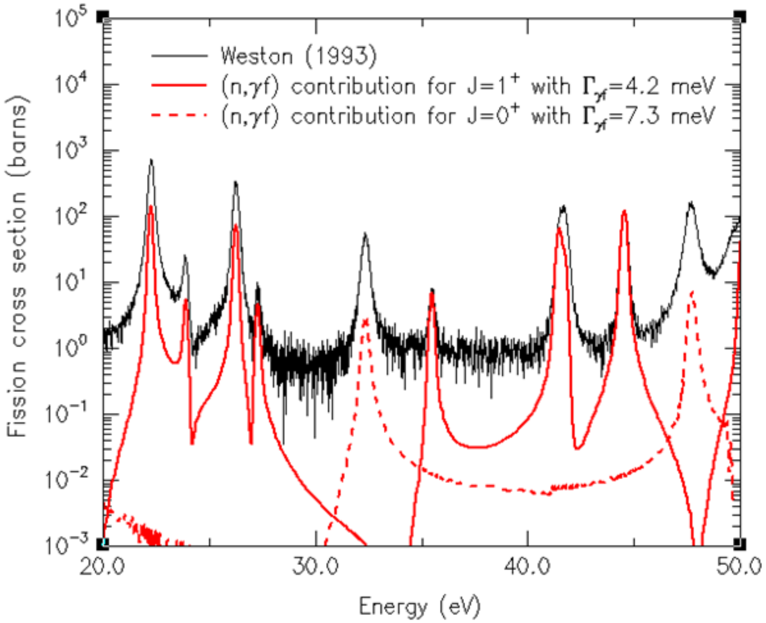
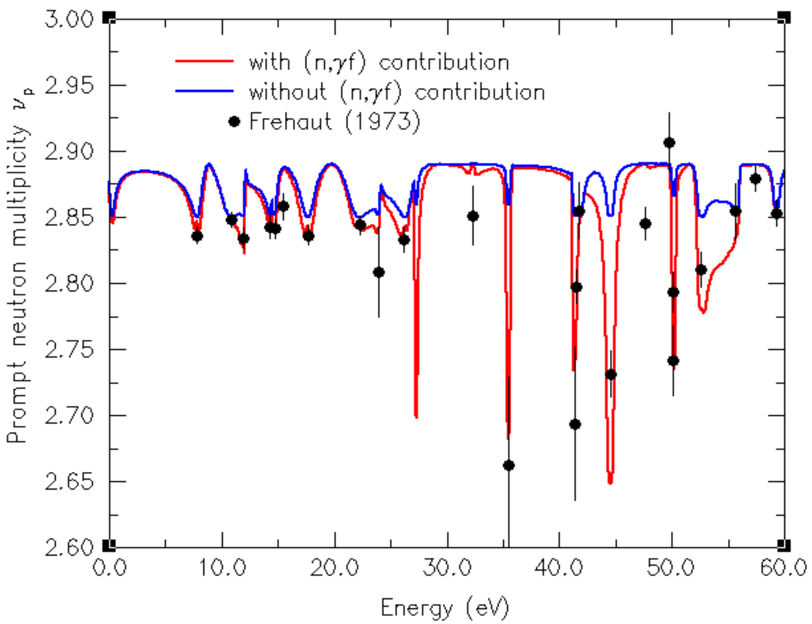
# FISSION ANALYSIS IN RESOLVED RESONANCE RANGE TOWARDS BETTER EVALUATION OF FISSION WIDTHS

Investigation of the two-step (n,γf) process*

- Still a topic of discussion
- No direct measurements of this reaction → challenge
- WPEC/SG34 provides some recent explanations for $^{239}$Pu




- Future evaluation artworks on $^{239}$Pu and others → include explicitly the two-step (n,γf) reaction (additional dedicated partial reaction width, $\Gamma_{\gamma f}$); usual fitted fission width becoming clear →one-step fission component only.

* E. Lynn, Rev. Mod. Phys. **52** (1980)

# FISSION ANALYSIS IN RESOLVED RESONANCE RANGE TOWARDS BETTER EVALUATION OF FISSION WIDTHS

3rd Perspective: 3.2

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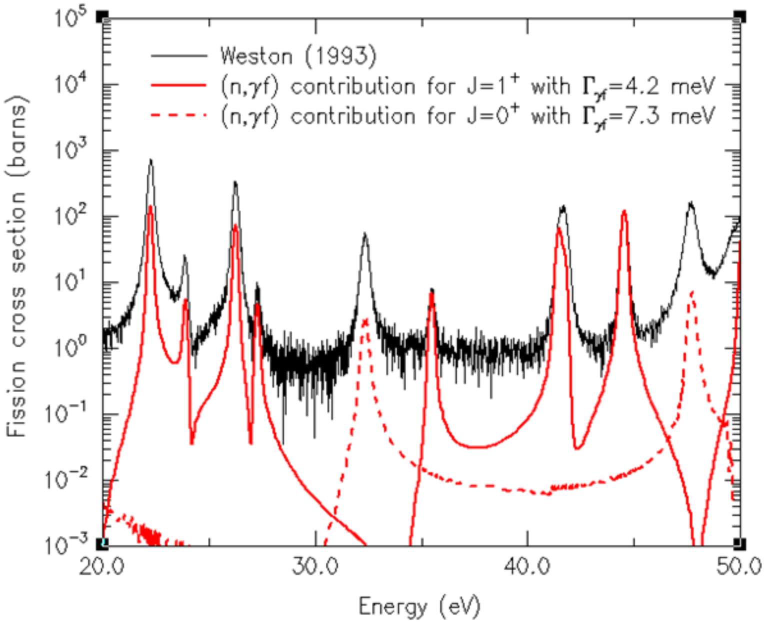


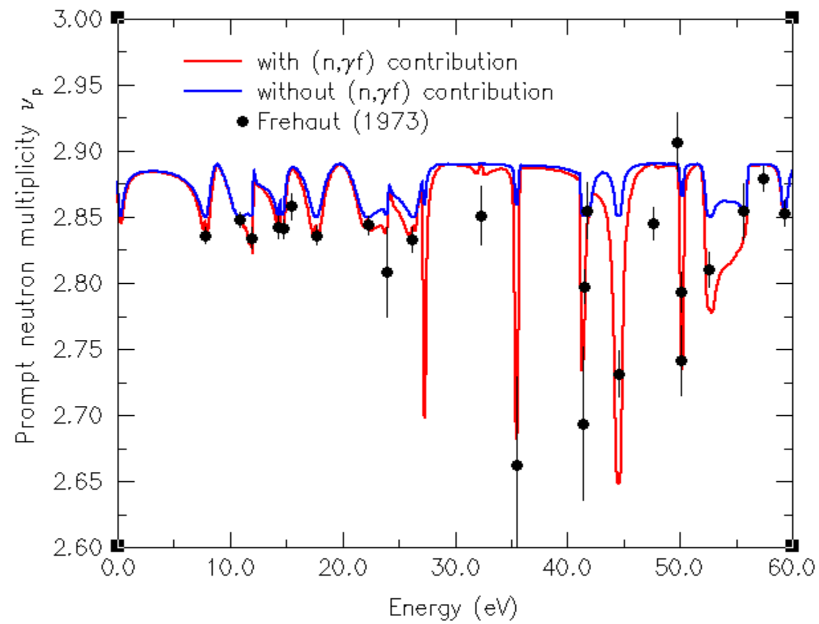


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DE LA RECHERCHE À L'INDUSTRIE

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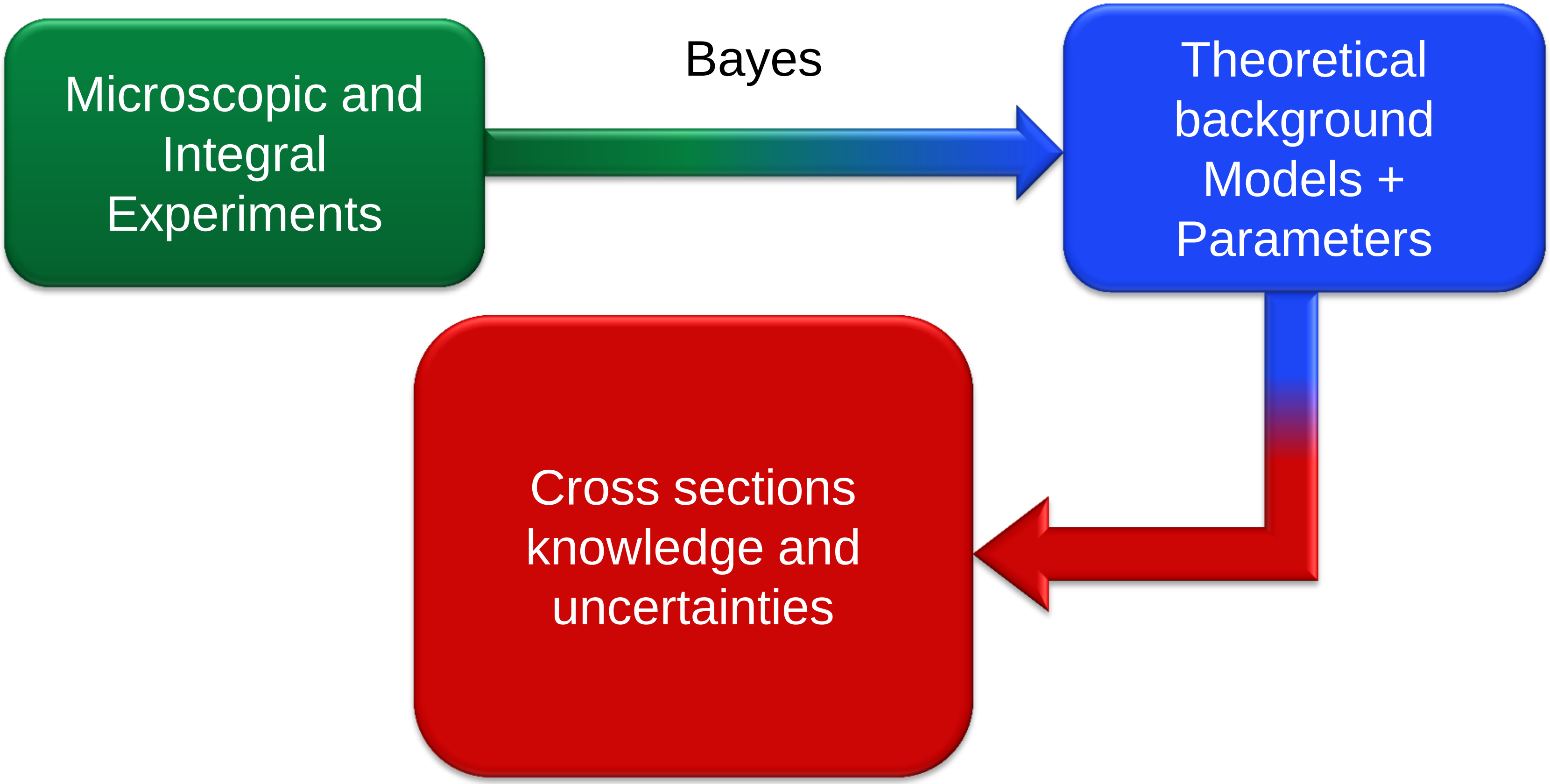
# Step Forwards for Cross Section evaluation in the resonance range

4 5 6

# What about Uncertainties from the Resonance Range to the Continuum?

# CROSS SECTIONS "KNOWLEDGE" EVALUATION IN THE RESONANCE RANGE AND HIGHER




**Issues** :

- **Systematic experimental uncertainties**
- **Phenomenological Nuclear reaction model theories + Parameters**
- **Model defects (Syst. Uncertainties)**
- Integral experiment assimilation
- **Common Physics from RRR to Continuum (previous slides)**

# Bayes' theory

Bayesian inference

New Data

Parameters

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

*A priori information*

## ➢ Description of $\vec{x}$

- Resonance parameters (RRR) — $\vec{x}_{RRR} = \{\gamma_{a\lambda}, E_\lambda, a_c, R'\}$
- Averaged resonance parameters(URR) — $\vec{x}_{URR} = \{\langle\Gamma_a\rangle, a_c, R^\infty, D_0, S_a\}$
- Continuum — $\vec{x}_{Cont} = \{\beta_2, a_c, d_c, \ldots\}$
- Fission Parameters — $\vec{x}_{Fission} = V, W, ClassII, \ldots$

## Bayes' theory

Bayesian inference

New Data

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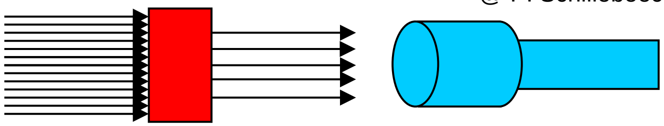
Parameters

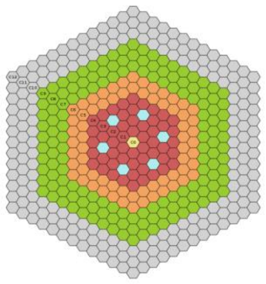
*A priori information*

### Description of $\vec{y}$

- Microscopic experiments (TOF)
  - Transmission,
  - **GELINA**, **nTOF**, DANCE, …
- Integral experiments
  - **ICBEP**
  - **PROFIL**, **PROFIL-2**, **PROFIL-R** et **PROFIL-M**
  - Spectral indices **MASURCA**

@ P. Schillebeeckx





# EVALUATIONS AND UNCERTAINTIES
# MULTI-MODEL EVALUATION

- Meta-Model from 0eV to 200MeV:

$$\sigma(E_n, \vec{x}_{RRR}, \vec{x}_{URR}, \vec{x}_{OM}, \vec{x}_{fission}, \dots)$$

- How to deal with it ?
  - Several teams with internal constraints
  - Several analysis methodologies
- Solutions :
  - Share Physics (see previous slides)
  - → coupling between RRR/URR/Continuum
  - External constraints (Experiments ; Mathematics)
  - Extensive use of Monte-Carlo / look at pdf's

## EVALUATIONS AND UNCERTAINTIES
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4th Perspective

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1 ; 2 ; 3

4th Perspective

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4.1

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# IMPOSING CONSTRAINTS ON SEVERAL MODELS
# GENERAL DESCRIPTION

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# GENERAL DESCRIPTION

- Unified model on an energy domain

@ Conrad

$[E_L, E_R]$ + Boundary at $E_C$:

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

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

Two models
Used on two separated energy domains

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- Given a microscopic experiment with statistical **and** systematic uncertainties on $[E_L,E_R]$
  - See effect of systematic uncertainties on nuclear model parameters
  - See effect of systematic uncertainties on cross section

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  - Mathematical framework
  - Cross sections continuity
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- Use of Integral experiments impacting several energy domains:
  - See effect of Integral Data Assimilation on cross sections/models

# Marginalization philosophy

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

Model parameters

« n ... rs

One Model / Several Experiments

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

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

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

Marginalization of the ... density:

$$p(\vec{x}, \vec{\theta} | \vec{y}, U) ...$$

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

Marginalization :

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

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

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- Didactic example : Sodium inelastic cross sections
  - Energy Range studied [1.9 – 2.1 MeV] ; Boundary at 2 MeV.
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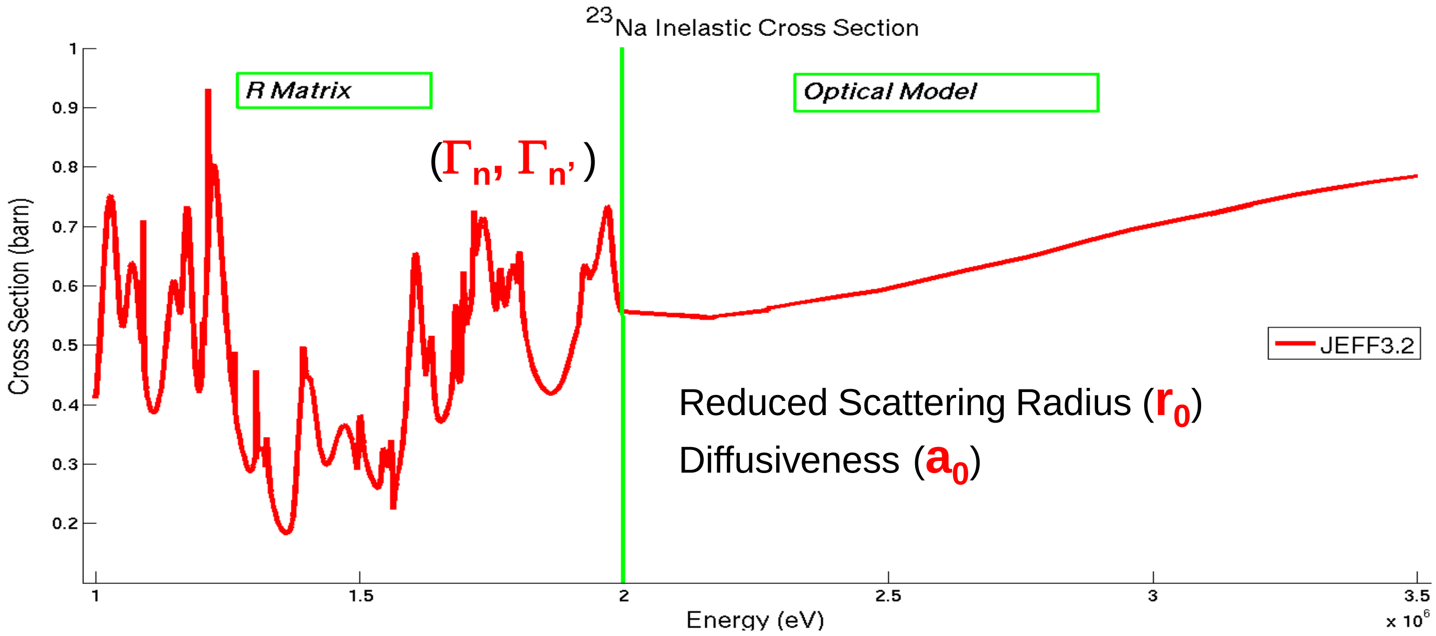


- “Simulated” experimental Data :
  - Based on theoretical points (**red**)
  - 3% statistical uncertainties
  - No/0.5/1/3% systematic uncertainties

4.1th Perspective
Analysis of wide range experiments

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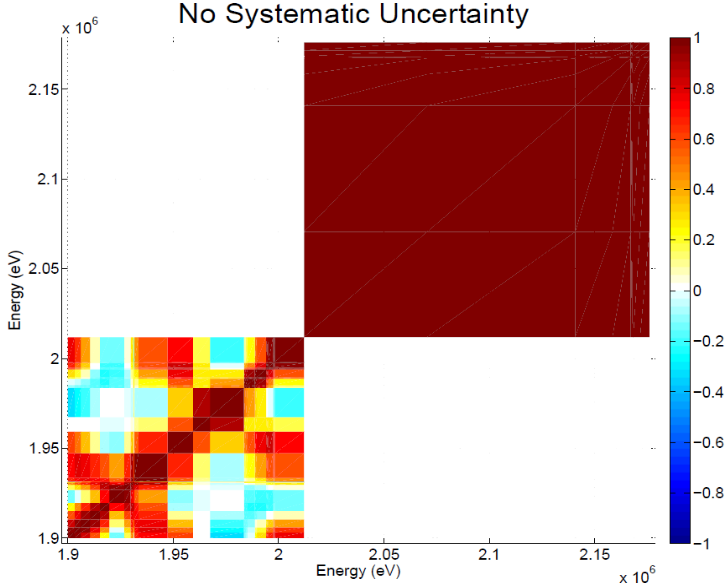
Statistical Uncertainty 3%
No Systematic Uncertainty




- Syst. Uncertainty

Tends to ensure cross section continuity
1st attempt with normalization
→ Generalize to other experimental
(background, resolution parameters., isotopic concentration)

4.1th Perspective
Analysis of wide range experiments



*Rouki et al., NIM in Physics Research Section A, **672** (2012)

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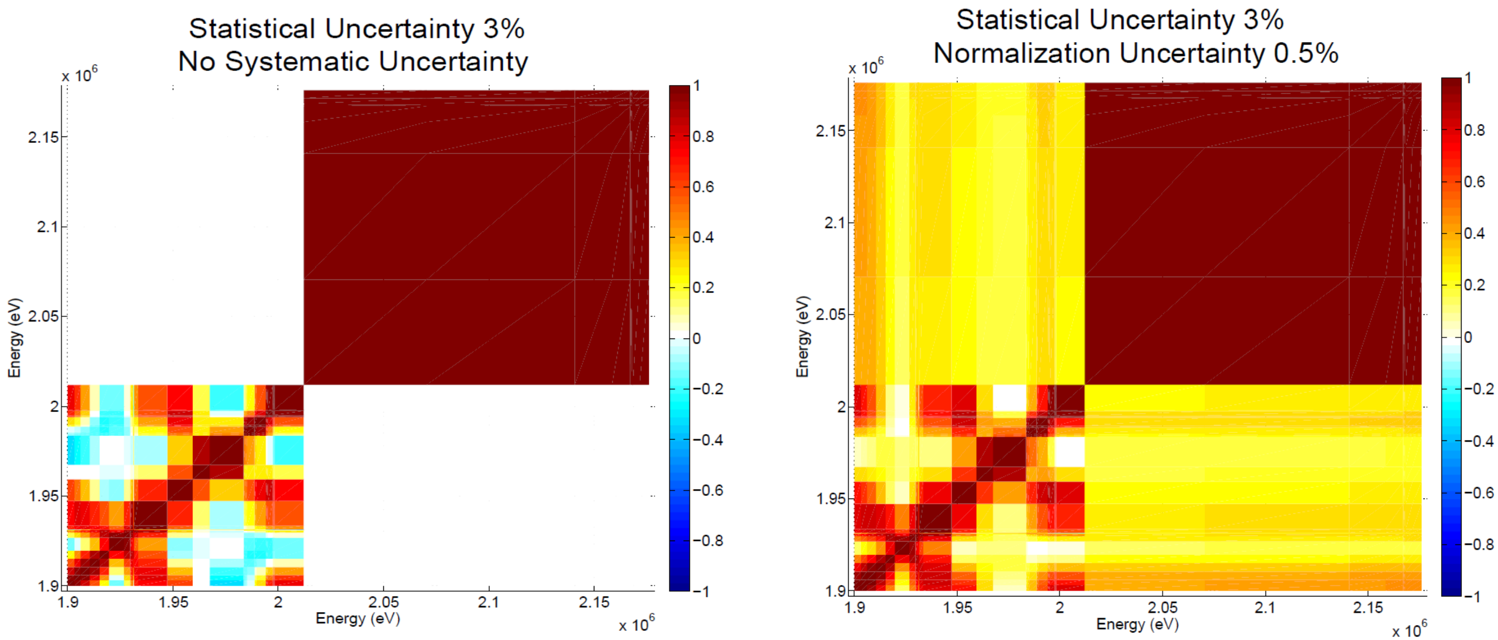


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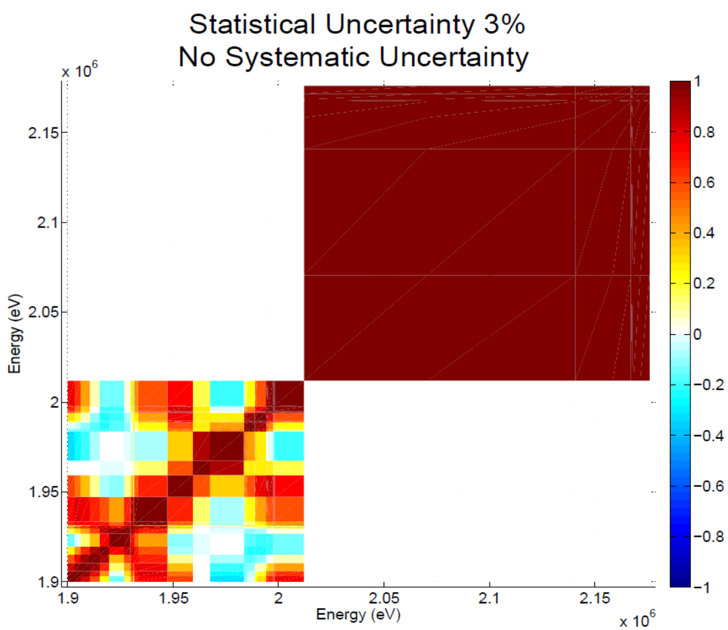


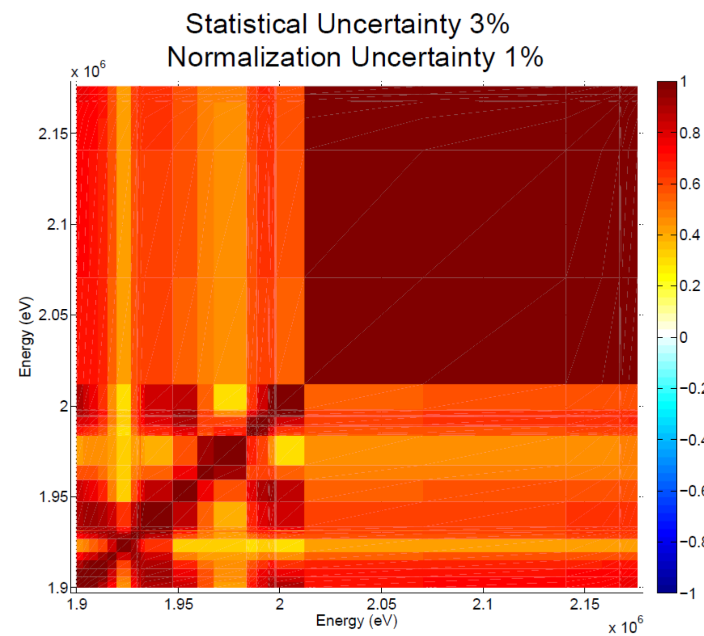


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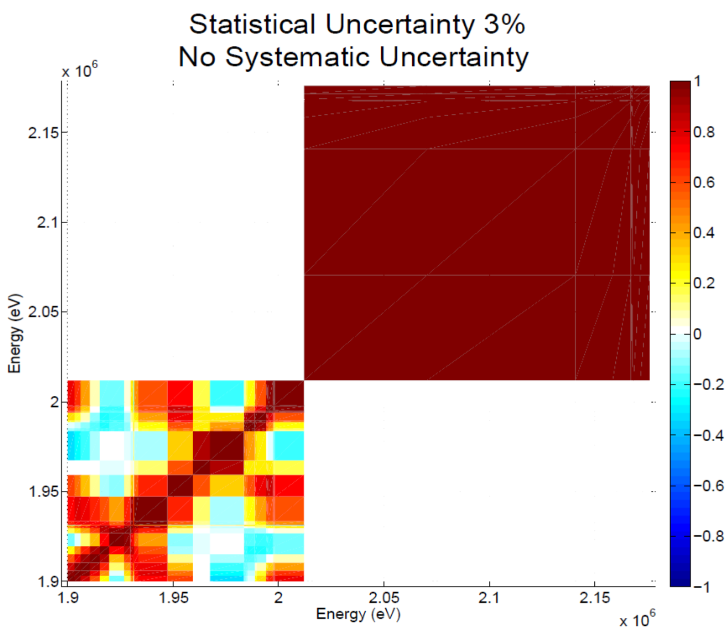


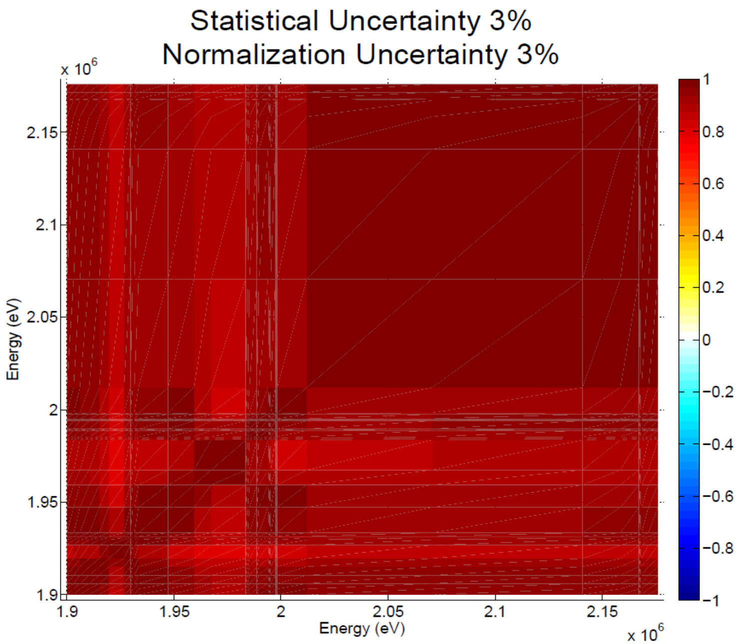


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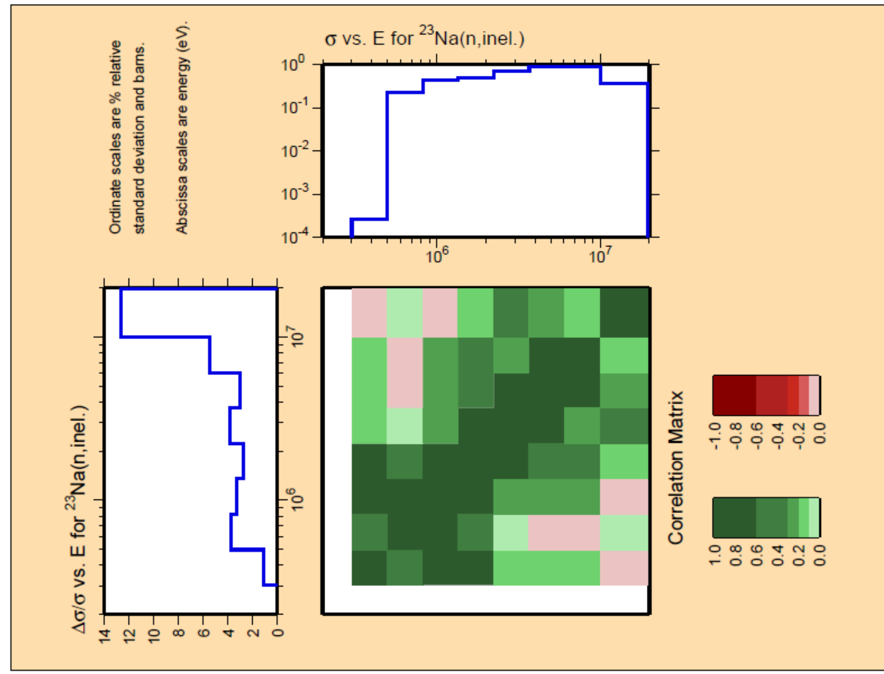
"Real" Evaluation done for time being
JEFF3.2 $^{23}$Na
Based on new (n,n') measurements*
(Syst. Unc. 2.6%)

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# IMPOSING CONSTRAINTS ON SEVERAL MODELS
# LAGRANGE MULTIPLIERS

# IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS

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

# IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS

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$$\Downarrow$$

$$\begin{aligned}\chi^2_{GLS+C} = {} & (\vec{x} - \vec{x}_m)^T M_x^{-1} (\vec{x} - \vec{x}_m) \\ & + \left(\vec{y} - \vec{t}\right)^T M_y^{-1} \left(\vec{y} - \vec{t}\right) \\ & + 2\left|C^T(\vec{x})\right| \cdot \lambda\end{aligned}$$

# IMPOSING CONSTRAINTS ON SEVERAL MODELS LAGRANGE MULTIPLIERS

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Constraints

Lagrange Multipliers

# IMPOSING CONSTRAINTS ON SEVERAL MODELS
# LAGRANGE MULTIPLIERS

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

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Constraints

Lagrange Multipliers

- Simple Mathematical description
- Difficult Mathematical resolution
  - Based on Uzawa algorithm
  - Slow convergence
  - Constraints calculations → time consuming

# IMPOSING CONSTRAINTS ON SEVERAL MODELS
# LAGRANGE MULTIPLIERS

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4.2th Perspective
Impose constraints

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

- Didactic example : Uranium Total cross section
  - Energy Range studied [25 – 750 keV] ; Boundary $E_C$ at 150 keV.
  - Below 150 keV : Average R matrix
  - Above 150 keV : Average R matrix or Optical Potential

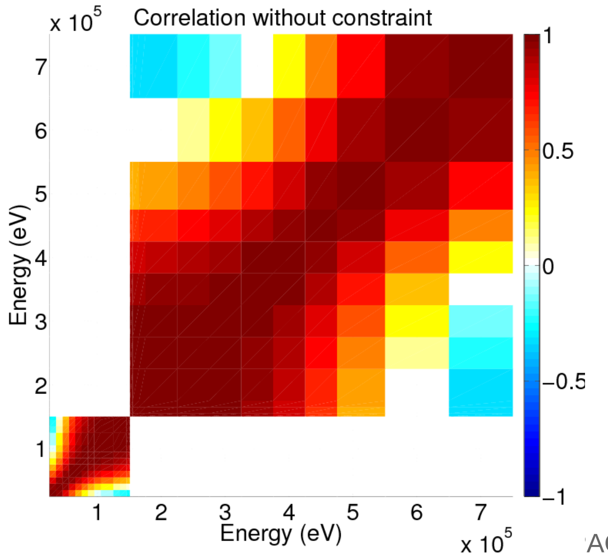
- Considered parameters :

*Unresolved Resonance Range* : Effective Radius (**R'**), Strength ($S_{l=0,1}$), Distant level ($R^{\infty}_{l=0,1}$ )

*Optical Model* : Reduced Scattering Radius ($r_0$) and Diffusiveness ($a_0$)

- Considered **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




- 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

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  - Above 150 keV : Average R matrix or Optical Potential

- Considered parameters :

*Unresolved Resonance Range* : Effective Radius (**R'**), Strength ($S_{l=0,1}$), Distant level ($R^{\infty}_{l=0,1}$)

*Optical Model* : Reduced Scattering Radius ($r_0$) and Diffusiveness ($a_0$)

- Considered **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

- Difficulty arises if :
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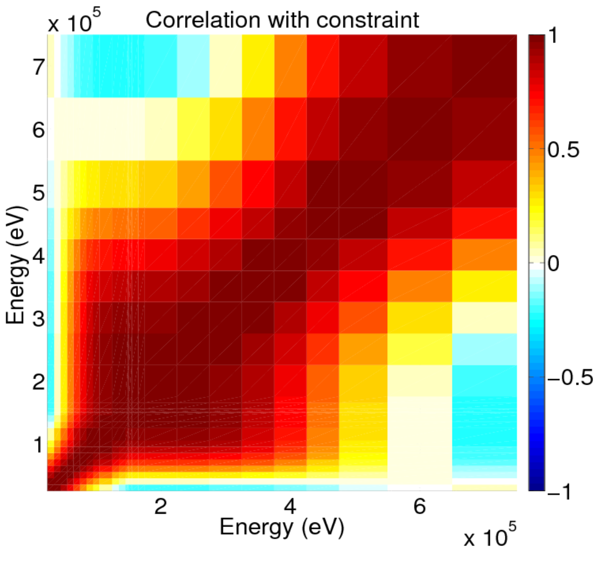
  - There are Model defects



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

- Didactic example : Uranium Total cross section
  - Energy Range studied [25 – 750 keV] ; Boundary $E_C$ at 150 keV.
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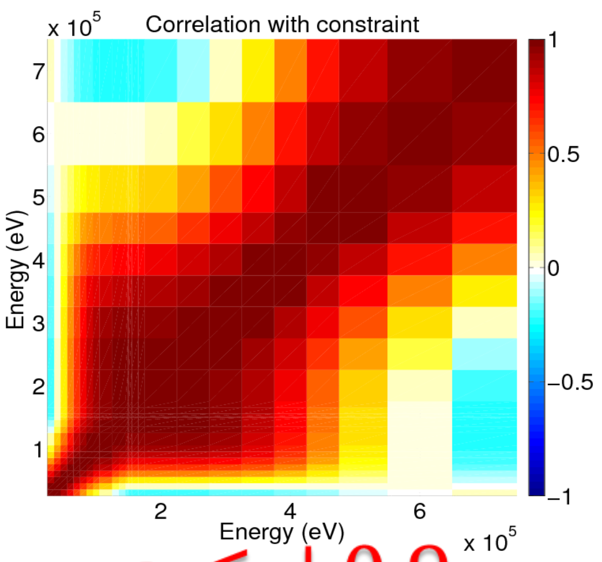


$\rho \leq \pm 0.9$

# UNCERTAINTIES : EVALUATION

$$\sigma(E_n, \vec{x}_{RRR}, \vec{x}_{URR}, \vec{x}_{OM}, \vec{x}_{fission}, \ldots)$$

- What ever is the methodology σ and x are considered as random variables (pdf)

→ Monte-Carlo Sampling is a natural ingredient

- Estimation of Uncertainties with Monte-Carlo during the evaluation process *:

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

- Sample of $p(\vec{x}\,|\,M,U)$ → $\vec{x}_k$

- For each $\vec{x}_k$ calculation of Likelihood $\ell_k[p(\vec{y}|M,\vec{x}_k,U)]$

*R. Capote and D. Smith, Nucl. Data Sheets **109**, 2768 (**2008**)
* and **C. De Saint Jean et al., Nuc. Sci. Eng., **161**, 363 (**2009**).
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5th Perspective →

UMC for the **whole energy range**
with integrated analysis tools
covering [0eV ; 200MeV]
With shared Physics (parameters)
With constraints
With Experiments
→ Treatment of Experimental parameters
and marginalisation** (“get rid of them properly”)
**FULL BAYESIAN****

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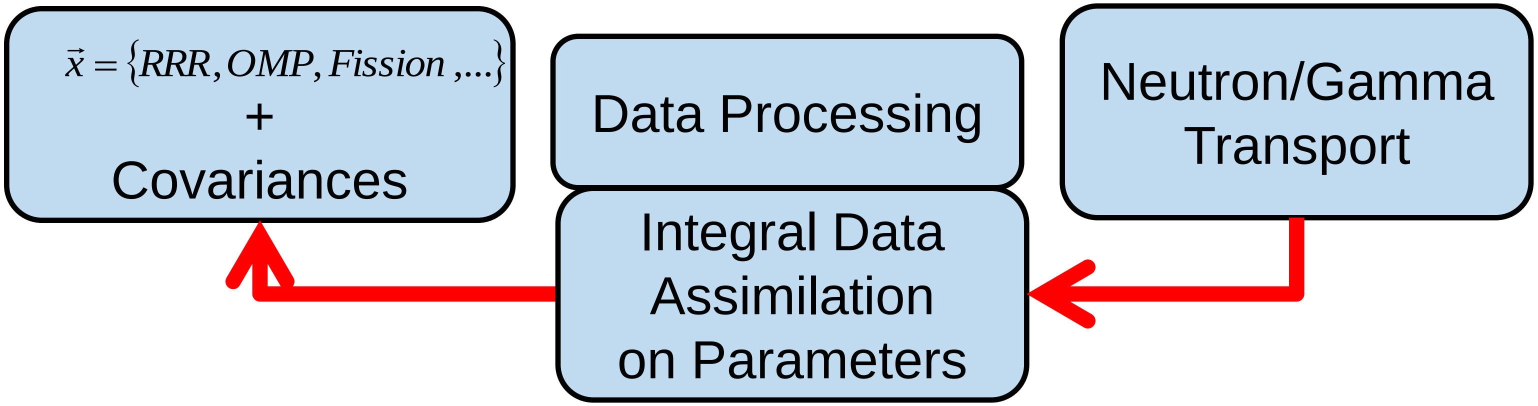
# UNCERTAINTIES AND INTEGRAL EXPERIMENTS?

$$\sigma(E_n, \vec{x}_{RRR}, \vec{x}_{URR}, \vec{x}_{OM}, \vec{x}_{fission}, \ldots) + \left\{\delta\left\langle\sigma_i\sigma_j\right\rangle\right\}$$

- What about propagation of uncertainties and/or integral data assimilations ?




- Need of a new generation of simulation codes :
  - Need of **Integrated** tools : Nuclear reaction codes ; data treatment codes ; transport codes (Analog Monte-Carlo simulation,…)
  - Need of "**parallelized**" codes →HPC horizon (for example Conrad is multi-threaded)
- Use Pdf of parameters ; Sampling →bunch of random numbers (1000 is a magic number ?) ; Statistical methods ; correlations (Cholesky) ;

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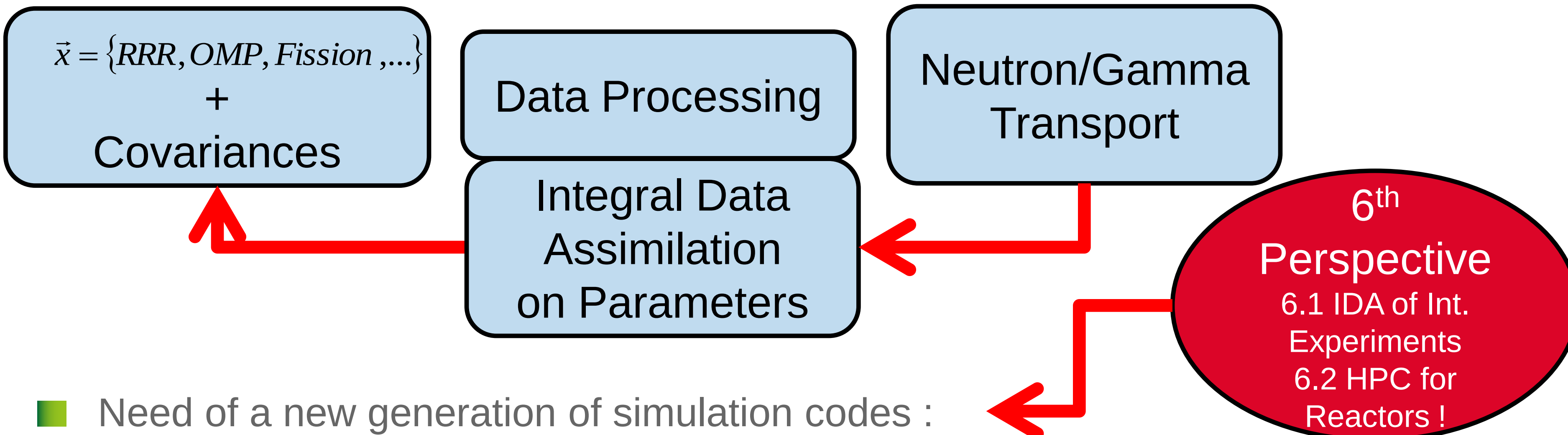


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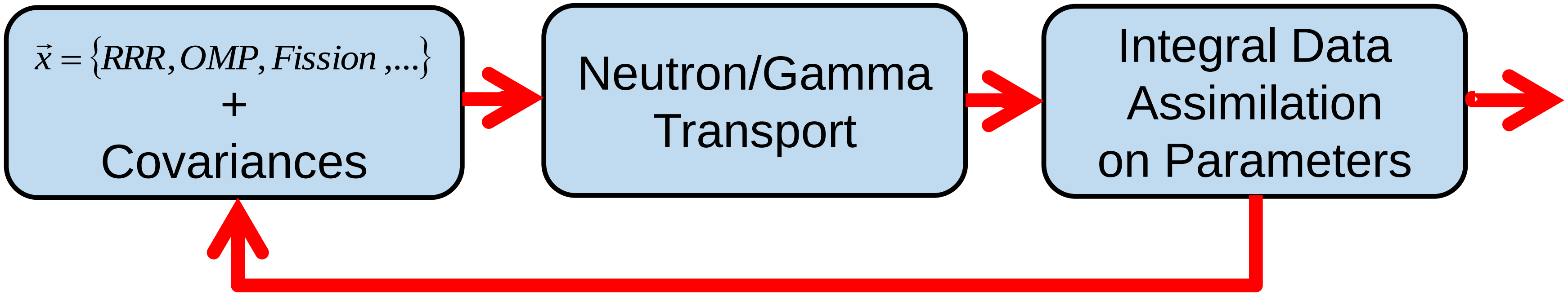
# INTEGRAL DATA ASSIMILATION

- Evaluation libraries are judged to their ability to reproduce public benchmark (ICSBEP,IRPHE,…)
- Some of these benchmarks are even used as judged of a single evaluation (JEZEBEL)
- Consistent Nuclear Data Evaluation ; Integral Data Assimilation *




- Generalization ; extensive use of Monte-Carlo neutron transport code (MCNP,Tripoli4,…)
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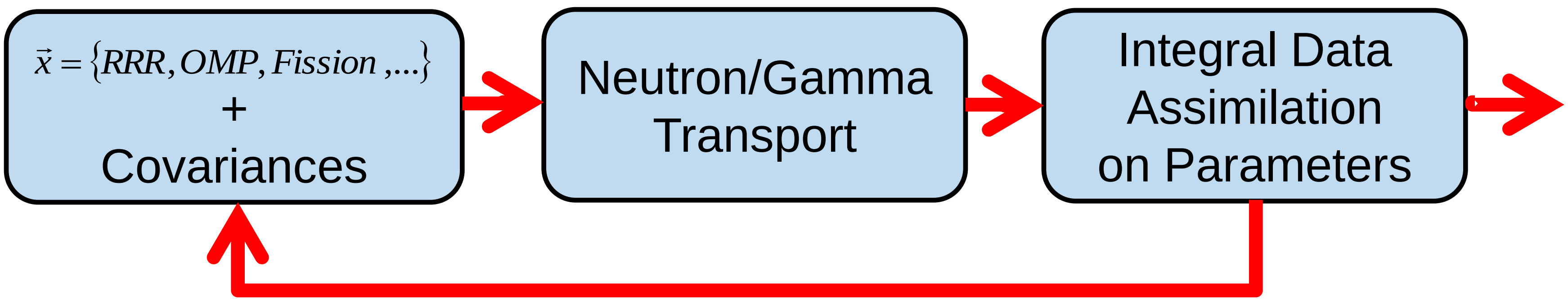


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6$^{th}$ Perspective
6.1 IDA of Int. Experiments
6.2 HPC for Reactors !



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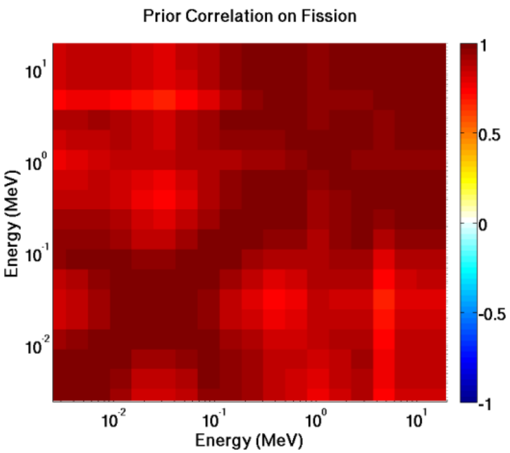
# $^{239}$PU COVARIANCE MATRICES




$$\sigma_g^r$$

$$\vec{x} = \{OMP, Fission, ...\}$$

**Multigroup cross section Data Assimilation**

**Nuclear model parameters Data Assimilation**

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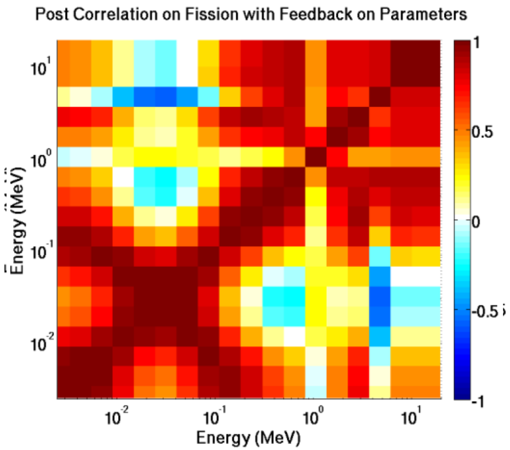


"Public" Integral Experiments

- ICSBEP (JEZEBEL)

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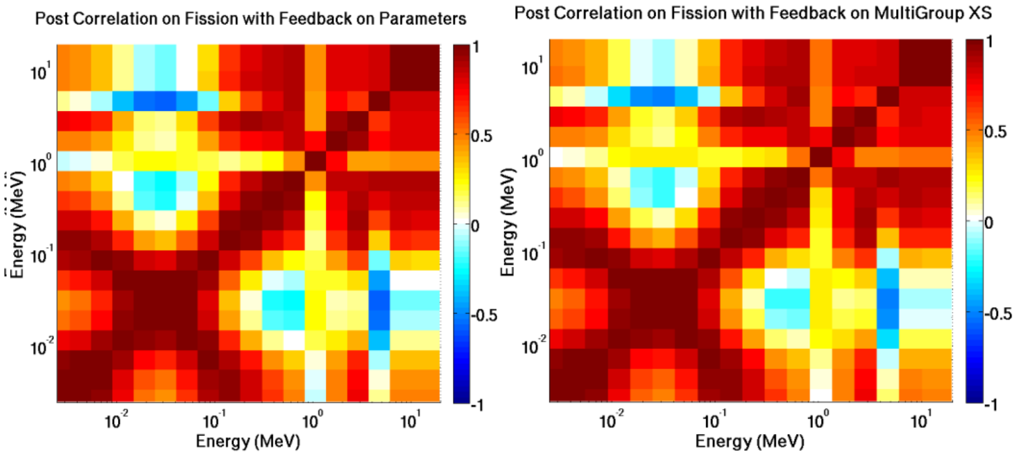


Correlation Matrix almost equivalent
$|C_{(param \rightarrow \sigma g)} - C_{(\sigma g)}|_{max} \sim 0.1$

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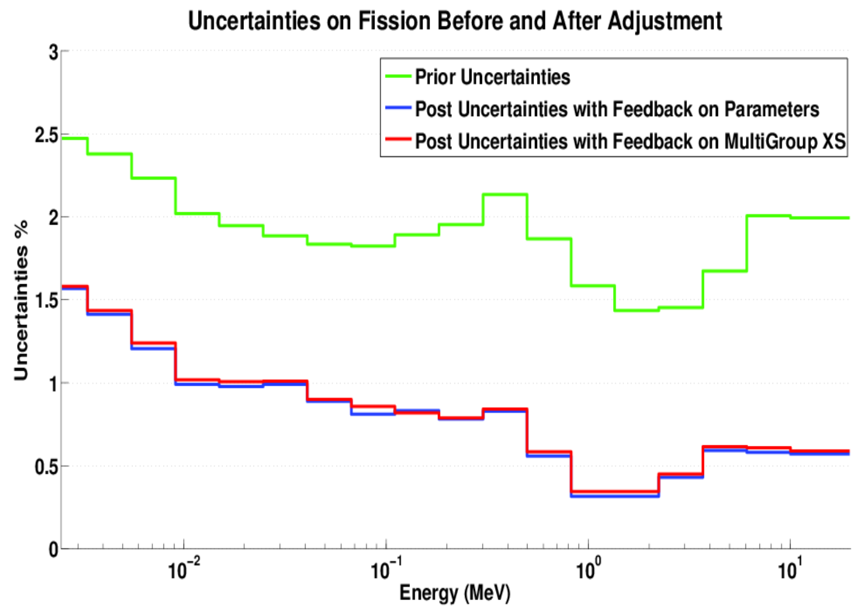


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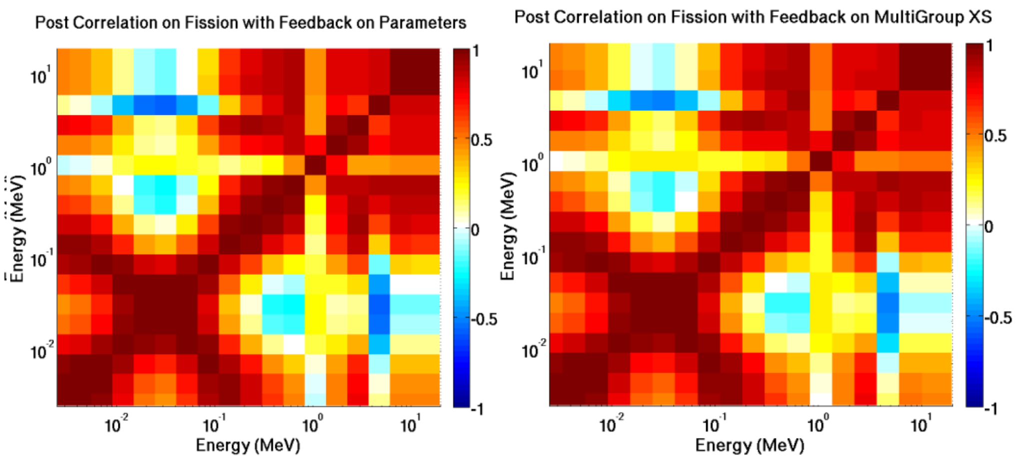


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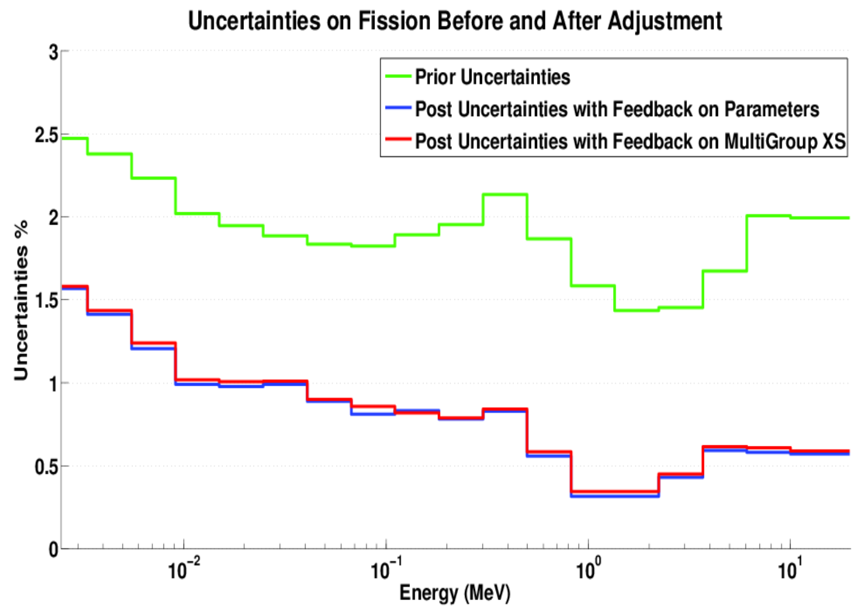


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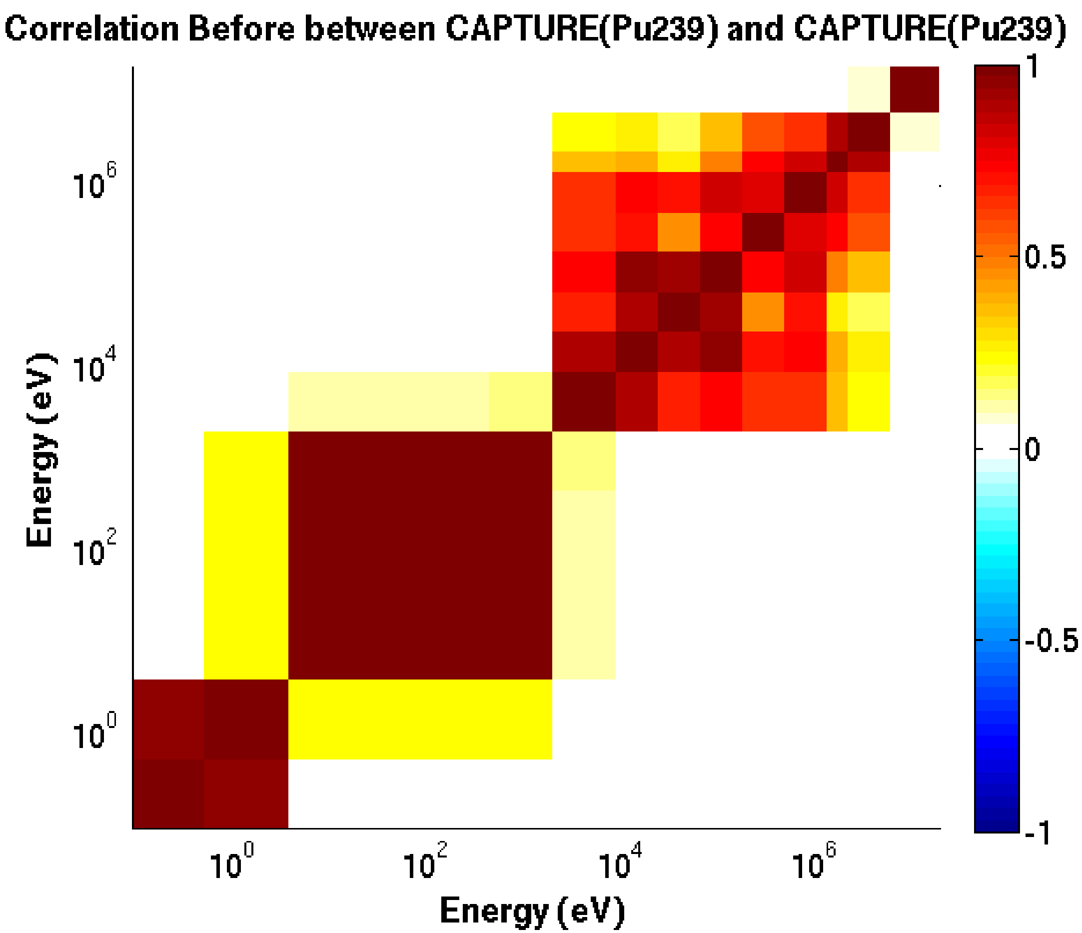


$\sigma_g^r$ and $\chi_g, \upsilon \ldots$
$+$ TRENDS

**Multigroup cross section Data Assimilation**

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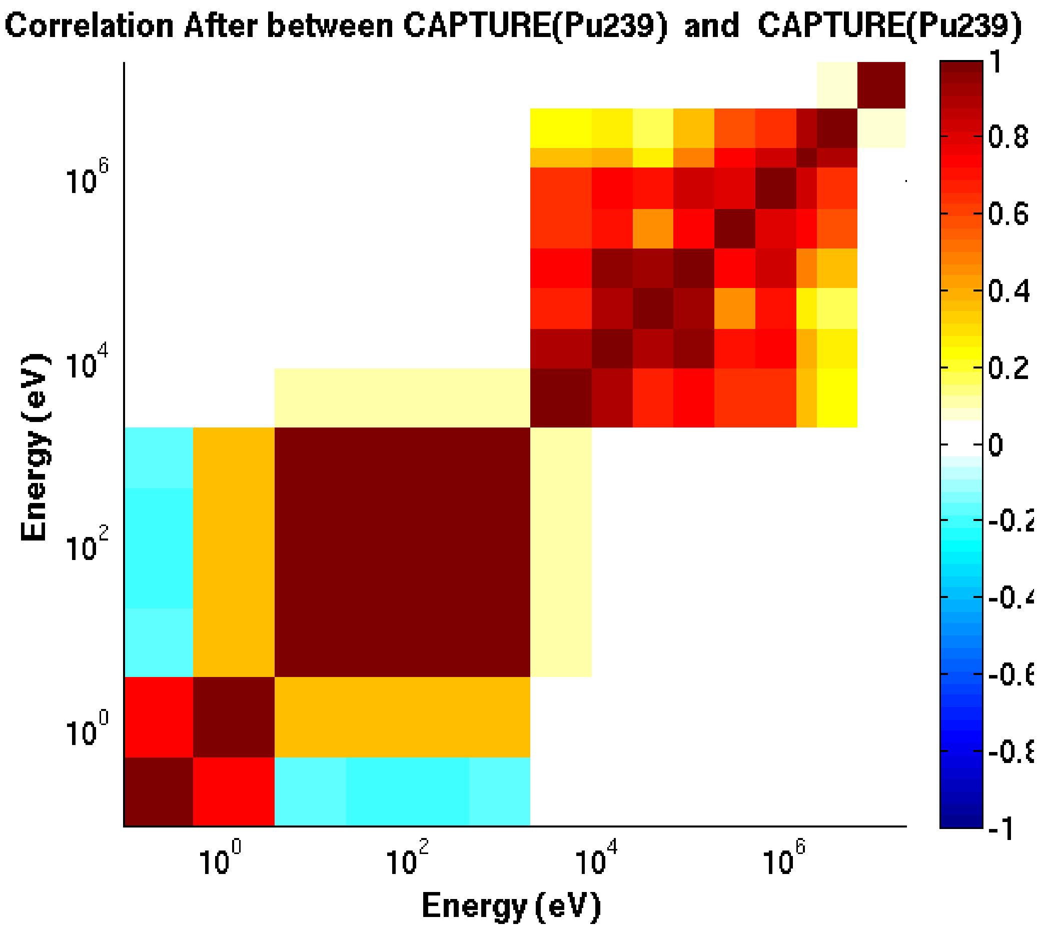
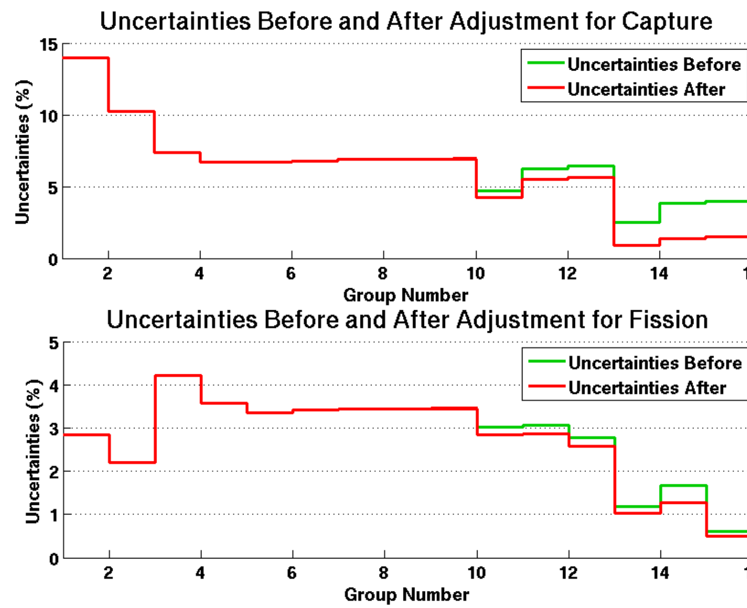



**Additional Integral Experiments**
**❑CERES Program in MINERVE/DIMPLE**

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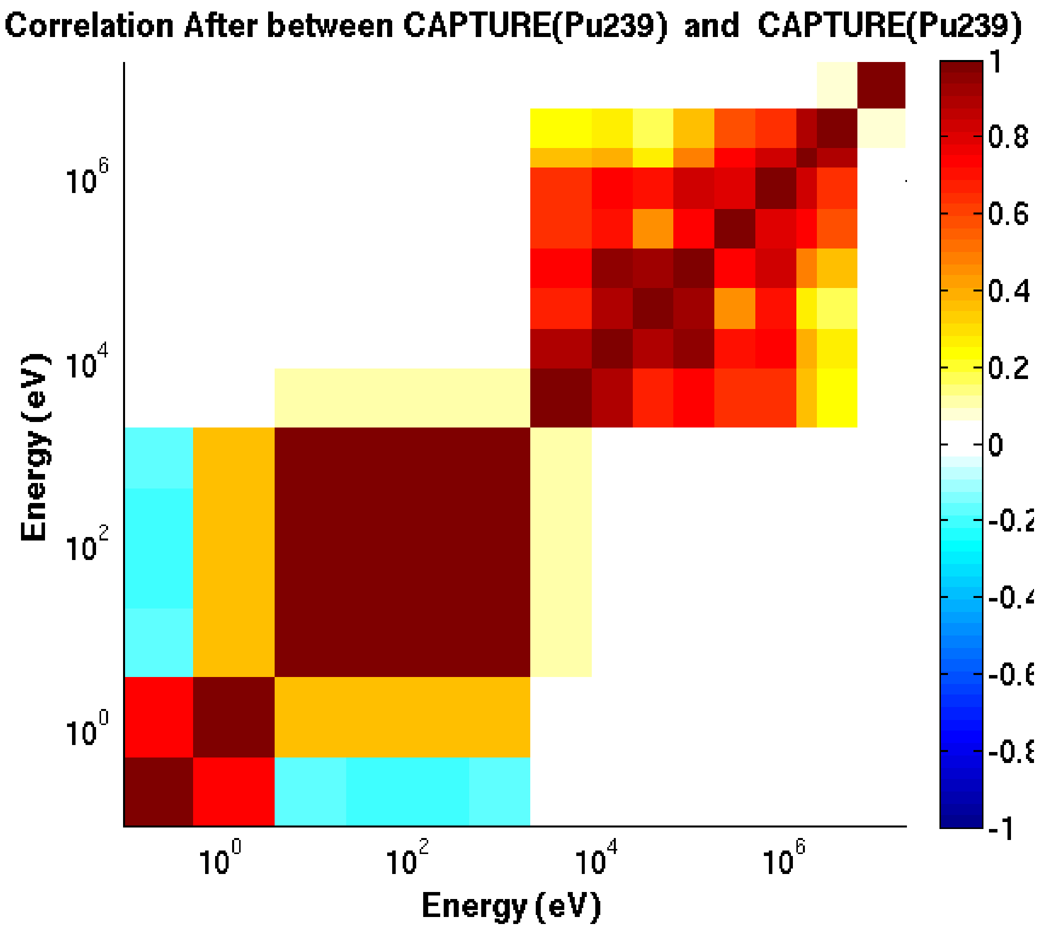


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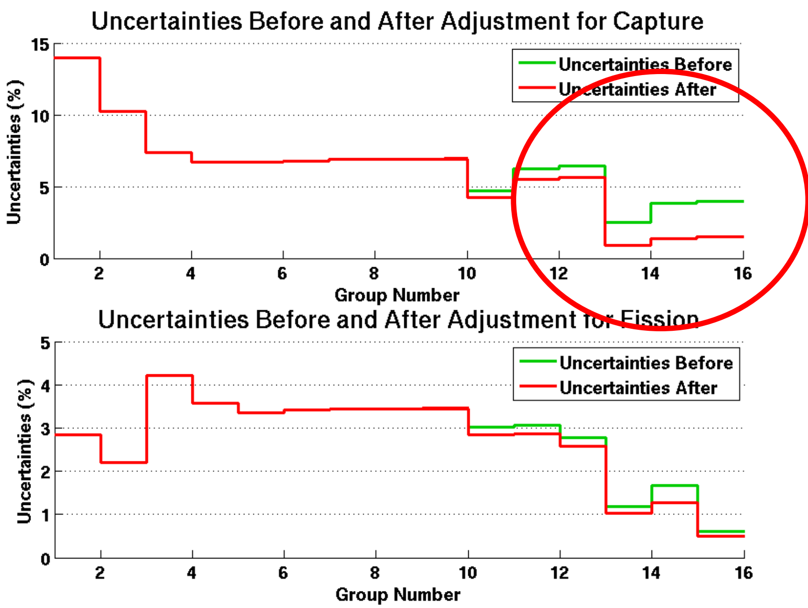


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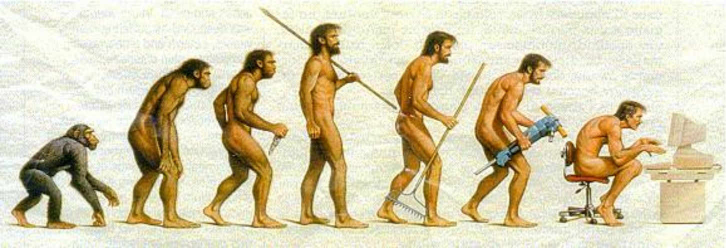
# CONCLUSIONS



- Several kind of Nuclear Data
- Several kind of Nuclear Reaction Models
- Several kind of Experiments
- Several kind of Covariance Matrices

- Progress on Methodologies needed:
  - Data assimilation techniques
  - Adding physical constraints (On several models)

- Progress on Experiments needed:
  - Reduction of systematic uncertainties for microscopic measurements
  - Integral experiments to target limited energy domain / reactions / isotopes

- Progress on Nuclear models needed:
  - Share Common physic features
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  - Avoid compensations

- Needs to define Covariance estimation benchmarks:
  - Fixed experiments
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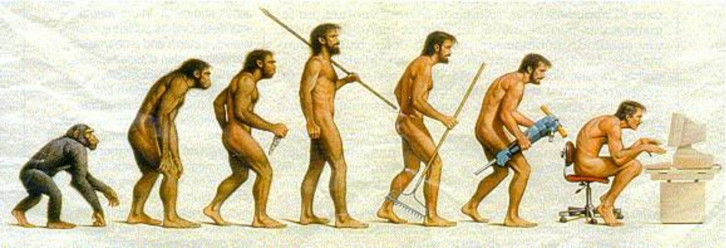

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1 ;2 ;3
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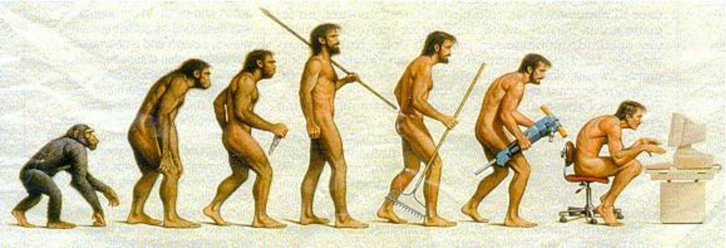

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4 ; 5 ; 6
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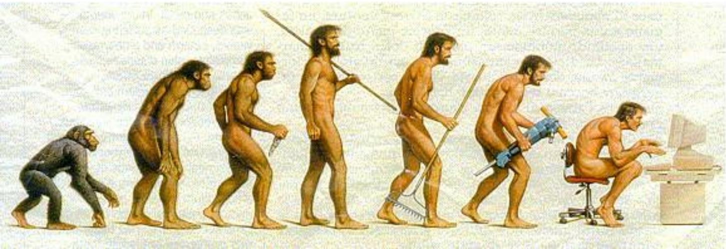

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8th Perspective

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7th Perspective

# OTHER PERSPECTIVES

1. Other theories (S,K,… ?)
2. Reich-Moore alternatives / Progress for Fission
3. Resonance shape analysis with double differential data (sodium/Fe/U,Pu,etc…)
4. Direct reaction treatment even in RRR
5. Microscopic Measurement :
   a) Systematic uncertainties
   b) Long range experiments (from RRR to Continuum)
   c) Cold/hot experiments (few K to 1000 K)
   d) Surrogate
   e) Multi-Observables
      I. fission+Capture, Fission xs / Fission yields ;
      II. Spectra …
6. Microscopic theories
7. ……………………………………