DE LA RECHERCHE À L'INDUSTRIE

Covariance Matrices for Differential and Angle-Integrated Neutron-Induced Elastic and Inelastic Scattering Cross Sections of ^{56}Fe

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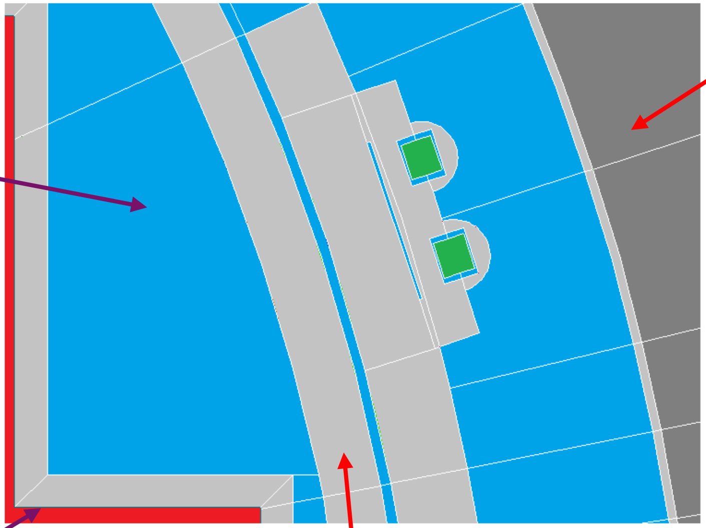
OUTLINE

- **Introduction**
- **Methods**
  - *Optical model*
  - *Statistical model*
  - *Bayes' theory*
- **Results**
  - *Cross sections*
  - *Correlation matrices*
- **Conclusions**

Context



Reflector:

- Flatten power distribution through neutron scatterings
- Reduce dose deposed in Reactor Pressure Vessel through neutron scatterings

Reactor Pressure Vessel:

- Radiation damage (Displacement per Atom or recoil energy) depends on neutron scatterings

Angular distribution & neutron-induced damage

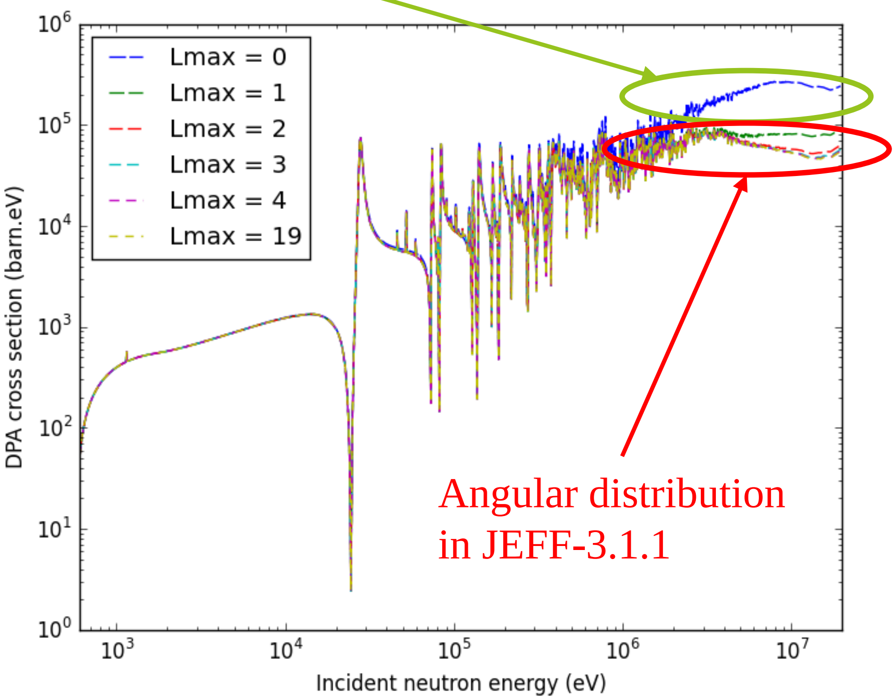
Angular distribution:

Legendre coefficients (evaluated in ENDF)

$$f(\mu, E) = \sum_{l=0}^{Lmax} \frac{2l+1}{2} a_l(E) P_l(\mu)$$

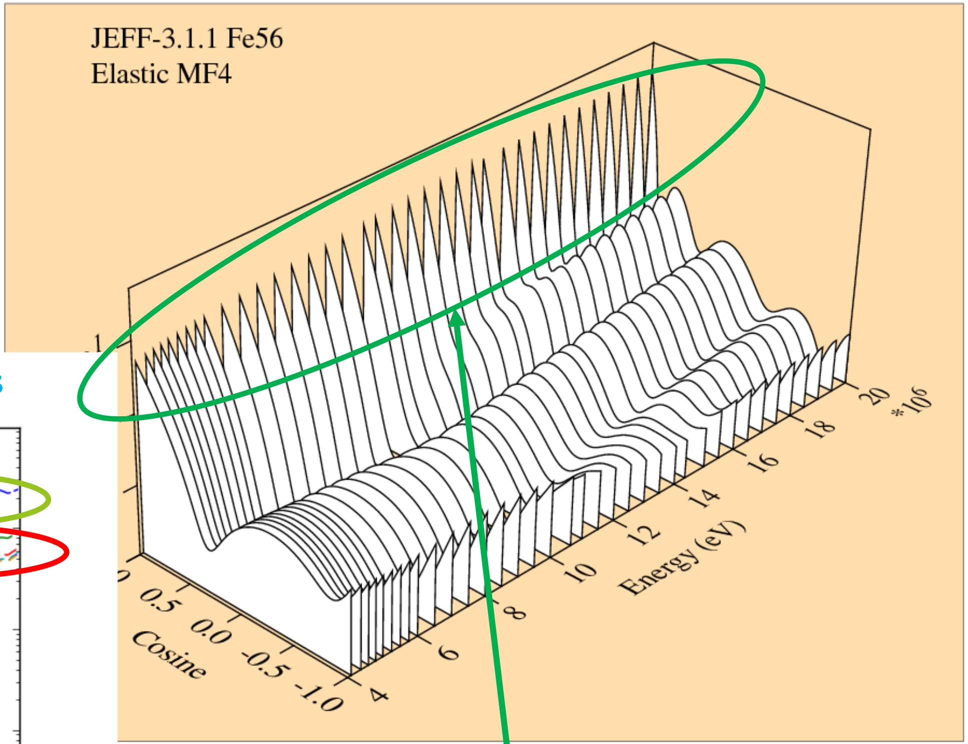
Isotropic angular distribution

Legendre polynomials



Angular distribution in JEFF-3.1.1

Neutron elastic scattering DPA cross sections of ^{56}Fe performed with different maximum Legendre polynomials



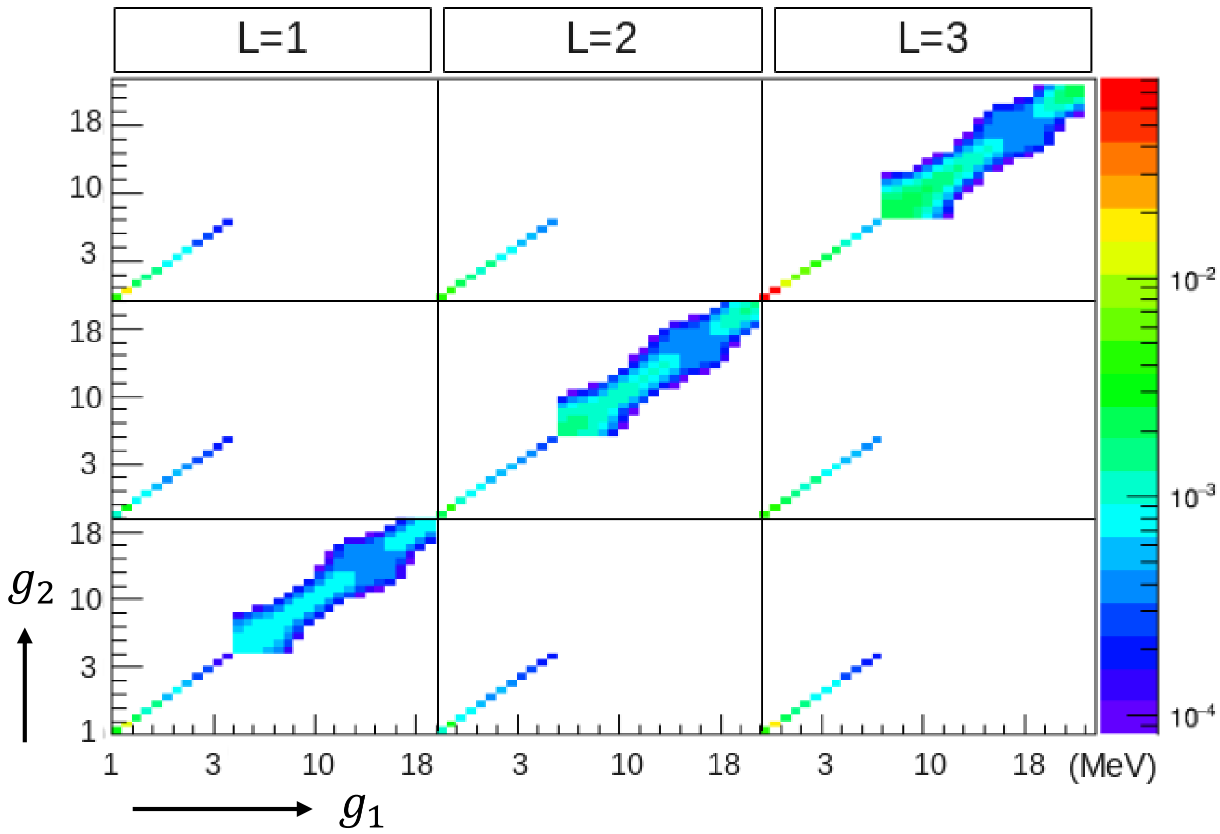
Angular distributions of the neutron elastic scattering reaction of ^{56}Fe in JEFF-3.1.1

High-order Legendre polynomials

Large influence of angular distributions on neutron-induced irradiation damage!

Covariance matrix

Covariance matrices of $a_l(E)$ for n+^{56}Fe elastic scattering in JEFF-3.2



- ➢ Correlations between different orders of Legendre coefficients
- ➢ Correlations only for elastic scattering $\Rightarrow$ **Lack of complete correlation matrix!**

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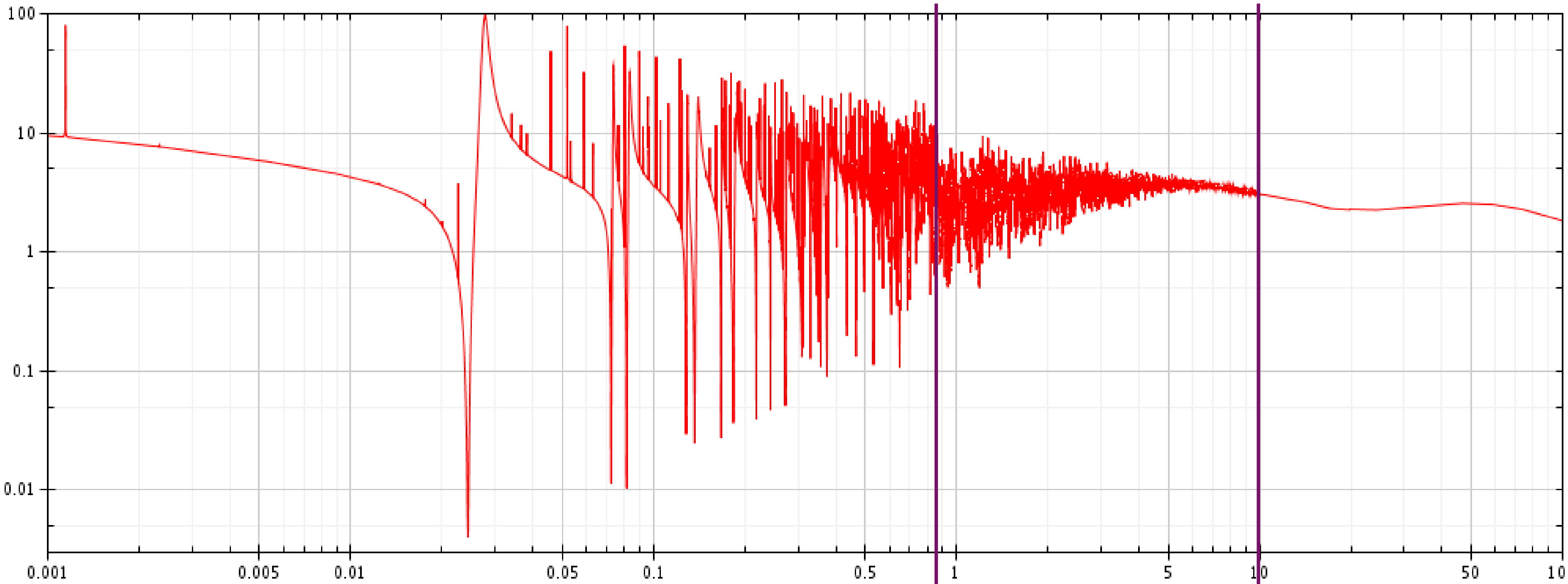
^{56}Fe elastic cross section in JEFF-3.1.1



Resolved Resonance Region

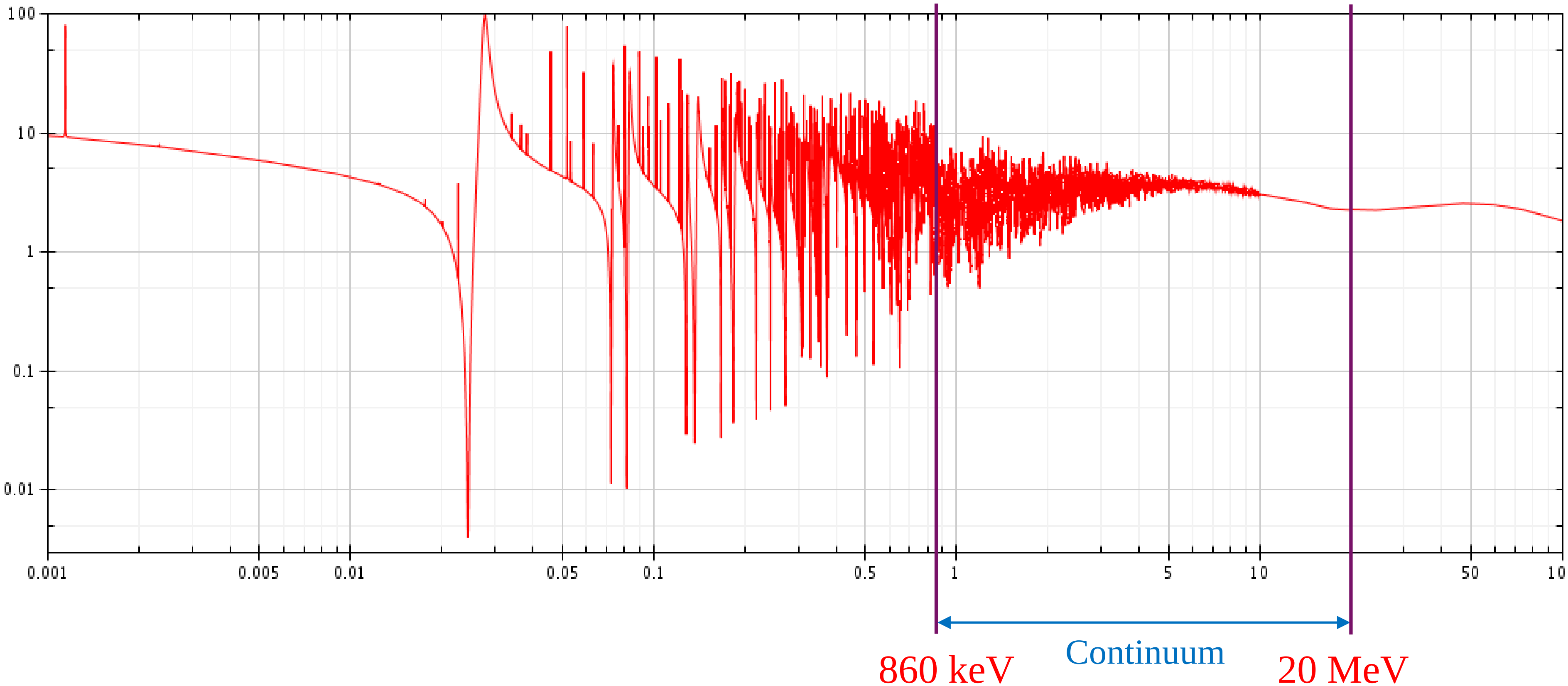
R-matrix formalism
Compound nucleus
Direct reaction

Interpolation of experimental data

Continuum

Optical Model
Hauser-Feshbach
Compound nucleus
Pre-equilibrium
Direct mechanism

New evaluation of the "Continuum"



Optical Model
Hauser-Feshbach
Compound nucleus
Pre-equilibrium
Direct mechanism

Principles of the optical model calculations

Optical potential
Spherical model
(Morillon-Romain)

$$U(r,E) = [V_V(E) + iW_V(E)]f(r,R,a)$$ *Volume*

$$+ [V_S(E) + iW_S(E)]g(r,R,a)$$ *Surface*

$$+ [V_{SO}(E) + iW_{SO}(E)]\frac{1}{r}\left(\frac{h}{m_\pi c}\right)^2 \times g(r,R,a)\mathbf{1}\cdot\boldsymbol{\sigma}$$ *Spin-Orbit*

$$f(r,R,a) = \frac{1}{1+\exp[(r-R)/a]}$$

$$g(r,R,a) = -4a\frac{d}{dr}f(r,R,a)$$

4 free parameters +
1 marginalized parameter

ECIS

Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = (-\frac{\hbar^2}{2m}\nabla^2 + V + iW)\Psi$$

Wave function

Total cross section
Shape elastic cross section
Reaction cross section

Principles of the statistical model calculations

- **Hauser-Feshbach formula for the angle-integrated partial cross sections**

From optical model calculation (ECIS)

Transmission coefficients (TALYS)

$$\sigma_{nX} \propto \frac{T_n T_X}{\sum_i T_i} W_{nX}, \qquad X = n, n'$$

2 free parameters

Width fluctuation correction factor
(Dresner's Integral, TALYS)

- **Blatt-Biedenharn formalism for differential elastic and inelastic scattering cross sections**

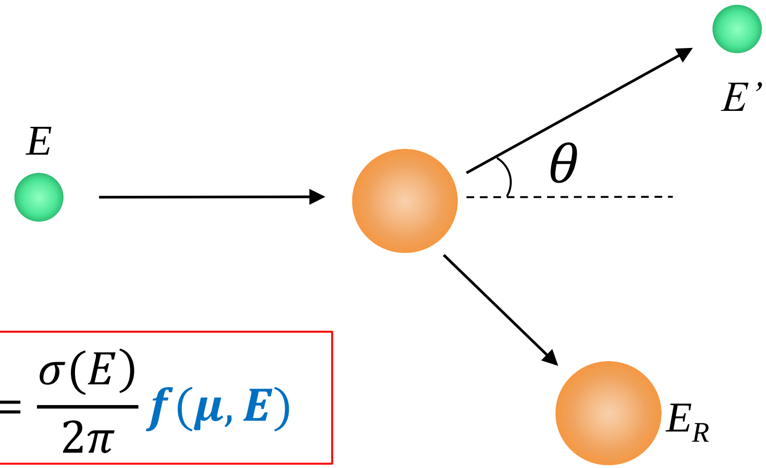
Clebsch-Gordan coefficients
(Racah, *Phys, Rev.* 61, 186 (1942))

$$\frac{d\sigma_{nX}}{d\Omega} \propto \sum_{L=0}^{\infty} B_L P_L(\cos\theta)$$

$$B_L = \sum_{l=0}^{\infty} \sum_{l'=|l-L|}^{l+L} (2l+1)(2l'+1)[(ll'00|ll'L0)]^2 \sin\delta_l \sin\delta_{l'} \cos(\delta_l - \delta_{l'})$$

Angular distribution & Legendre coefficients

- **Angular distribution:**



$$\sigma(\theta,\varphi,E) = \sigma(E)\boldsymbol{F(\theta,\varphi,E)}$$

Isotropic φ

$\mu = \cos\theta$

$$\boxed{\sigma(\theta,\varphi,E) \equiv \sigma(\mu,E) = \frac{\sigma(E)}{2\pi}\boldsymbol{f(\mu,E)}}$$

- **Angular distribution & Legendre polynomials:**

Legendre coefficients ⇔ Angular distribution

$$f(\mu,E) = \sum_{l=0}^{NL} \frac{2l+1}{2} \boldsymbol{a_l(E)} P_l(\mu)$$

Legendre polynomials

- **Multi-group coefficients of Legendre polynomials:**

$$a_{l,n} = a_l\left(\exp\left[\frac{\ln\left(E_{n,inf}\right) + \ln\left(E_{n,sup}\right)}{2}\right]\right)$$

Data assimilation with CONRAD

Bayes' theorem (posterior prob. density):

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

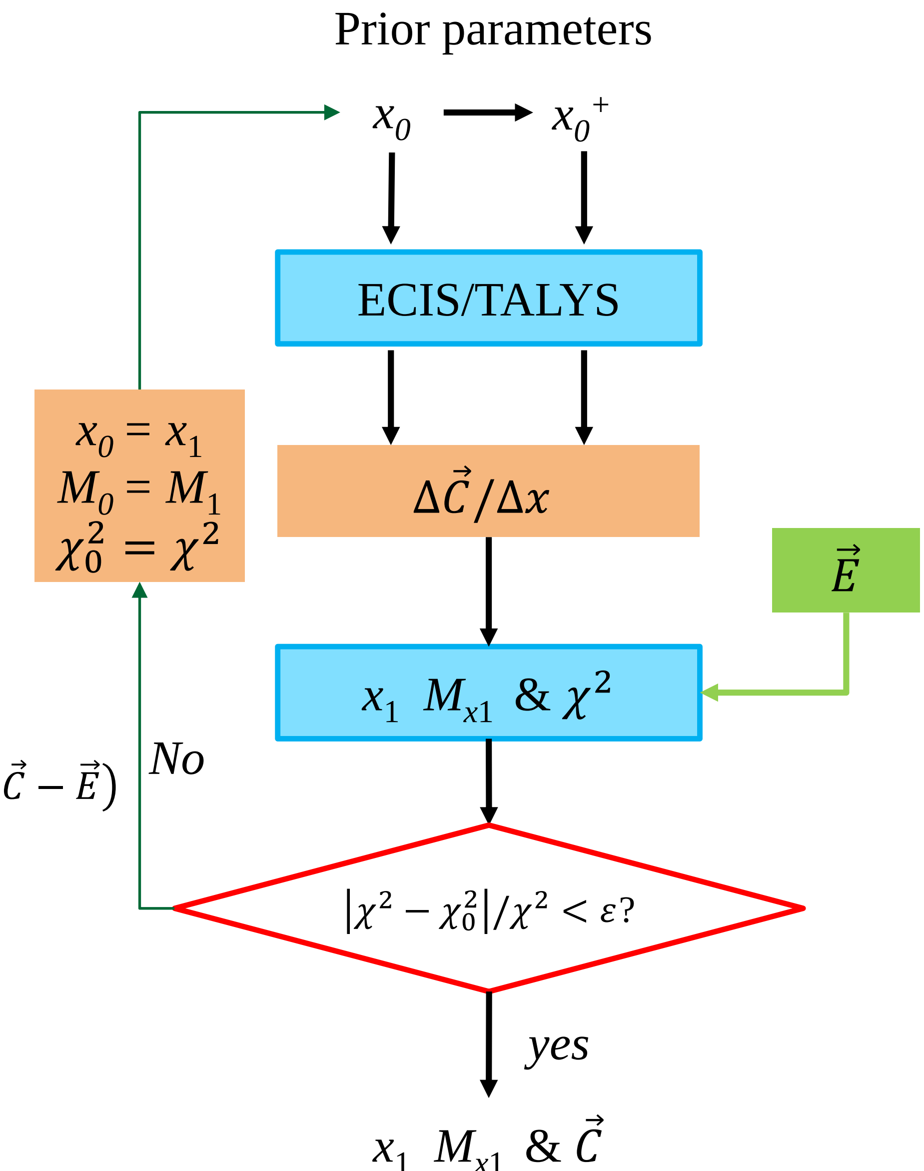
$\vec{x}$: parameters in physical model
$\vec{E}$: experimental data
U : prior information

GLS cost function:

$$\chi^2_{GLS}=(\vec{x}-\vec{x}_0)^T M_x^{-1}(\vec{x}-\vec{x}_0)+(\vec{C}-\vec{E})^T M_E^{-1}(\vec{C}-\vec{E})$$

Hypothesis: Gaussian distribution of $\vec{x}$

$$\boxed{\max_x p(\vec{x}|\vec{E},U) \Leftrightarrow \min_x \chi^2(x,\vec{E})}$$



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1st step: model parameters established with JEFF-3.1.1

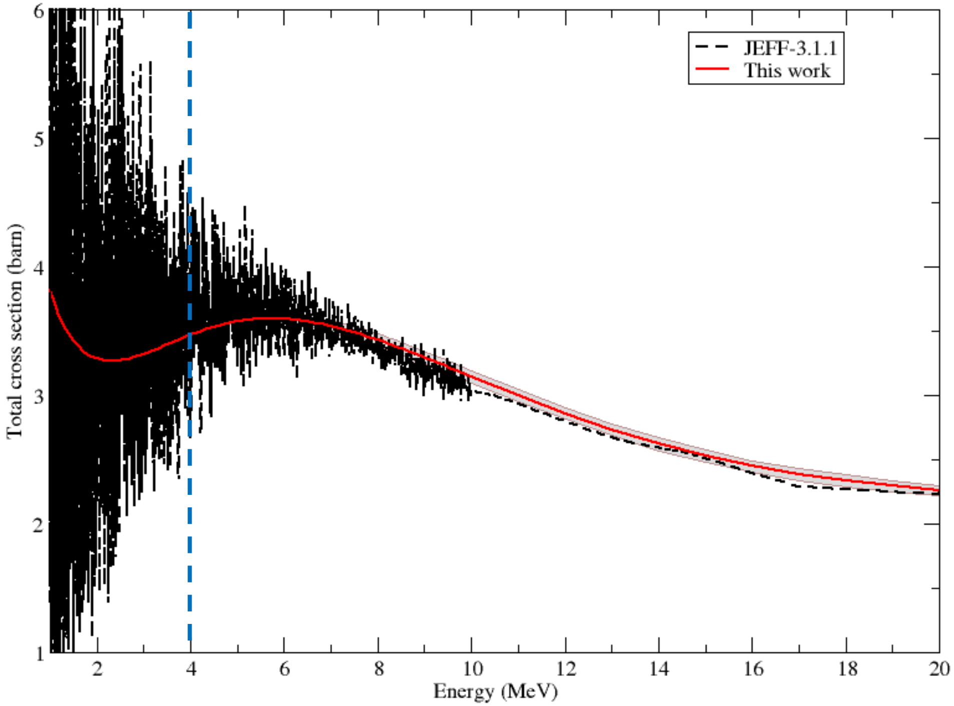
- with the aim of reproducing the uncertainties
- Covariance matrices corresponding to JEFF-3.1.1 data

  $\Rightarrow$ uncertainty quantification for calculations based on JEFF-3.1.1

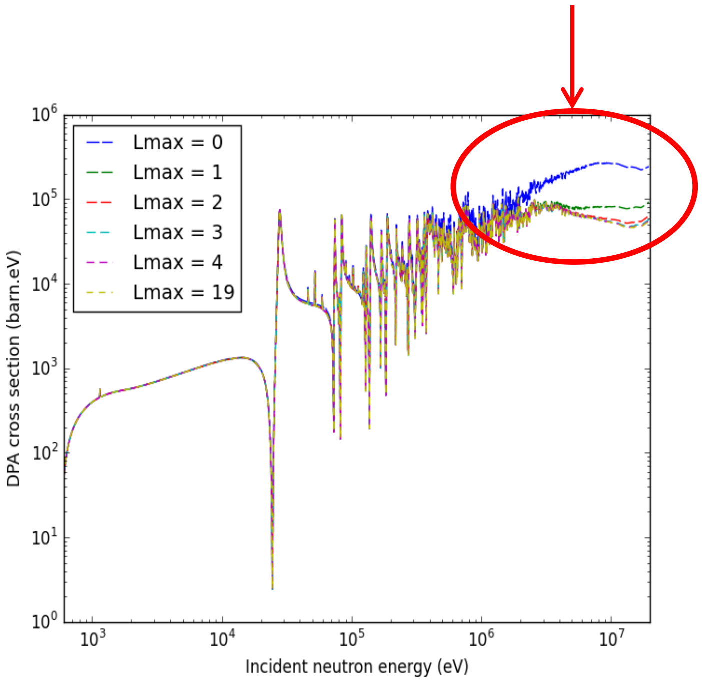
2nd step: prior parameters come from 1st step + experimental data (EXFOR)

- with the aim of reevaluating cross sections
- Realistic uncertainties based on Bayes' theorem
- Complete covariance matrices

Results for the total cross section (ECIS)



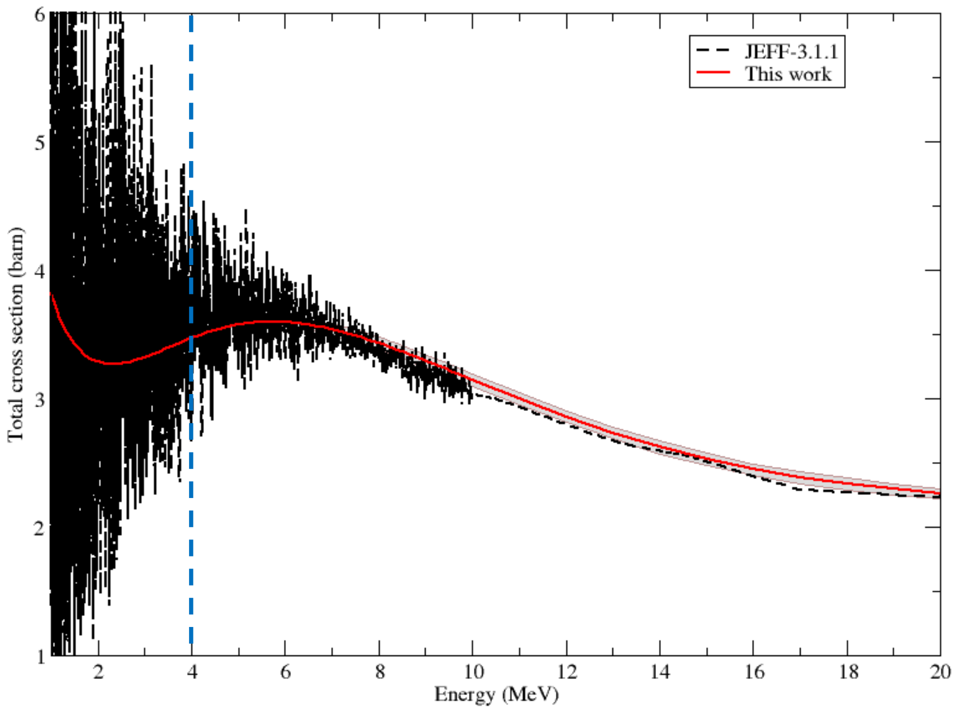
Total cross section



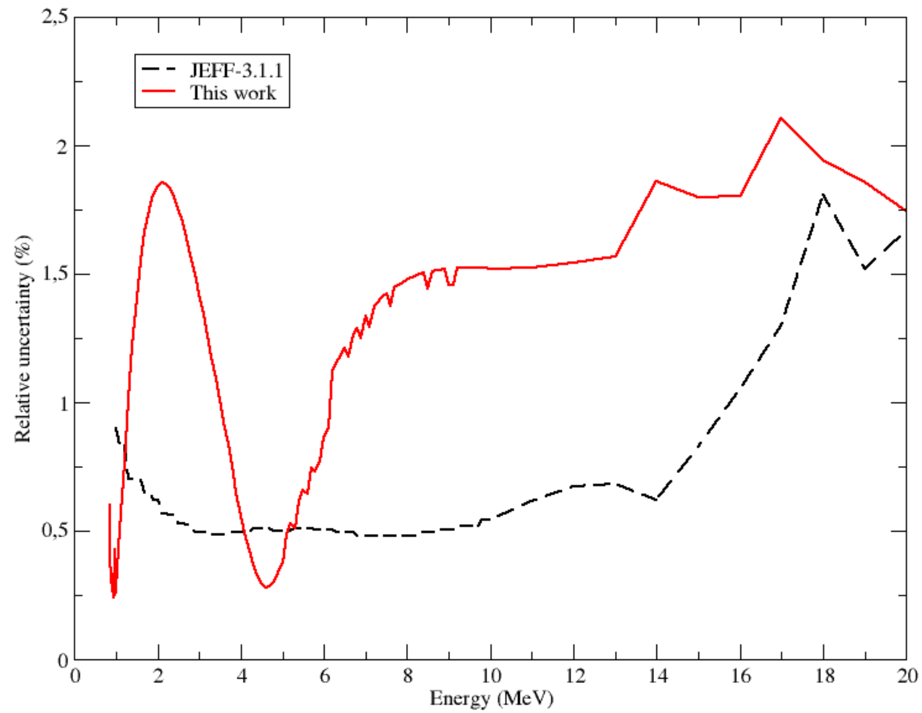
- Reasonable agreement with the total cross section of JEFF-3.1.1 above 4 MeV

- Below 4 MeV, optical model not appropriate to reproduce the resonant structures
  $\Rightarrow$ However, such an approach is sufficient for producing suitable covariance information for our nuclear application

Results for the total cross section (ECIS)



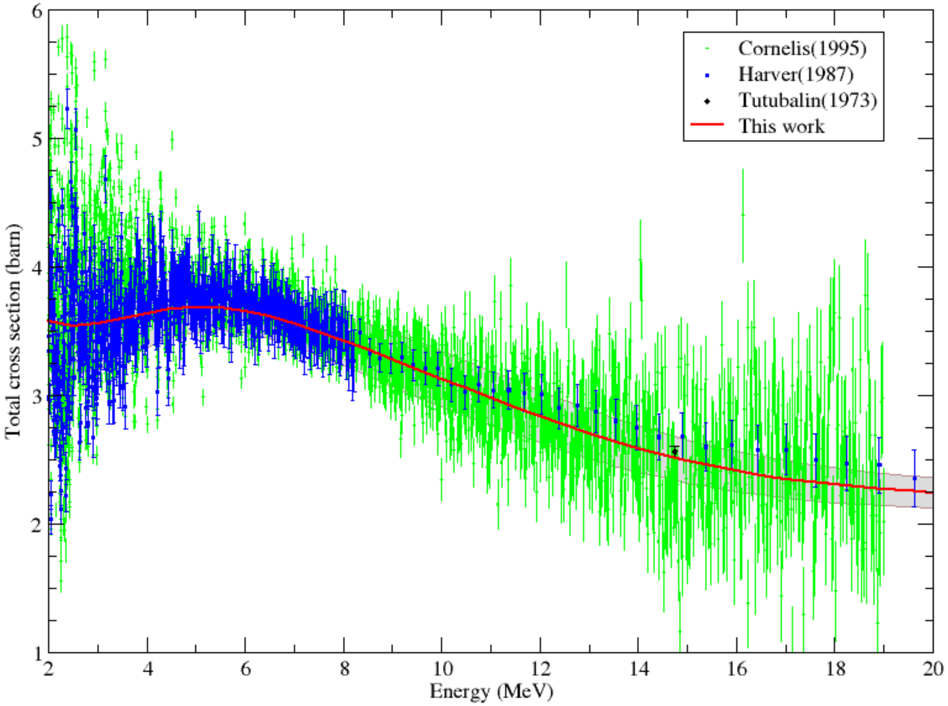
Total cross section



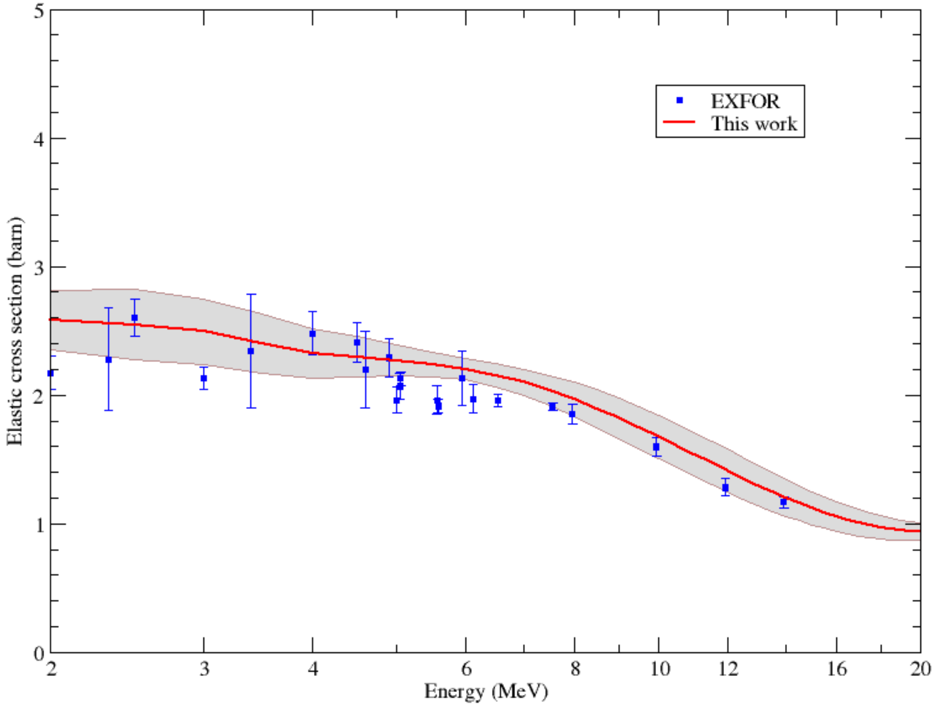
Relative uncertainty of total cross section

- Above 6 MeV, we obtain a more realistic relative uncertainty on the total cross section which is close to 1.8% in average
- Below 6 MeV, our work need to be improved

Comparison with experimental data



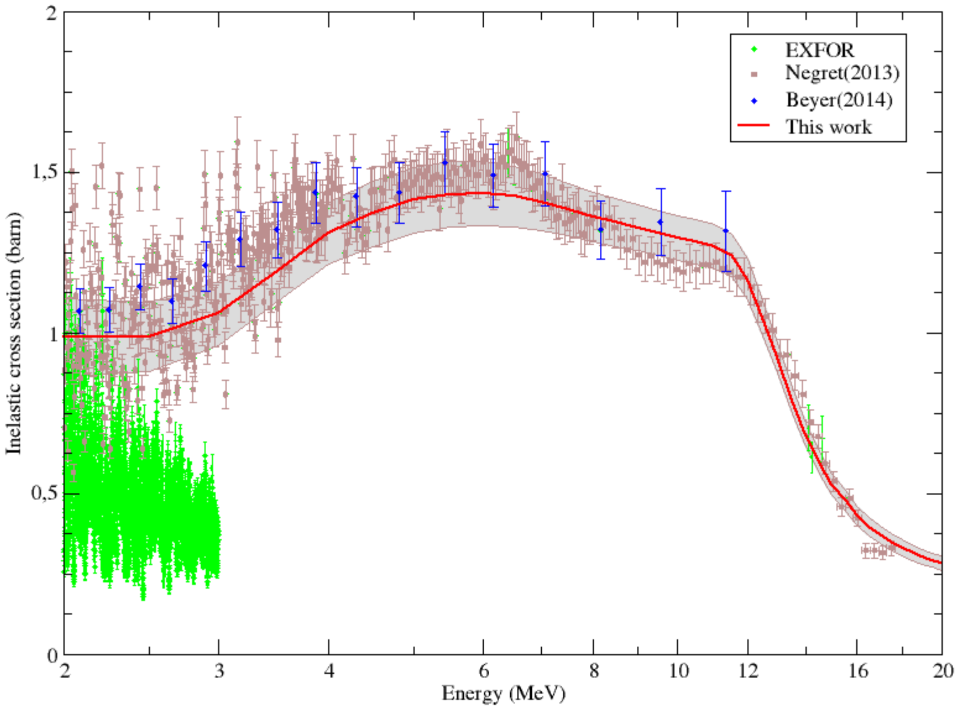
Total cross section



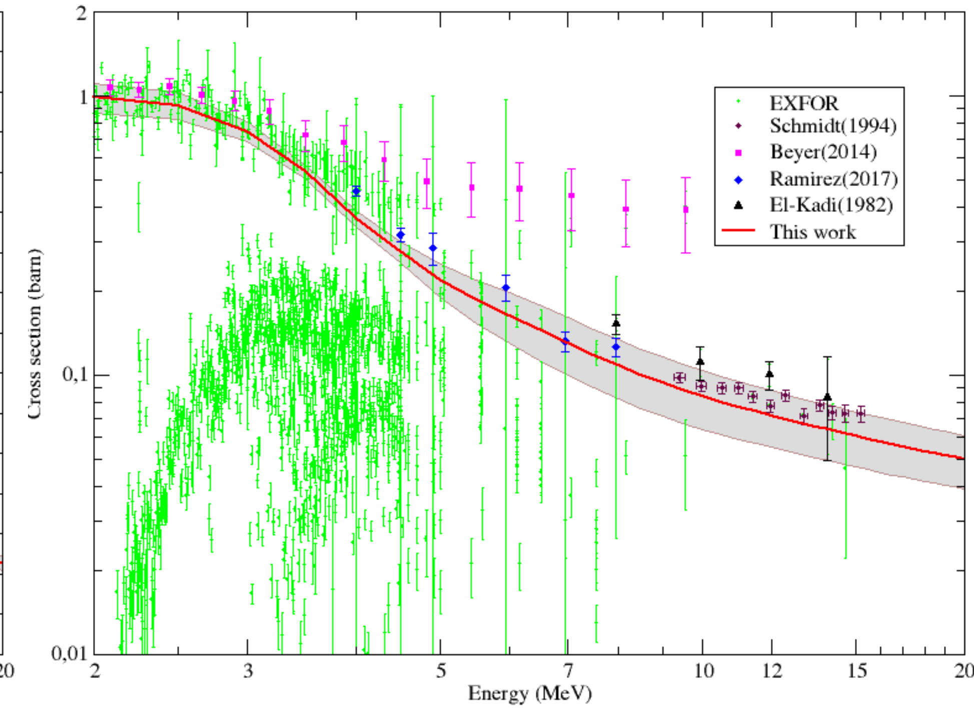
Elastic cross section

- The smooth trends of our cross sections are in good agreement with experimental data
- More realistic uncertainties are obtained (5%, discrepancies among experimental data)

Comparison with experimental data



Total inelastic cross section



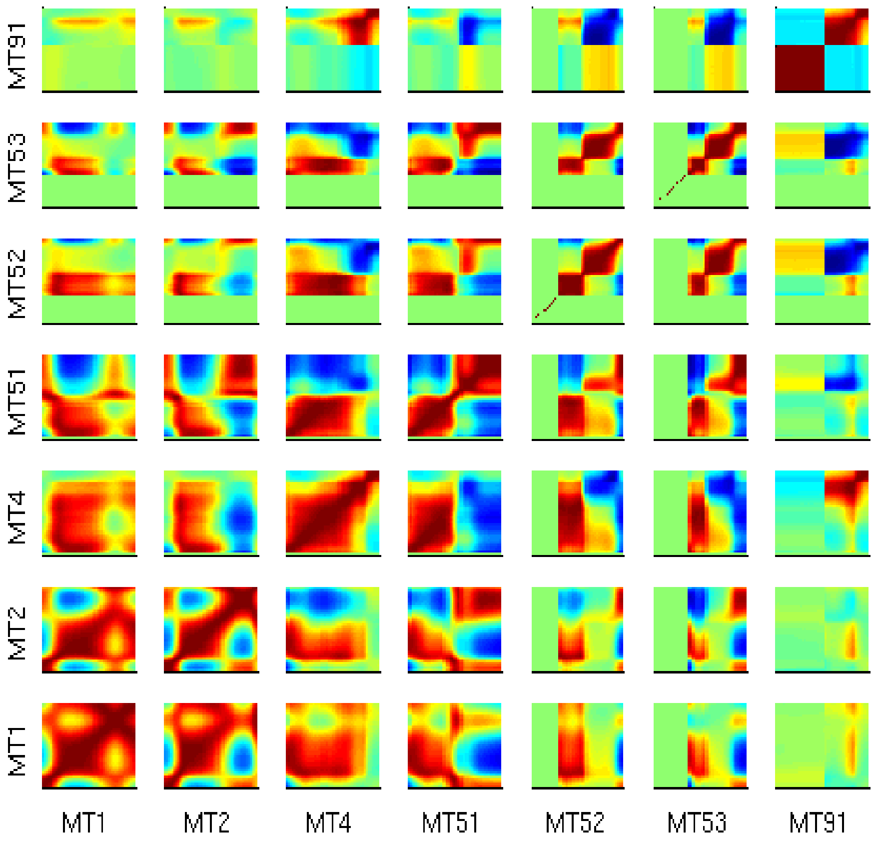
First-level-inelastic scattering cross section

- Neglecting fluctuation
- Agreement with Beryer & Negret > 4 MeV

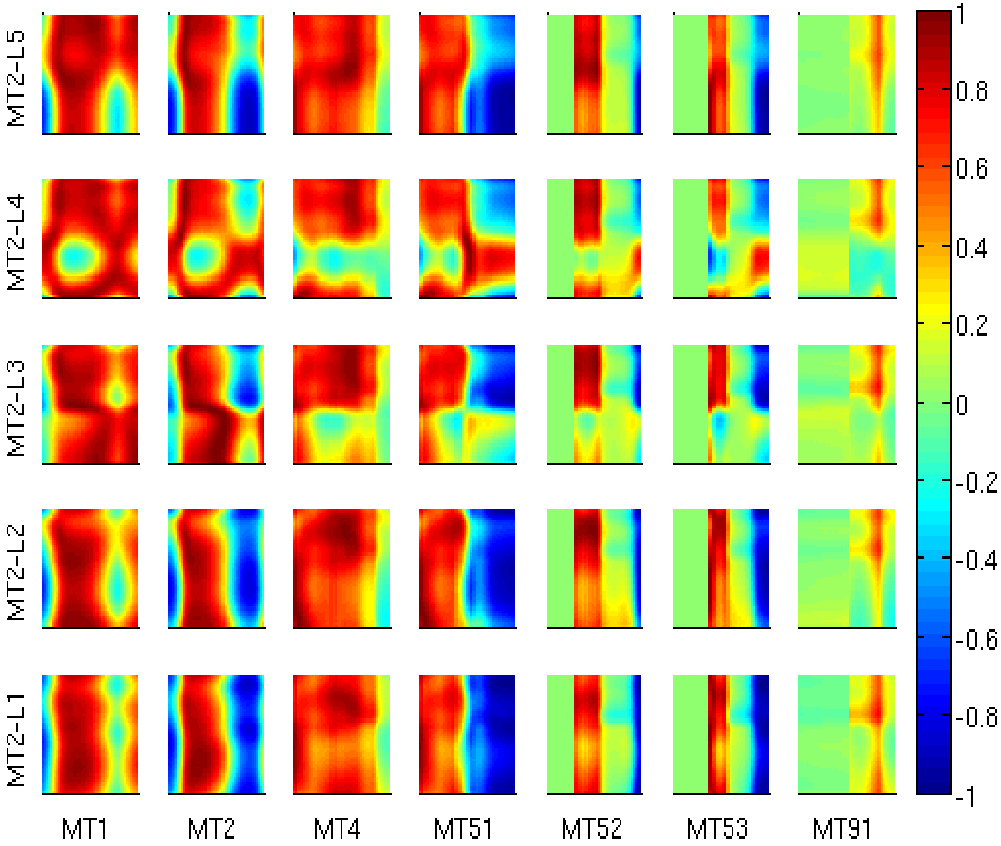
- Neglecting fluctuation
- Agreement with Schmidt & Ramirez (& El-Kadi)

Correlation matrix

Incident energy [860 keV, 20 MeV], divided into 80 groups



Correlations between different **cross sections**

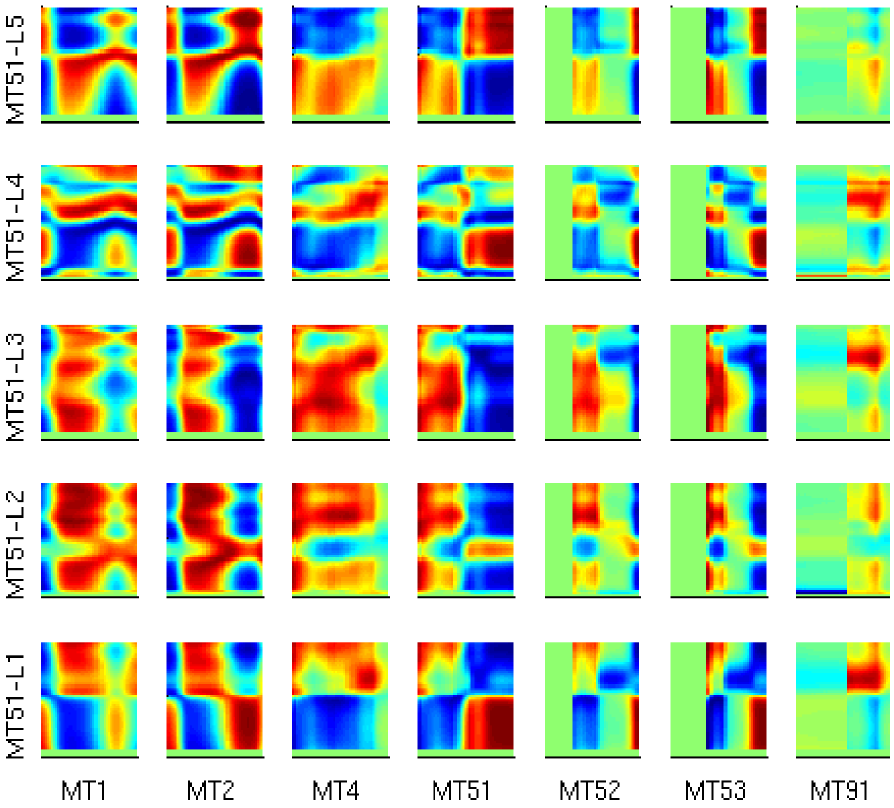


Correlations between different **cross sections** and **angular distribution** of <u>elastic</u> scattering

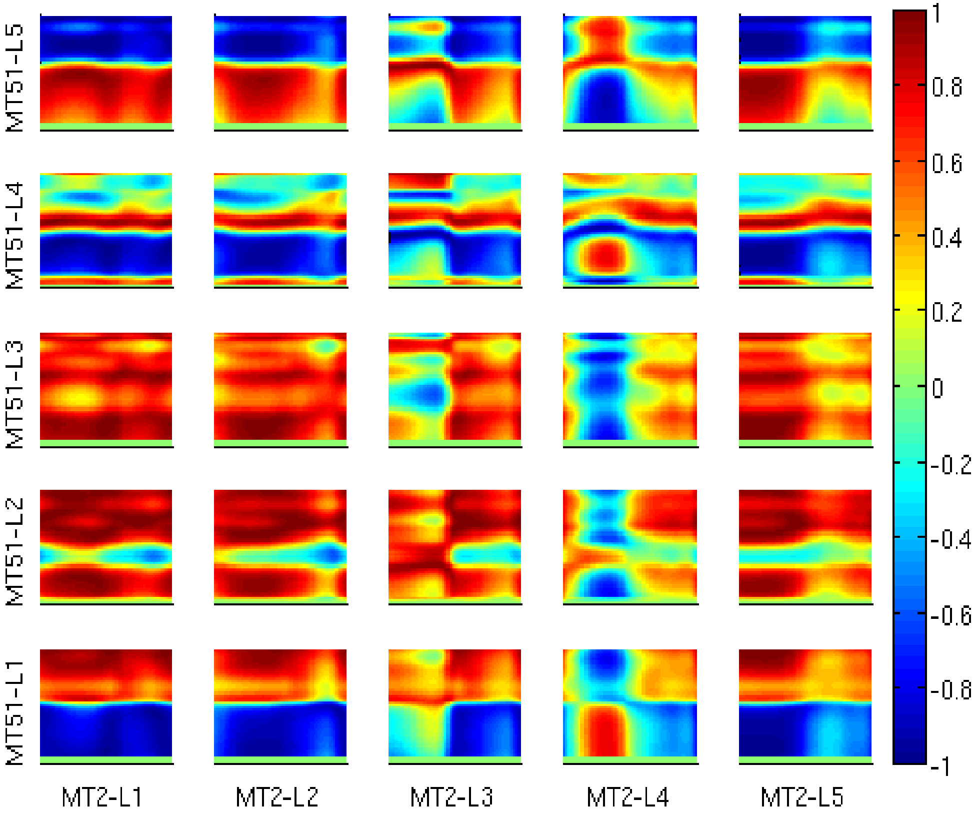
Correlation between different cross sections and elastic scattering angular distributions!

Correlation matrix

Incident energy [860 keV, 20 MeV], divided into 80 groups



Correlations between different **cross sections** and **angular distribution** of first-level-inelastic scattering



Correlations between different **angular distributions** of elastic scattering and first-level-inelastic scattering

Correlation between different cross sections and angular distributions of first-level-inelastic scattering!

Correlation between different angular distributions!

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Conclusions & prospects

- **Reproduction of cross sections in JEFF-3.1.1**
- **New evaluations from 2 MeV to 20 MeV (ECIS and TALYS)**
  - No cross section fluctuations
  - Good agreement with experimental data
- **Uncertainty Quantification using Bayes' theorem (CONRAD)**
- **Correlations between cross sections and angular distributions**

Prospects:

- **R-matrix limited evaluation in the resonance region (M. Diakaki, in progress)**
- **Integral validation of cross sections and angular distributions**
- **Uncertainty propagation to neutron fluence (CEA SERMA) & DPA (PhD subject) in reactor vessel & starting blocks**

Thanks for your attention!

Commissariat à l'énergie atomique et aux énergies alternatives
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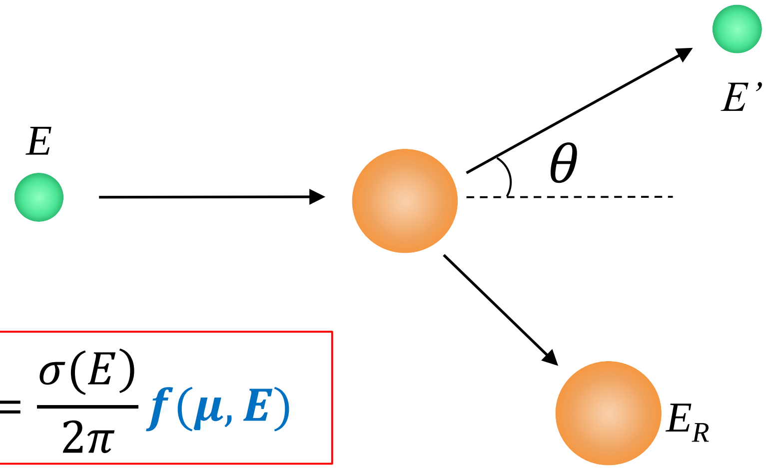
Angular distribution & Legendre coefficients



Angular distribution:

$$\sigma(\theta,\varphi,E)=\sigma(E)\boldsymbol{F(\theta,\varphi,E)}$$

$$\left.\begin{array}{l}\text{Isotropic } \varphi\\ \mu=\cos\theta\end{array}\right\}\quad \boxed{\sigma(\theta,\varphi,E)\equiv\sigma(\mu,E)=\frac{\sigma(E)}{2\pi}\boldsymbol{f(\mu,E)}}$$

Angular distribution & Legendre polynomials:

Legendre coefficients ⇔ Angular distribution

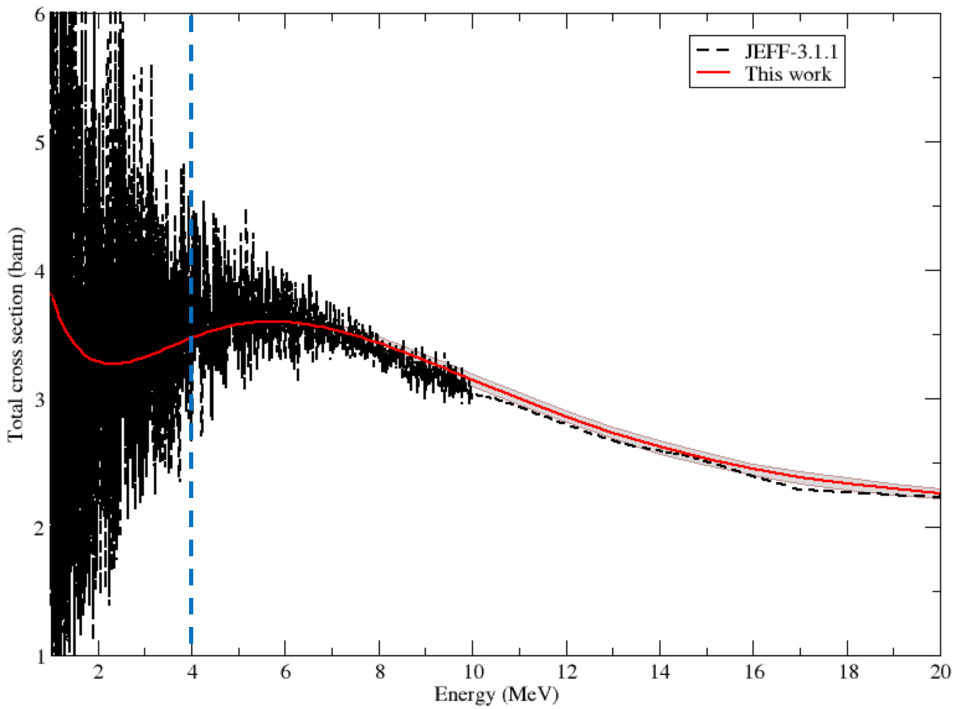
$$f(\mu,E)=\sum_{l=0}^{NL}\frac{2l+1}{2}\boldsymbol{a_l(E)}P_l(\mu)$$

Legendre polynomials

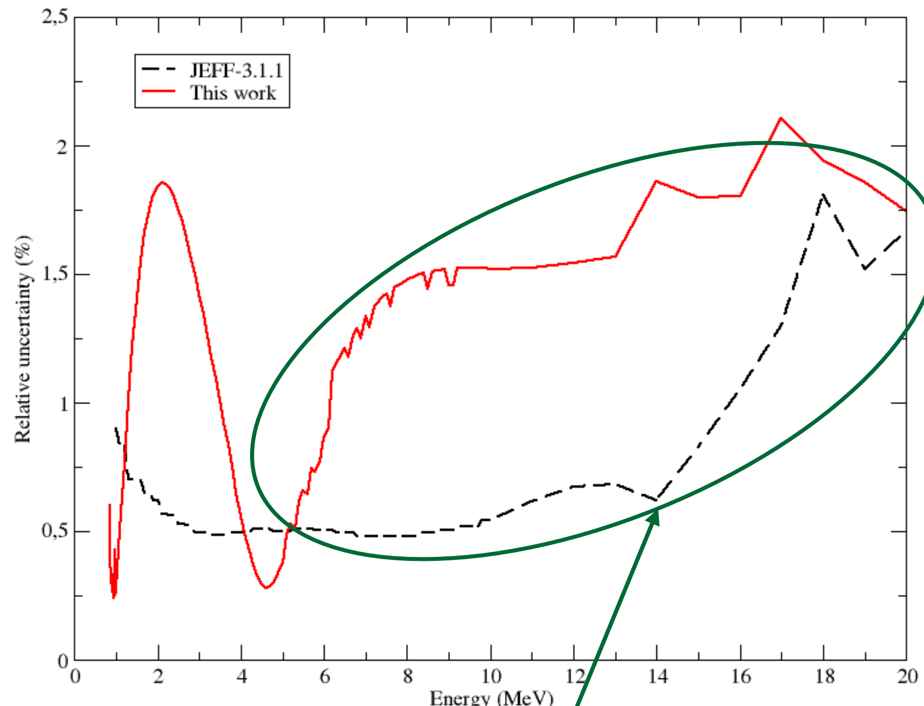
Multi-group coefficients of Legendre polynomials:

$$a_{l,n}=\frac{\int_{E_{n,inf}}^{E_{n,sup}}a_l(E)\sigma(E)dE}{\int_{E_{n,inf}}^{E_{n,sup}}\sigma(E)dE}\quad \text{or}\quad a_{l,n}=a_l\left(\exp\left[\frac{\ln\left(E_{n,inf}\right)+\ln\left(E_{n,sup}\right)}{2}\right]\right)$$

Results for the total cross section (ECIS)



Total cross section

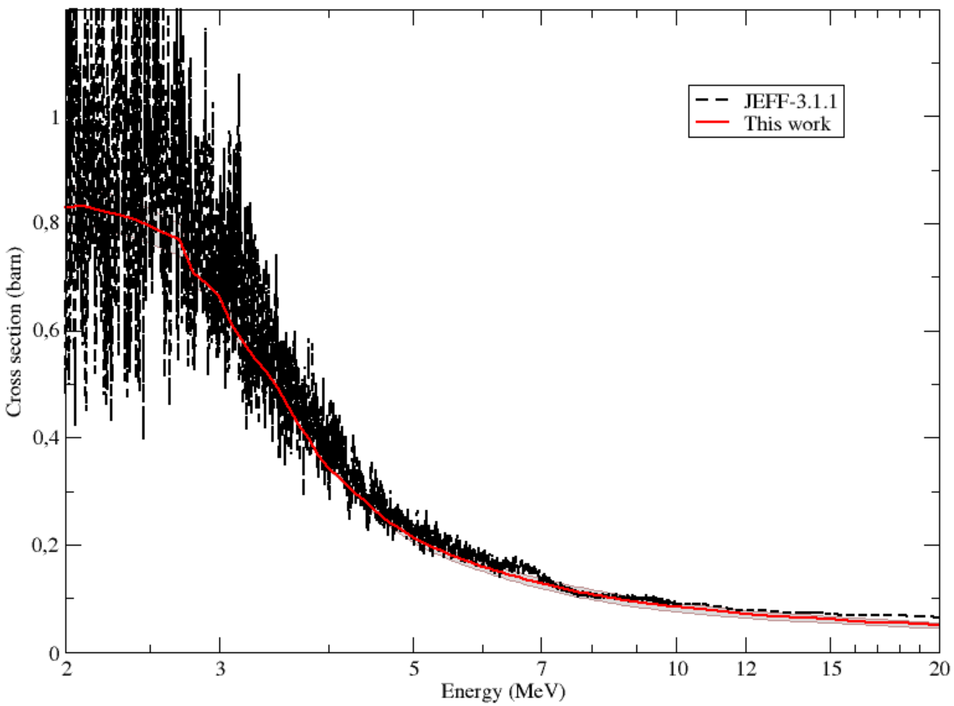


Relative uncertainty of total cross section

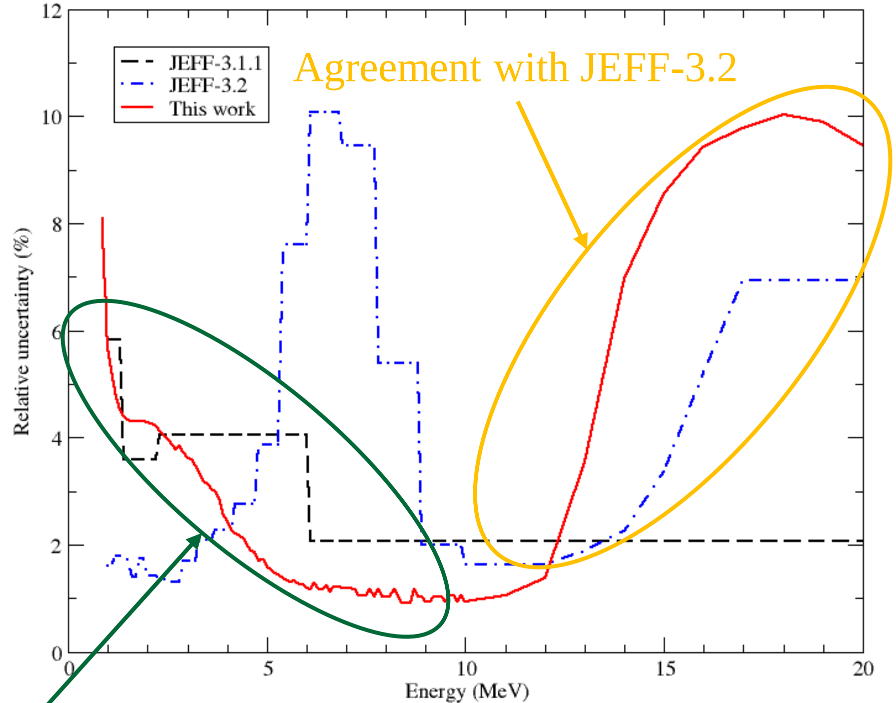
- Above 6 MeV, we obtain a more realistic relative uncertainty on the total cross section which is close to 1.8% in average
- Below 6 MeV, our work need to be improved

Higher uncertainty than JEFF-3.1.1
(from elastic & inelastic scatterings)

Results for the inelastic cross sections (TALYS)



First-level-inelastic scattering cross section

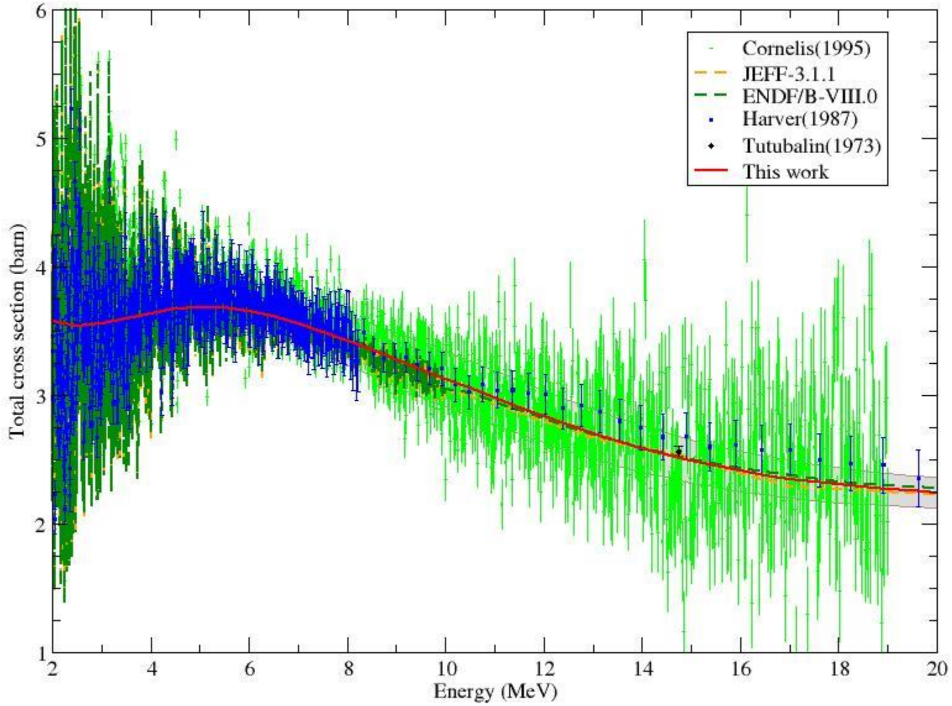


Relative uncertainty of total inelastic scattering cross section

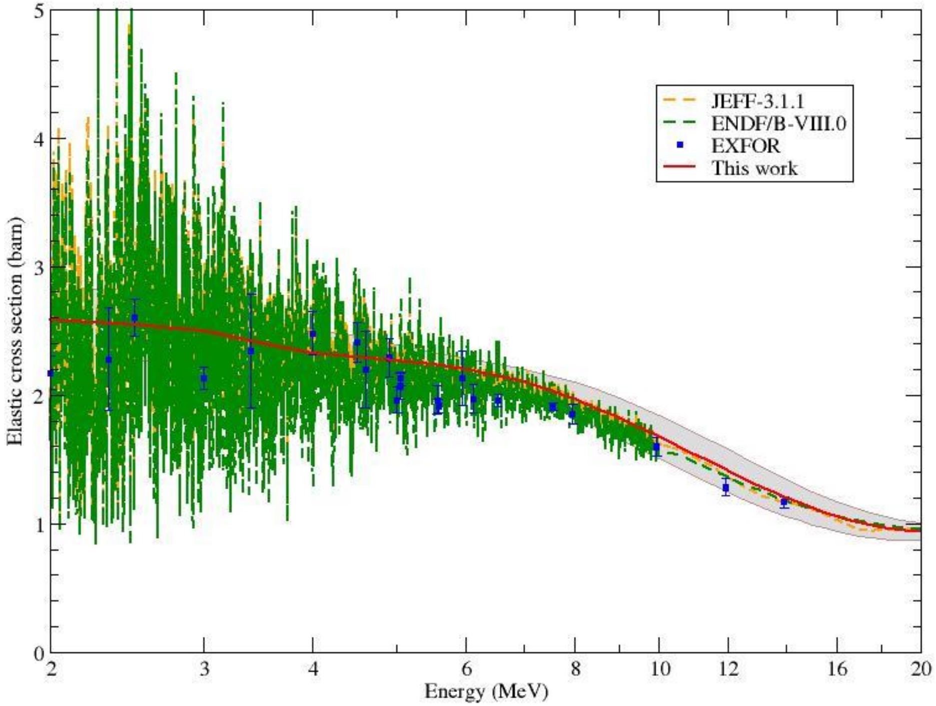
Agreement with JEFF-3.1.1

- Agreement between JEFF-3.1.1 and our TALYS calculations is difficult to improve due to the large resonant structures in the inelastic channel
- However, we succeeded to obtain relative uncertainties in good agreement with those from JEFF-3.1.1

Total & elastic cross sections



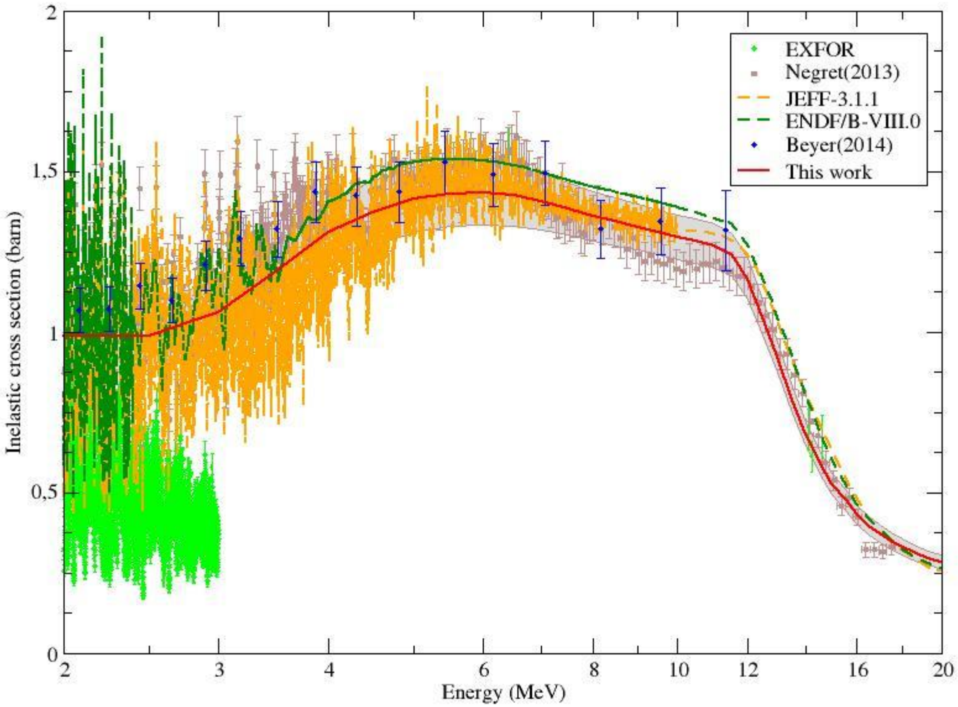
Recalculated **total** XS & experimental data



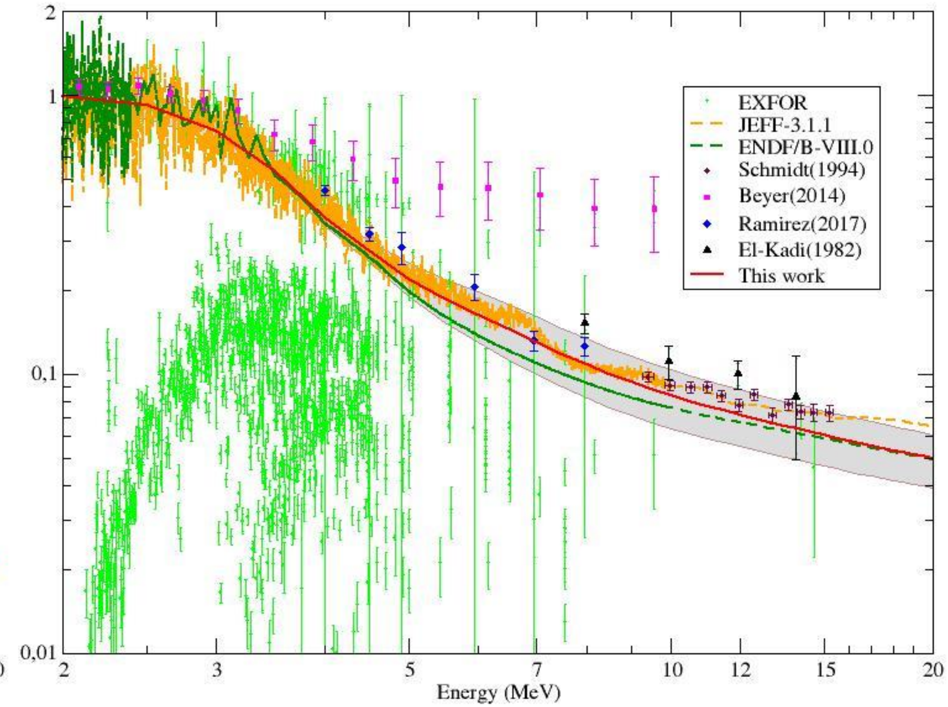
Recalculated **elastic** XS & experimental data

- Good agreement with experimental data and evaluated data
- Realistic uncertainties (5%, discrepancies among experimental data)

Total & 1st level inelastic scattering cross sections



Recalculated **total inelastic** XS & experimental data



Recalculated **first-level-inelastic** XS & experimental data

- Neglecting fluctuation (agree with B8.0)
- Agreement with Beryer & Negret > 4 MeV

- Neglecting fluctuation (agree with B8.0)
- Better agreement with Schmidt & Ramirez (& El-Kadi) than B8.0