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Kernel approximation and ^{52}Cr, ^{56}Fe, ^{58}Ni covariances in the resonance region

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What was our challenge?

Under AFCI covariance project the NNDC is responsible for structural materials, of which 56-Fe, 52-Cr and 58-Ni represent top priority. The resonance region is of primary importance since it extends up to 0.8 MeV - 1 MeV.

During FY2008-2009 we tried several strategies to meet this obligation, but AFCI (fast reactor) users at INL and ANL kept telling us that our uncertainties are far too small.

In FY2010 we radically changed the strategy and developed new approach in the resonance region based on kernel approximation.

Genesis of kernel approximation

Basic idea is not new, it goes back to 1980:

Proposed by J.D. Smith, ORNL, master thesis.

Employed by PUFF and NJOY to process MF32 capture and fission into cross section covariances.

Advocated by F. Fröhner for estimating covariances using statistical model of neutron resonance reactions (Hauser-Feshbach with width fluctuation corrections).

Used by S. Mughabghab for quick estimates of covariances.

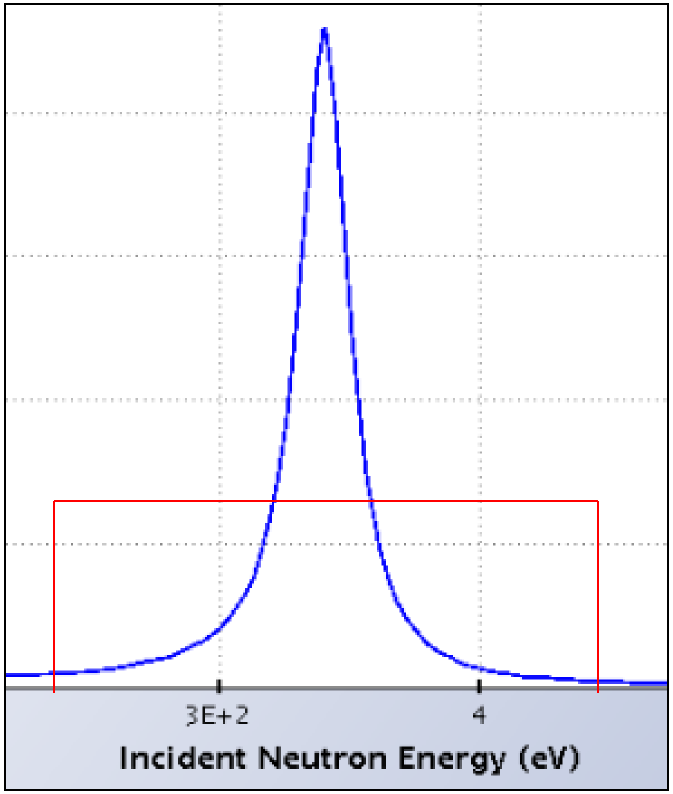
Detailed formalism for capture and elastic scattering developed by the NNDC in FY2010. Applied to 55-Mn, 52-Cr, 56-Fe and 58-Ni, …

What is kernel approximation?

Three step procedure:

1. Replace detailed resonance shape with average cross section.
2. Compute uncertainties of these averages by propagating parameter uncertainties from Atlas.
3. Combine uncertainties into covariance matrix by adding suitable level-level correlations.

55-Mn(n,g)



Area under the peak is proportional to capture kernel, $A_\gamma = g\Gamma_n \Gamma_\gamma/\Gamma$, which can be derived from Breit-Wigner or Hauser-Feshbach.

Why kernel approximation?

Advantages

It is transparent

- Formalism is analytical
- Results are easy to reproduce
- Results are easy to explain

It addresses several MF32 issues

- Lack of systematic uncertainties (level-level correlations)
- Lack of potential scattering uncertainty
- Avoids dubious adjustment of thermal region with RRR
- Does not rely on processing codes

Disadvantages

It is approximate

- Covariances are produced in broad energy bins
- Relatively crude treatment of interferences

MF32 systematic uncertainty issue

F. Fröhner, ND1994, Gatlinburg: “For modern TOF data statistical uncertainties are a tiny fraction of the true, correlated uncertainties. The SAMMY fits[1)] to high resolution resonance data for 56-Fe are most impressive, but the published statistical uncertainties are misleading. The reported s-wave radius parameter R’=5.437 0.002 fm gives no hint of the actual uncertainty. The same is true for the reported neutron widths, *e.g.*, Γ_n = 1409.3 1.1 eV for the big s-wave resonance at 27.8 keV.”

1) Perey *et al*, “56-Fe resonance parameters…”, ORNL/TM-11742 (1990).

Perey:	R’= 5.4 0.002fm	(0.04%)	Γ_n = 1409.3 1.1eV	(0.08%)
Atlas:	5.9 0.3 fm	(5.1%)	1409 60 eV	(4.2%)

MF32 potential scattering issue

WPEC Subgroup 2 "*Generation of Covariance Files for Fe-56 and Natural Fe*", coordinator H. Vonach, monitor H. Gruppelaar (1989-2001), final report:

"A complete set of covariances for the resonance parameters of 56Fe was derived by F. Fröhner and put into ENDF format (file 32). There are, however, serious problems in the use of this information as the important potential scattering radii uncertainties cannot at present be stored in the ENDF-6 format. Therefore also the existing codes neglect the uncertainties of the potential scattering radii and thus lead to unrealistically small cross-section uncertainties."

56-Fe MF32 was not included into JEFF-3 due to ΔR' issue. Fröhner's 1993 proposal to CSEWG for ΔR' format extension got lost.
Comment: Proposal recovered by D. Muir from his archive in summer 2010.

ΔR' format extension was adopted by CSEWG in 2009. However, it is too simple, and none of current MF32 files in ENDF/A include ΔR'.

Formalism

Thermal region

- $\Delta\sigma(E) \approx \Delta\sigma(E_{th})$ for capture, $\sigma(E)$ follows 1/v law
- $\Delta\sigma(E) \approx \Delta\sigma(E_{th})$ for elastic scattering, $\sigma(E) \approx$ const

Resonance region

- kernel approximation for capture
- kernel approximation for elastic scattering

Kernel formalism for capture

Average cross sections

It can be derived from Breit-Wigner:

$$A_\gamma = \int_{-\infty}^{+\infty} \sigma_\gamma(E)dE,$$

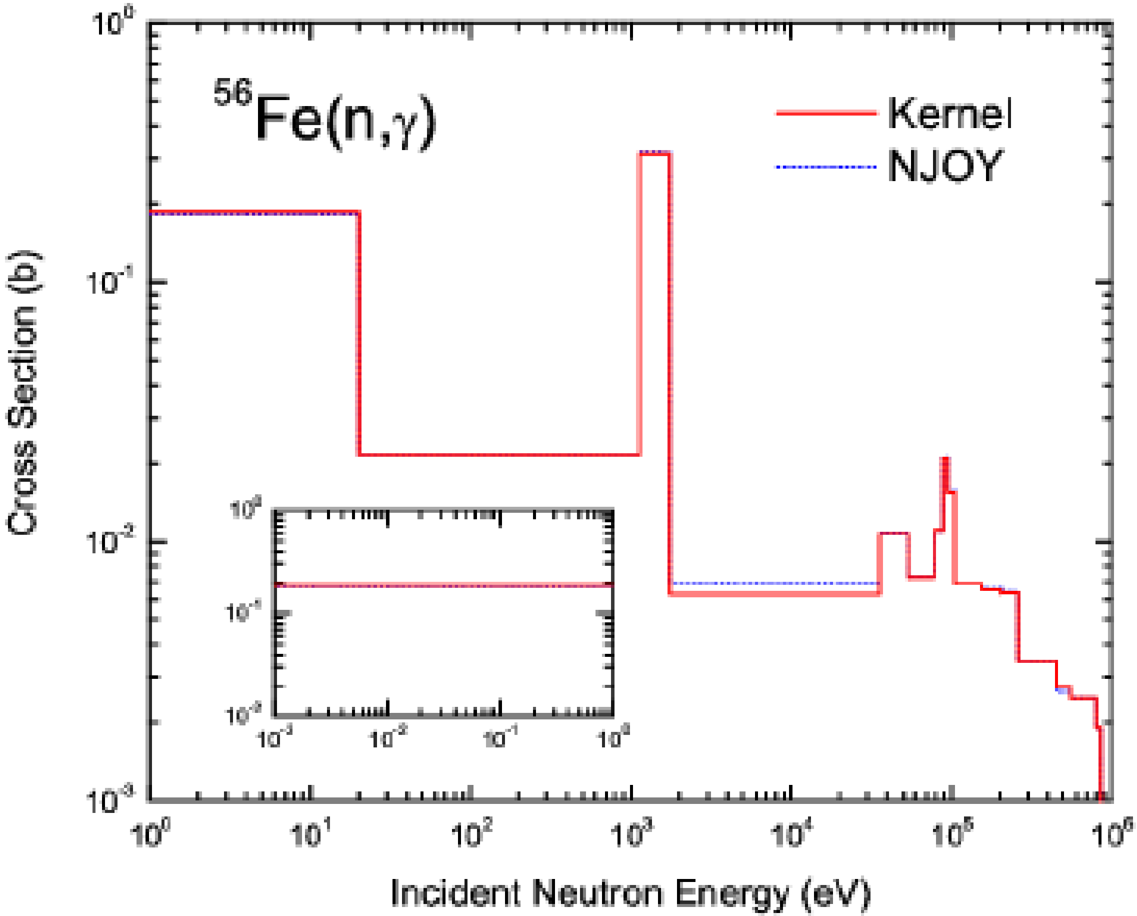
$$A_\gamma = 2\pi^2 \lambda\!\!\!^{-2} g \frac{\Gamma_n \Gamma_\gamma}{\Gamma}.$$

$$\Delta E = E_1 - E_2$$

$$\bar{\sigma}_\gamma = \frac{1}{\Delta E} \int_{E_2}^{E_1} \sigma_\gamma(E)dE \approx \frac{1}{\Delta E} \int_{-\infty}^{+\infty} \sigma_\gamma(E)dE = a\frac{g\Gamma_n\Gamma_\gamma}{\Gamma},$$

Example: Average cs for 56-Fe(n,g)

Kernel approximation works well for capture as can be seen from comparison with average cross sections obtained by NJOY. Thermal region (1/v law) extends up to ~1 keV.



Kernel formalism for capture, cntn'd

Sensitivities, uncertainties

Single resonance:

$$\frac{\partial\bar{\sigma}_\gamma}{\partial\Gamma_n} = a\frac{g\Gamma_n\Gamma_\gamma}{\Gamma}\frac{\Gamma_\gamma}{\Gamma}\frac{1}{\Gamma_n} = \bar{\sigma}_\gamma\frac{\Gamma_\gamma}{\Gamma}\frac{1}{\Gamma_n}$$

$$\frac{\partial\bar{\sigma}_\gamma}{\partial\Gamma_\gamma} = a\frac{g\Gamma_n\Gamma_\gamma}{\Gamma}\frac{\Gamma_n}{\Gamma}\frac{1}{\Gamma_\gamma} = \bar{\sigma}_\gamma\frac{\Gamma_n}{\Gamma}\frac{1}{\Gamma_\gamma}.$$

$$\left(\Delta\bar{\sigma}_\gamma\right)^2 = \left(\frac{\Gamma_\gamma}{\Gamma}\Delta\Gamma_n\right)^2 + 2\frac{\Gamma_n\Gamma_\gamma}{\Gamma^2}\left\langle\Delta\Gamma_n\Delta\Gamma_\gamma\right\rangle + \left(\frac{\Gamma_n}{\Gamma}\Delta\Gamma_\gamma\right)^2$$

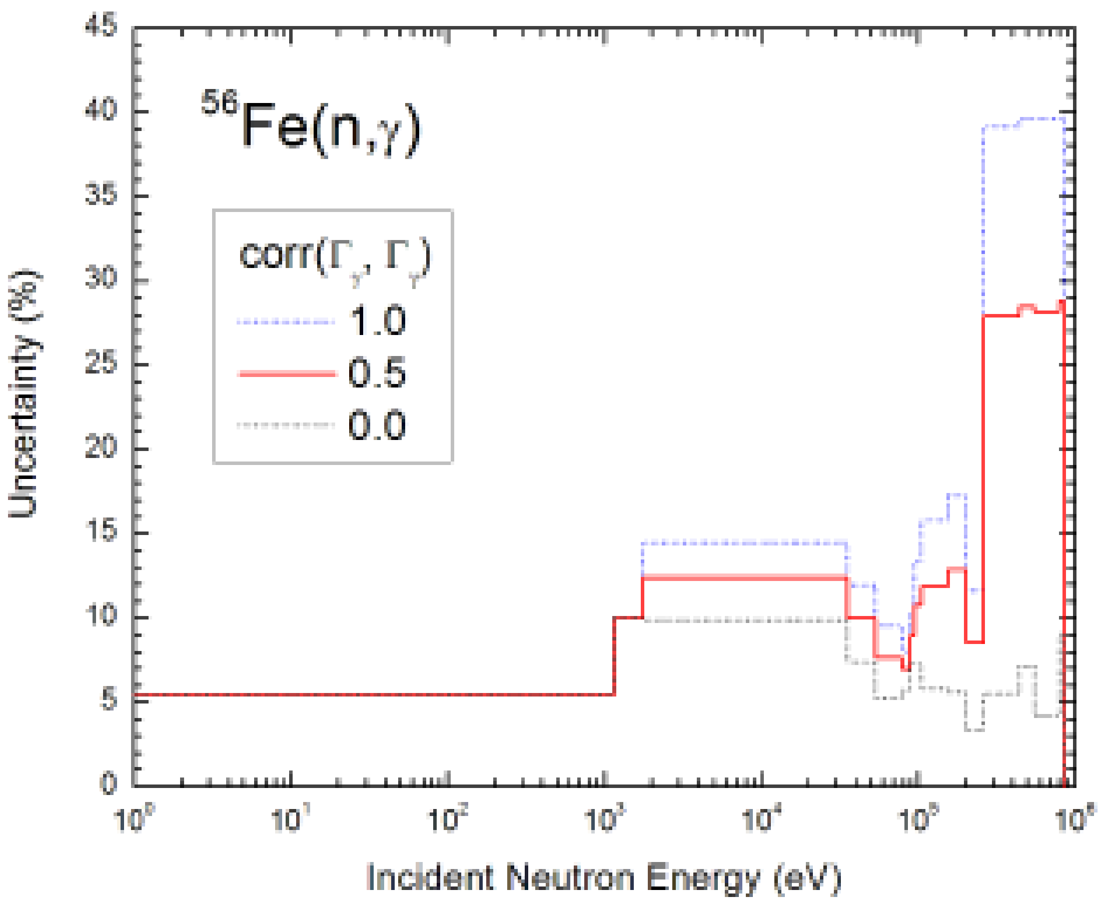
Example: Uncertainties for 56-Fe capture

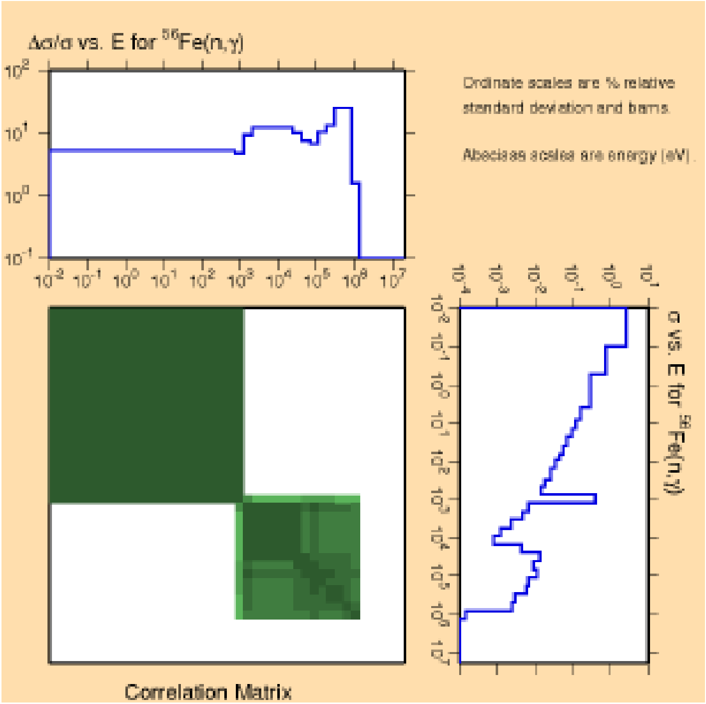
290 resonances, strong impact of level-level correlation

56-Fe: $\Gamma n \gg \Gamma_\gamma$, therefore kernel $(\Gamma_n/\Gamma)\Gamma_\gamma \approx \Gamma_\gamma$; $\Delta\Gamma_\gamma \approx$ const

If corr = 1 then $\Delta\sigma \approx \Delta\Gamma_\gamma$, if corr = 0 then $\Delta\sigma \approx \Delta\Gamma_\gamma/N^{1/2}$

For N ≈ 50 the difference is about a factor of 7 !!





Kernel formalism for elastic scattering
Average cross sections

It can be derived from Breit-Wigner:

$$\sigma_{\mathrm{el}}(E) = 4\pi\lambdabar^2(2l+1)\sin^2\phi_l + \pi\lambdabar^2 g \frac{\Gamma_n^2 - 2\Gamma_n\Gamma\sin^2\phi_l + 2(E-E_0)\Gamma_n\sin(2\phi_l)}{(E-E_0)^2 + \frac{1}{4}\Gamma^2}$$

$$\bar{\sigma}_{\mathrm{el}} = \frac{1}{E_2 - E_1}\int_{E_1}^{E_2}\sigma_{\mathrm{el}}(E)\,dE = \bar{\sigma}_{\mathrm{el}}^{pot} + \bar{\sigma}_{\mathrm{el}}^{res}$$

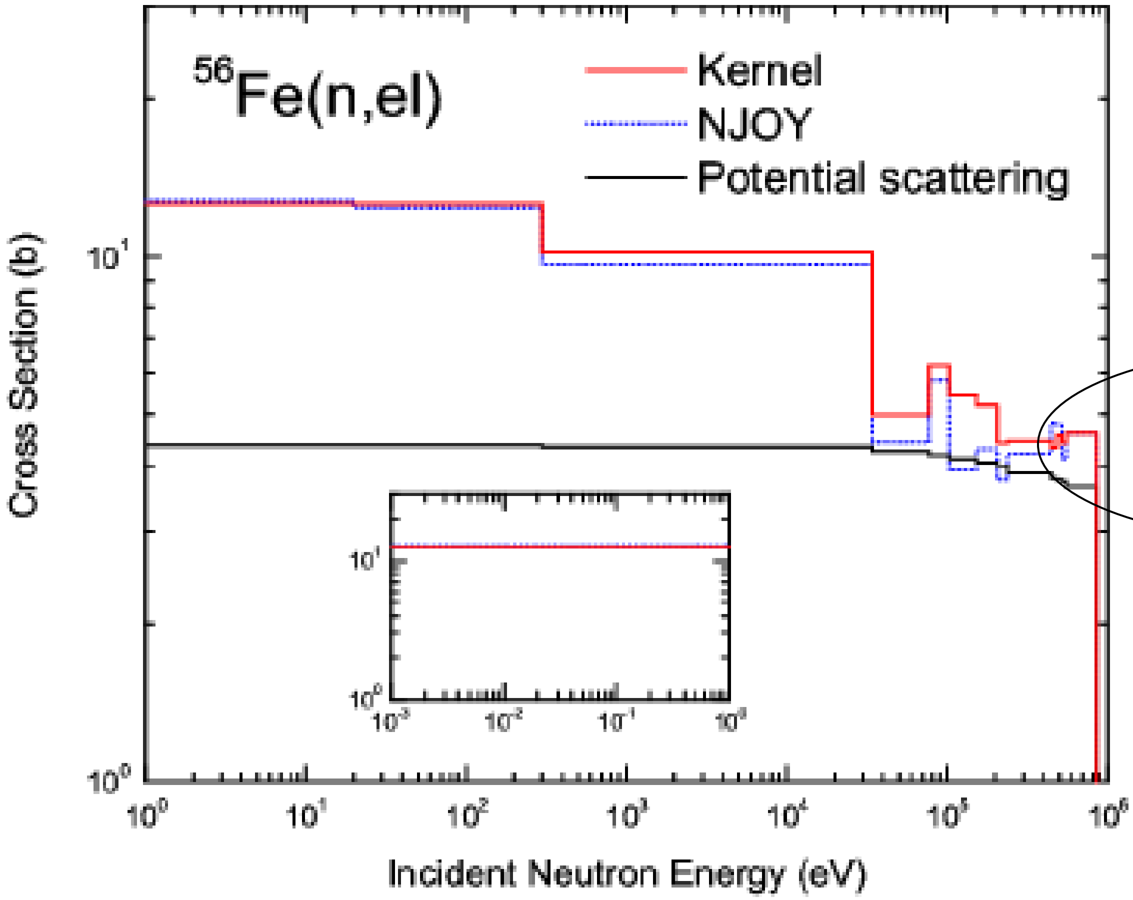
$$\bar{\sigma}_{\mathrm{el}}^{pot} = 4\pi\lambdabar^2(2l+1)\sin^2\phi_l \approx 4\pi R'^2$$

$$\bar{\sigma}_{\mathrm{el}}^{res} \approx \frac{\pi\lambdabar^2 g}{E_2 - E_1}\frac{g\Gamma_n(\Gamma_n - 2\Gamma\sin^2\phi_l)}{\Gamma} \approx \frac{\mathrm{const}}{E}\frac{g\Gamma_n\Gamma_n}{\Gamma}$$

Important points:
- negative and positive interference terms approximately cancel out
- average cross section is sum of potential and resonance terms
- potential scattering term is approximately constant
- resonance term vanishes with the energy

Example: 56-Fe(n,el) average cs

Kernel approximation for elastic is acceptable, though not perfect.
σ_{res} decreases with E, σ_{pot} makes major contribution at high E, therefore $\Delta R'$ would contribute considerably to $\Delta\sigma_{el}$



$\sigma_{res} \approx 1$ b

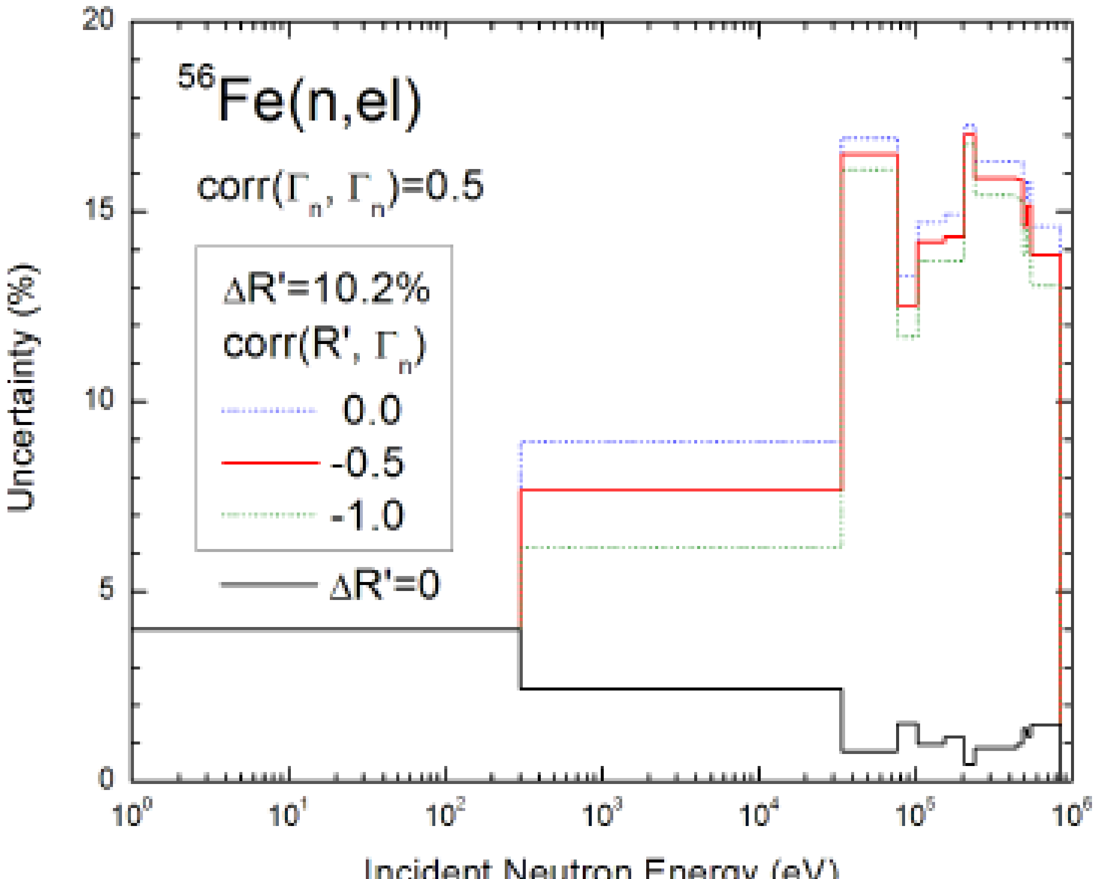
$\sigma_{pot} \approx 3.7$ b

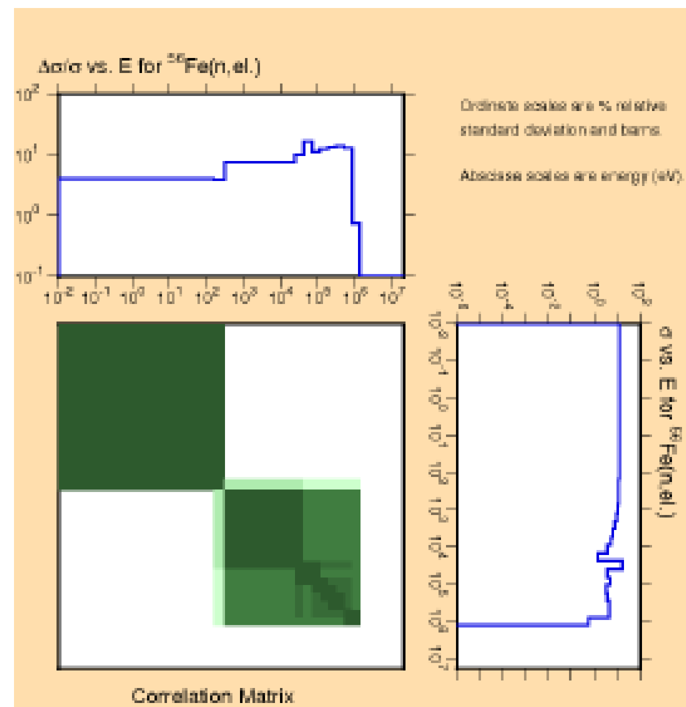
Example: 56-Fe(n,el) uncertainties

Contribution from ΔR' is crucial

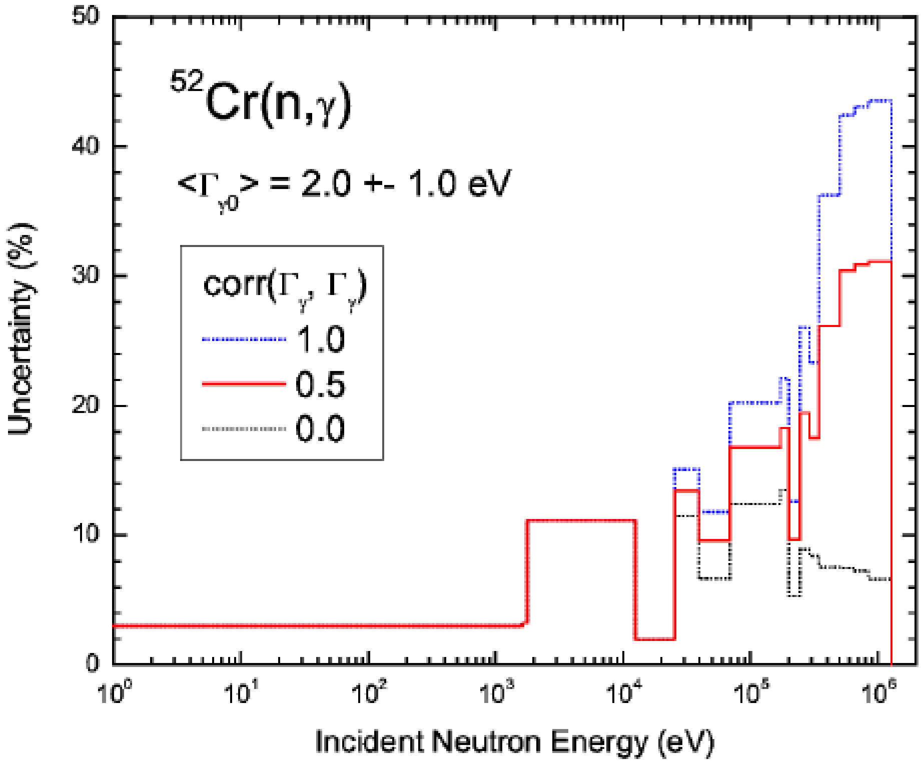
Elastic cs at high resonance energies is dominated by potential scattering.

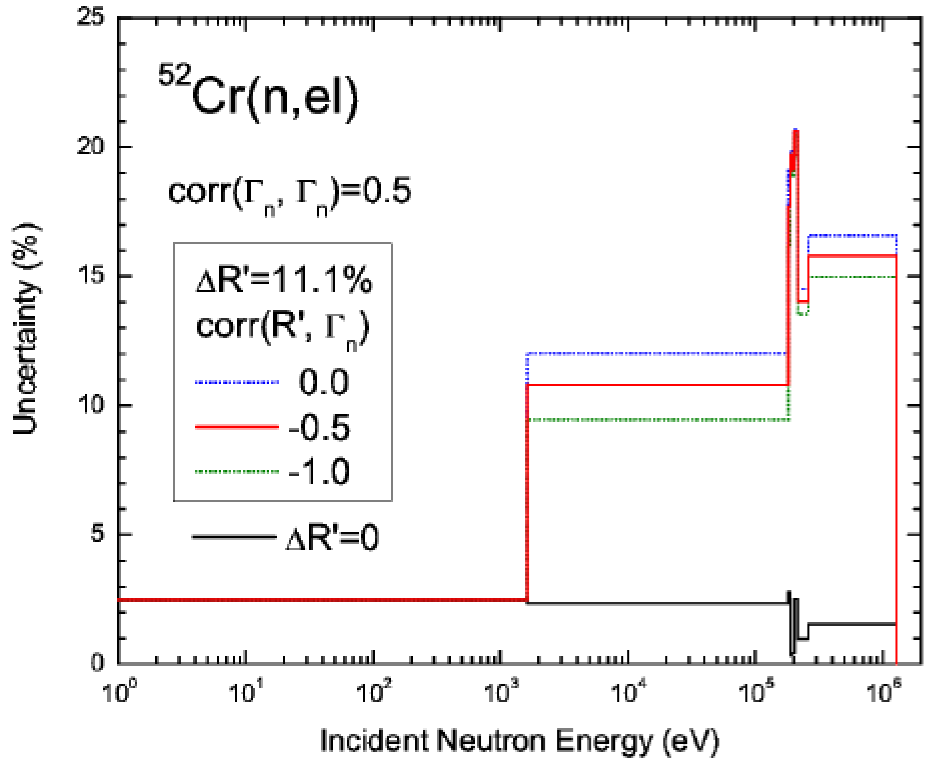
ΔR' in Atlas is valid for thermal energy! We assume $\Delta R'(E_{res}) = 2\Delta R'(E_{th})$





52-Cr capture and elastic
Dramatic difference with MF32 at 1 MeV

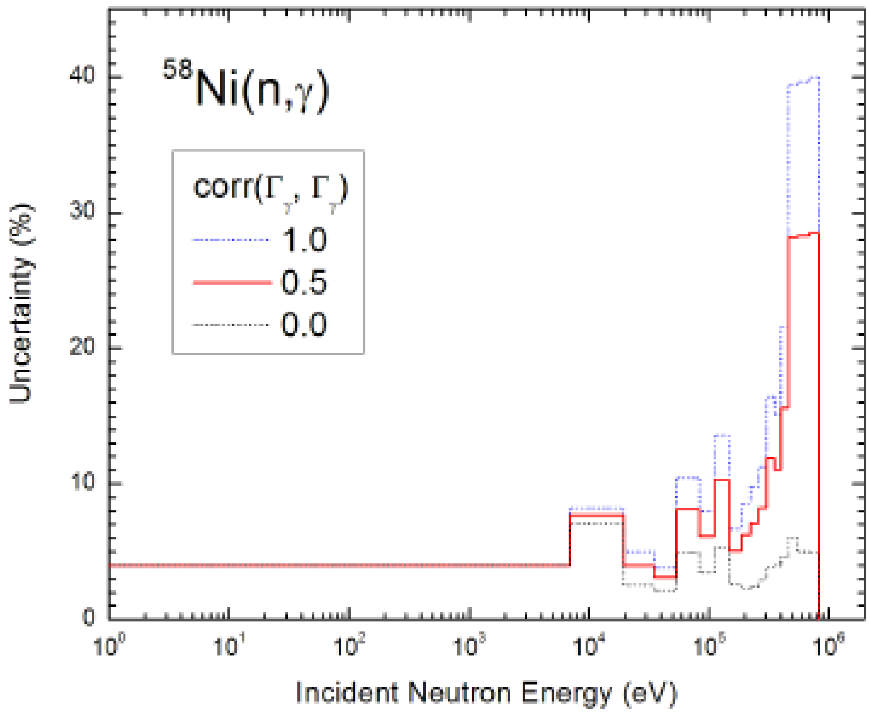


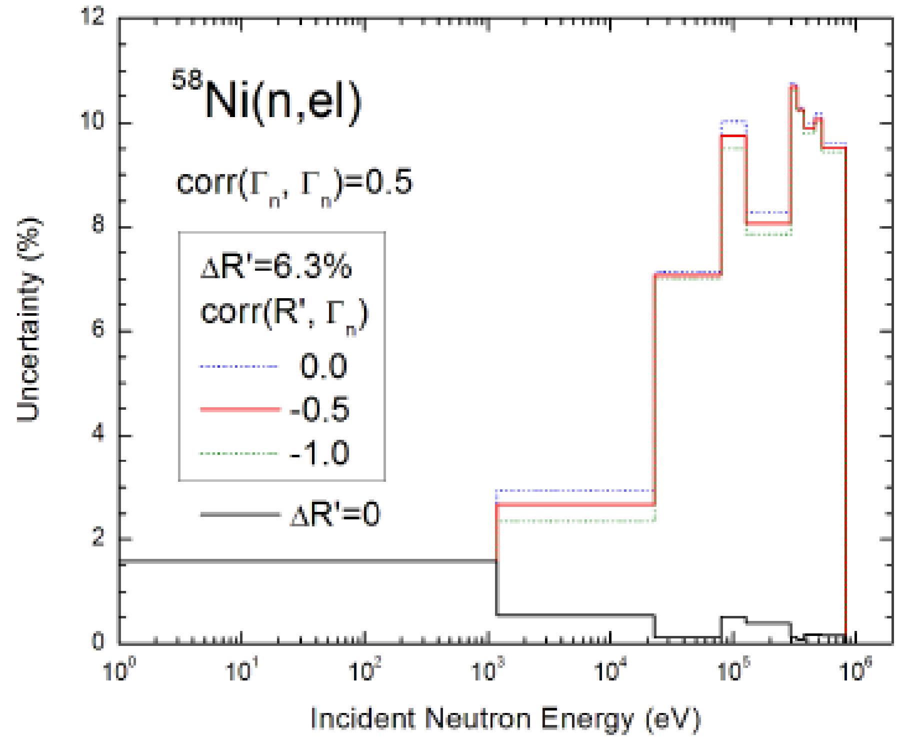


Reaction	Energy	Uncertainty Present	Uncertainty ENDF/A	Uncertainty JENDL-4.0	Comment
^{52}Cr(n,γ)	Thermal	3%	20%	2%	Error in ENDF/A
	1 MeV	30%	3%	2%	Lack of corr in ENDF/A?
^{52}Cr(n,el)	Thermal	2.5%	6.5%	1%	Error in ENDFA
	1 MeV	15%	2%	0.3%	No $\Delta R'$ in ENDF/A

58-Ni capture and elastic

Dramatic difference with MF32 at 600-800 keV





Reaction	Energy	Uncertainty Present	Uncertainty ENDF/A	Comment
^{58}Ni(n,γ)	Thermal	4%	3.5%	Agreement
	10-10^3 eV	4%	22%	Due to direct capture in ENDF/A?
	600-800 keV	28%	3%	No correlation in ENDF/A?
^{58}Ni(n,el)	Thermal	1.6%	1.8%	Agreement
	10-10^3 eV	2.5%	2%	Agreement
	600-800 keV	9.5%	1.5%	No ΔR' in ENDF/A

Quality Assurance

Format: MF33, complies with ENDF-6 format

Mathematics: symmetry, Schwarz inequality, positive-definiteness

Physics: plausibility of uncertainties

- Checked for 33 groups, minimal value set to 2%
- Uncertainties of integral quantities (thermal, RI, 30-keV Maxw)

Reaction	Thermal		Resonance Int.		30-keV Maxwellian	
	This work[a]	Atlas	This work[b]	Atlas	This work[c]	KADoNiS
^{52}Cr(n,γ)	3.0%	2.3%	2.8%	-	8.3% (8.7 mb)	26% (8.8 mb)
(n,el)	2.5%	0.7%				
^{56}Fe(n,γ)	5.4%	5.4%	4.9%	11%	7.8% (11.5 mb)	4.3% (11.7 mb)
(n,el)	4.0%	3.9%				
^{58}Ni(n,γ)	4.0%	2.3%	3.8%	9.5%	4.5% (39.9 mb)	3.9% (38.7 mb)
(n,el)	1.6%	1.6%				

Summary and Conclusions

We developed new method using kernel approximation for covariances in the resonance region. Its major strength is transparency. The method can handle level-level correlations and potential scattering.

The method was applied to major structural materials. It was shown that capture strongly depends on level-level correlations, while elastic scattering is driven by potential scattering. Basic QA was performed and no major deficiencies were identified.

Comparison with MF32 data (ENDF/A) found fairly good agreement in thermal region, but sharp discrepancies were observed particularly at the high end of the resonance region. Our results suggest that MF32 data suffer from the lack of highly correlated systematic uncertainties including potential scattering uncertainty.