Covariances

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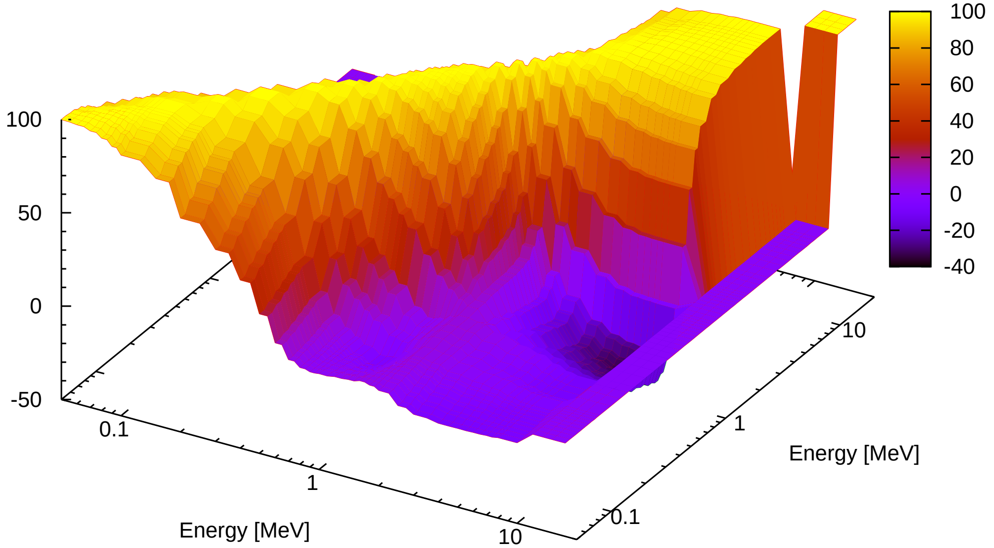


Covariance data needed (by nuclear data users)

- Estimation of margins/uncertainties in :
  - neutron multiplicities, k_{eff}, for the next generation reactors, ADS, criticality safety
  - isotope productions, MA, LLFP, fertile/fissile
- Quantities sensitive to k_{eff}
  - Cross section (MF3)
  - Resonance parameters (MF2)
  - $\overline{\mu}$, P_1 for elastic scattering (MF4, MT2)
  - Prompt fission neutron spectrum (MF5, MT18)
  - ν_p (MF1, MT456)

Evaluation Method

C.S. evaluated based on the experimental data

- Estimate a covariance by a Least-squares fitting to those measurements with GMA or SOK.
- Covariance of experimental data were re-constructed by evaluators.
- Examples — σ_t, σ_f, σ_{2n}, $\overline{\nu}$, *etc.*

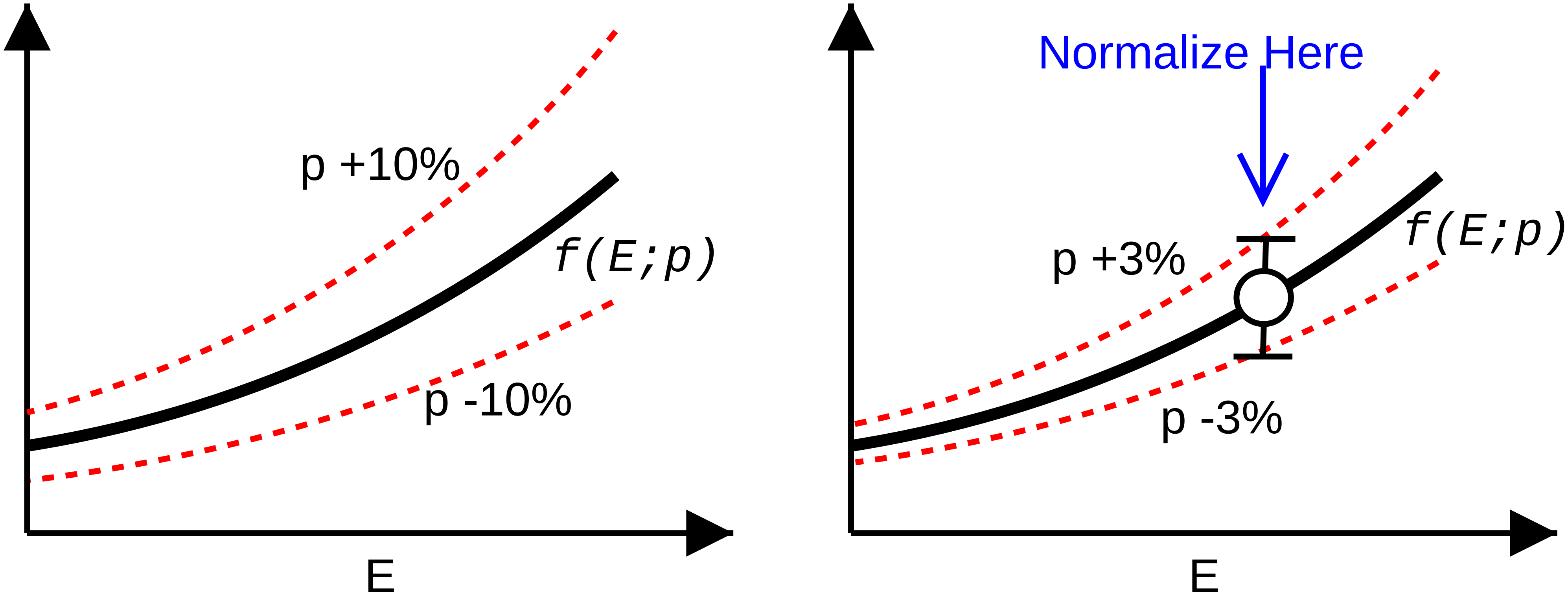
C.S. evaluated with a nuclear model

- Estimate the covariance with the KALMAN code.
- KALMAN calculates an error propagation from experimental data to the evaluated quantities though the covariance of model parameters.
- Examples: — σ_t (if OM used), σ_{inel}, χ, Legendre-coeff., resolved/unresolved resonance parameters.

Basic Idea

Inter/Extrapolation of experimental uncertainties

- Calculate sensitivities of model parameters
- Estimate uncertainties in the parameters by experimental data
- Calculate uncertainties in the cross sections by the parameter uncertainties



Covariance Data obtained by Fitting

Generalized Least-squares Fitting

- Estimate uncertainties at each energy-gird and correlations among them.
  - GMA : moves an experimental energy point to the nearest energy-grid.
  - SOK : assumes that $\sigma(E)$ varies linearly or it is constant between two energy-grids.
- No correlation if experimental data are uncorrelated.

Model Parameter Fitting

- Interpolation is made with some physical background.
- We believe that the model is “true.”
- Correlation exists even if experimental data are uncorrelated.

KALMAN Calculation

Covariance Evaluation with the KALMAN code

- includes
  - Statistical / systematic errors in the experimental data.
    - correlation from the systematic errors
  - Constraint by a physical model employed.
    - correlation from a model which is used for interpolation
- has advantages:
  - Inter/extra-polation of uncertainties to the region where no experimental data are available.
  - Deduction of uncertainties those can be obtained by calculations.

Covariance Evaluation for Gd Isotopes

We have generated covariance data for:

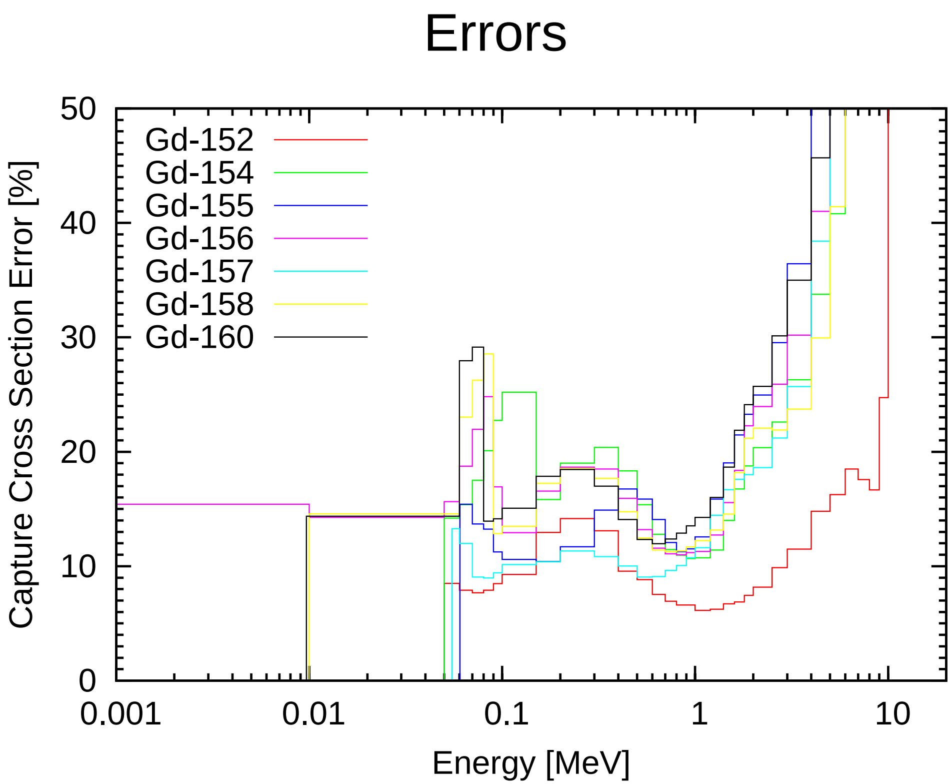
- Gd-152, 154, 155, 156, 157, 158, and 160, above resonance energy regions (LANL).
  - Total cross section
  - Neutron radiative capture cross section
  - Inelastic scattering cross section
  - Neutron emission reactions — $(n, 2n)$ and $(n, 3n)$
- Resonance parameters (ORNL).
  - Covariance of resonance parameters were generated with SAMMY

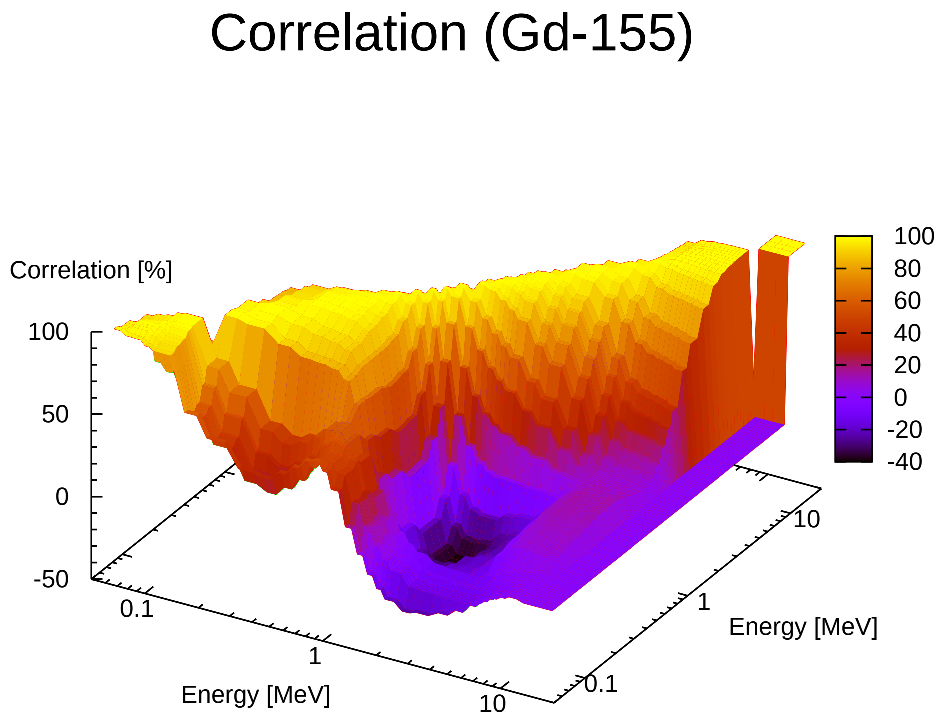
Covariance Evaluation Methods

- Covariance of the total cross section was estimated using a Least-squares analysis of experimental data.
  - The L-S method was adopted for the natural element of Gd, was then used for all isotopes.
- Covariances of the neutron capture and inelastic scattering cross sections, obtained from nuclear theory, are evaluated with the KALMAN code — which calculates uncertainties in the cross sections with the Bayesian parameter estimation method.
  - The statistical Hauser-Feshbach model was used to calculate cross sections and their model parameter covariances.
- An approximated (but reasonable) method was used to estimate covariances of $(n, 2n)$ reaction cross section, because they are less important for the criticality safety applications due to high-threshold energies.

Evaluated Uncertainties and Correlation

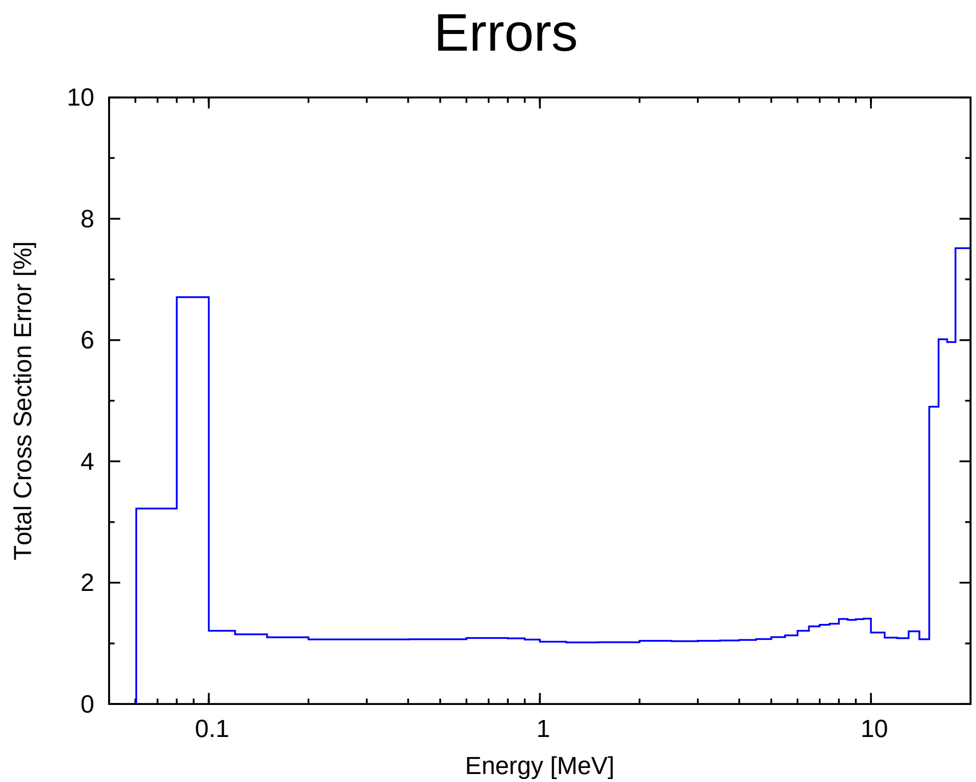
KALMAN Calculation for Neutron Capture

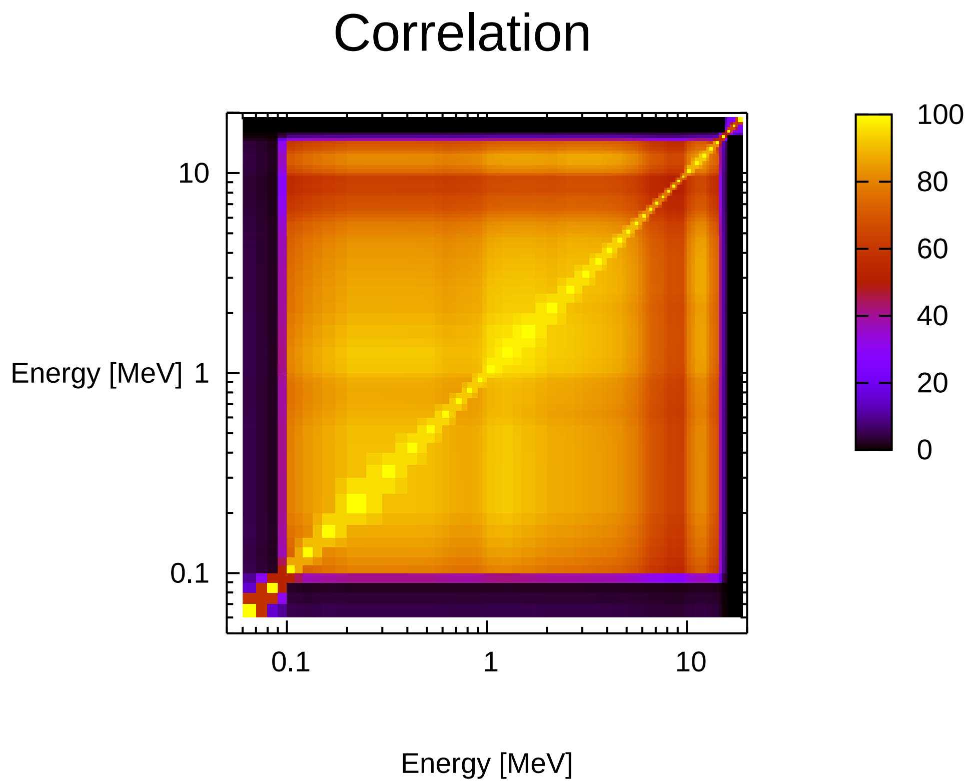




Evaluated Uncertainties and Correlation

SOK Calculation for Total C.S.





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Resonance Parameter Covariances

- Few information about resonance analyses in ancient times is available.
- Generation of covariance data for existing libraries in a simple way.
  - Larson implemented “**Retroactive Method**” to estimate a covariance matrix of resonance parameters in SAMMY.

Retroactive Method

- Generate simulated experimental data — calculate cross sections with the resonance parameters provided.
- Realistic energy points / resolution / background *etc.*, assumed by taking old experiments (ORELA, for example) into account.
- Estimate / assume uncertainties for the simulated data
- Generate a resonance covariance so as to reproduce the simulated uncertainties.

Resonance Parameter Covariances

SAMMY Output

- Standard ENDF/B-6 format, which can be processed with ERRORJ
- New “compact format”, which also can be processed with ERRORJ now.

Combined Data

- Leal evaluated the covariance of resolved/unresolved resonance region for all isotopes, and combined with the high energy data of LANL. They were processed with NJOY and ERRORJ.
- Comprehensive tests have not been done yet.

Comparison with N.Larson's Retroactive Method

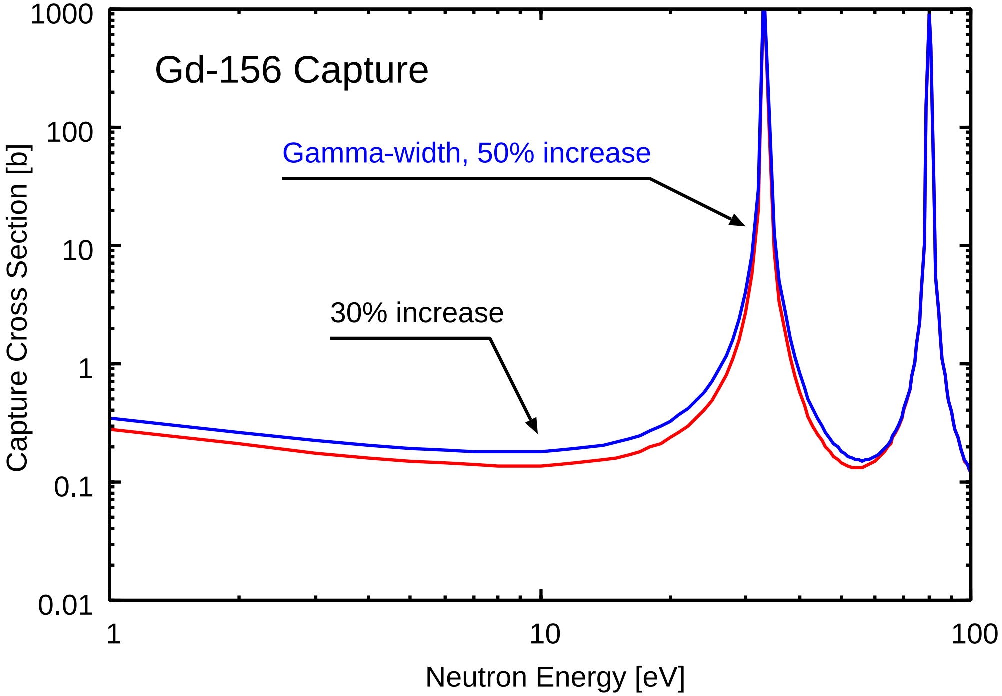
	JENDL	SAMMY Retroactive
Data point	averaged over several resonances	taken from typical experiments
Resolution	N/A	taken from typical experiments
Uncertainties	inferred from real experiments, but rounded into a single value — 5% for example	estimated from real experiments, can be rounded into a single value
Correction	N/A	Doppler broadening, multiple scattering
Sensitivity	sensitivity to the $\overline{\sigma}$	at each data point

In this study, we employ the RM/MLBW code, which was developed at the JENDL covariance evaluation, and "simulate" the SAMMY's retroactive method.

The Simplest Case

Gd-156 Capture Cross Section

- Increase in Γ_γ of 50% at 33 eV resonance
- result in increase in σ_{capt} of 30% at 10 eV
- The relative sensitivity is $30/50 = 0.6$.
- The actual sensitivity is a function of energy.



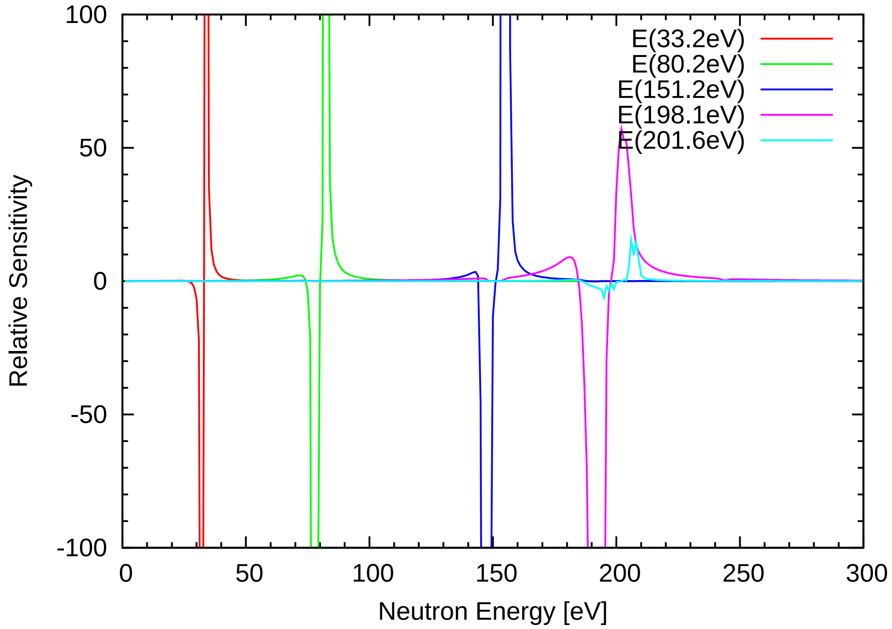
If we assume that the uncertainty in σ_{capt} is 5%, 8.3% (=5/0.6) uncertainty in the Γ_γ will reproduce the 5% uncertainty.

Sensitivity, Resonance Energy

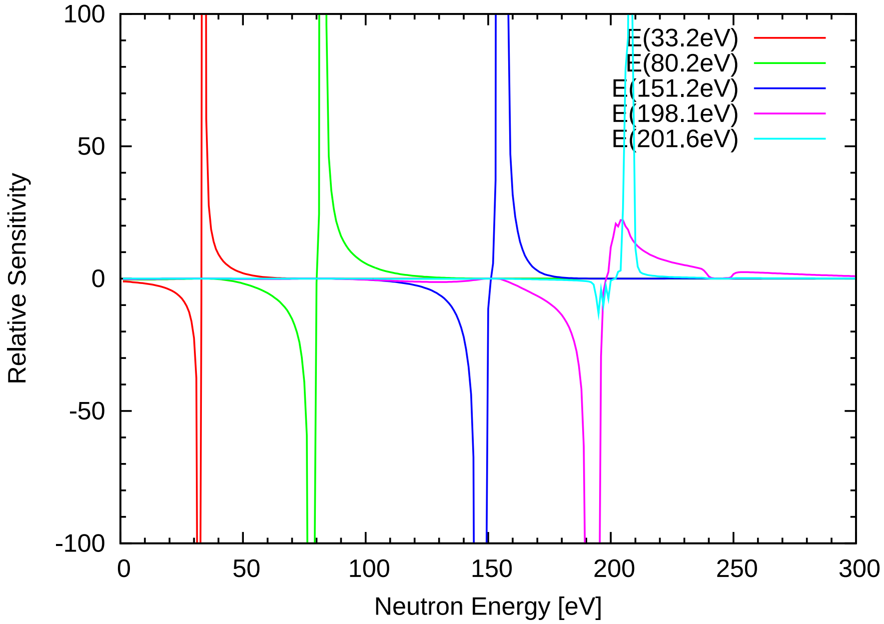
Relative Sensitivities of Resonance Energies

- Gd-156, resonance parameter (s-wave) taken from ENDF/B-VI
- The resonances at 33, 80, 151, 198, and 202 eV are included.

Total



Capture



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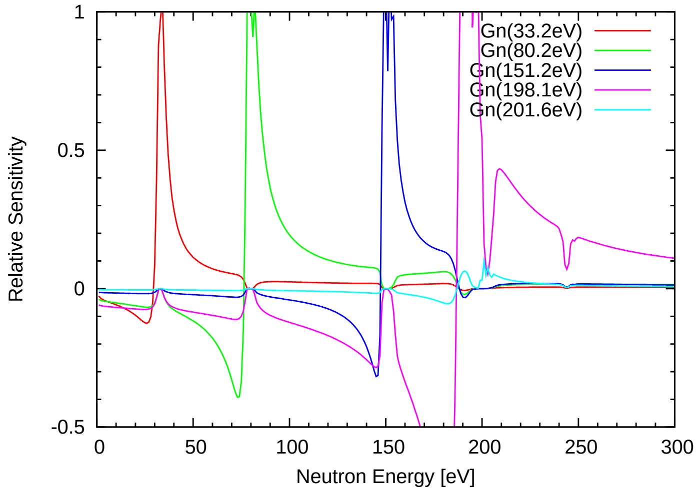
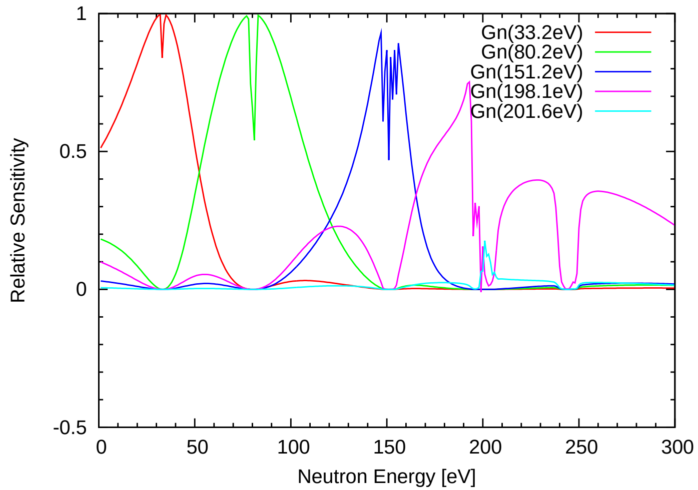
Sensitivity, Resonance Width

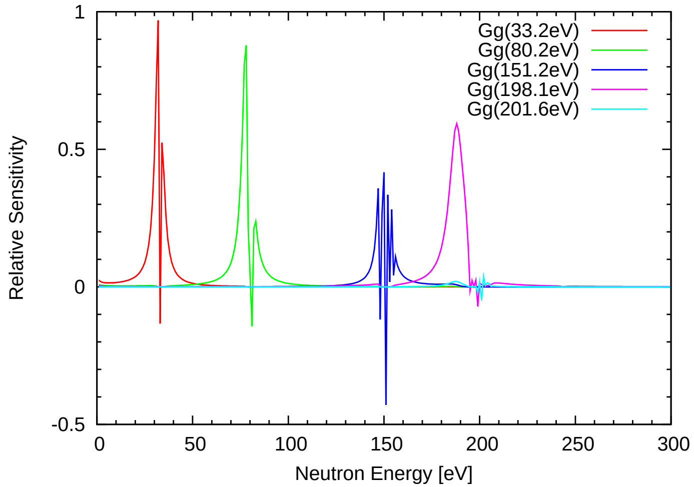
Neutron Width (upper), Gamma Width (lower)

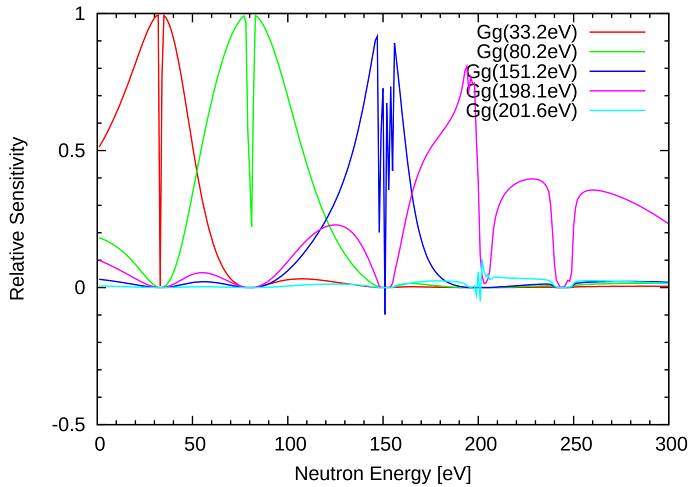
Total



Capture







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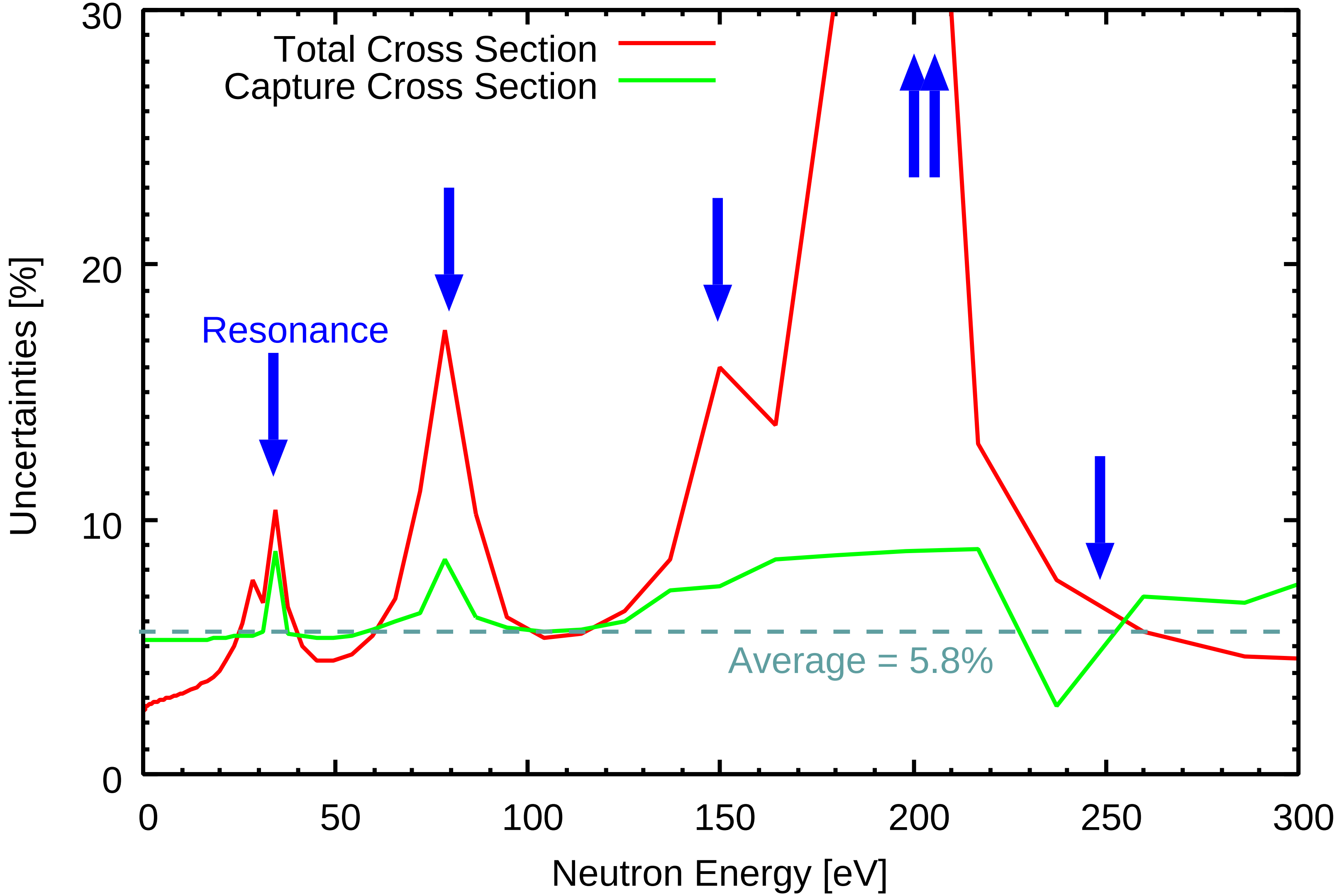
Capture Cross Sections

Realistic Experimental Condition Taken from KURRI TOF

- A series of capture measurements for fission products in the resolved / unresolved range at Kyoto University
  - Neutron Time-of-Flight with 46-MeV LINAC (12.7m)
  - BGO scintillator
- Energy resolution (FWHM), 1 – 3%
- ToF data interval, $\sim$ 100 points below 1 keV
- Sources of uncertainties for capture measurement, in the case of ^{99}Tc measurement
  - Statistical errors, about 3 – 10% (near resonances)
  - Normalization errors, about 6%
  - Corrections for background, self-shielding, multiple-scattering, about 2%
- Energy resolution and ToF data points, same as KURRI
- Uncertainties associated with experiments, 10% in capture cross section, with 50% correlation due to normalization

Gd-156 Cross Section Uncertainties (I)

If we can assume that capture measurements were carried out with the similar condition.



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Total Cross Sections

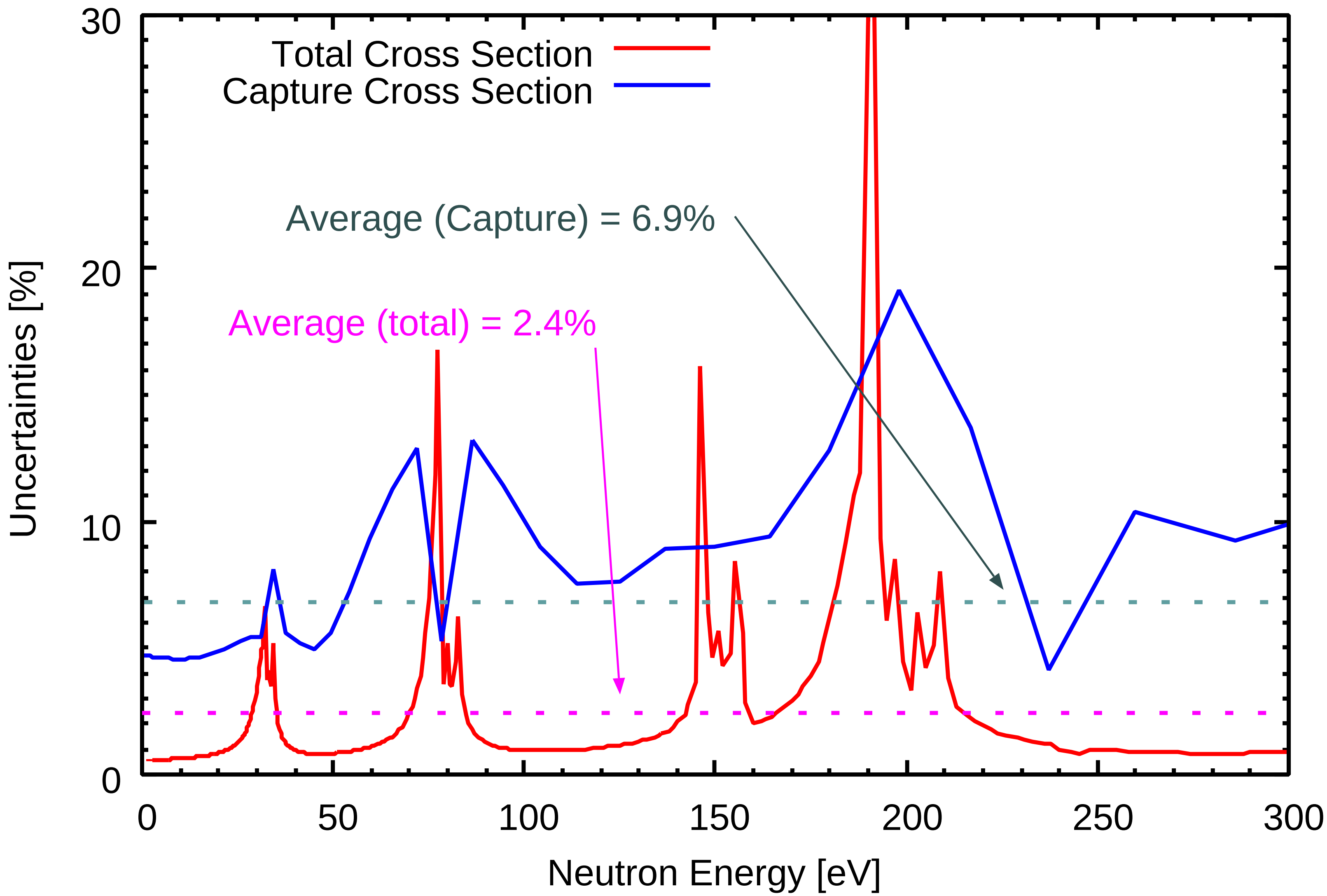
Gd Resonance Analysis at BNL, Mughabghab and Chrien

- No experimental transmission data available.
  - low-energy run, $\sim$ 100 eV / 1024 channels
  - high-energy run, $\sim$ 1 keV / 1024 channels

Assumed Transmission Experiment

- Transmission data interval, $\delta E \sim 0.01 E_n$
- Energy resolution assumed to be 1%
- Data in the off-resonance region are not used
- Uncertainties associated with experiments, 10% in total cross section, with 10% correlation due to normalization

Gd-156 Cross Section Uncertainties (II)



Resonance Parameter Covariance

Covariance Matrix for the First 3 Resonances

```
0-E0  3.32E+01 0.012   1000
0-Gn  1.46E-02 4.0     -197 1000
0-Gg  9.00E-02 7.8      382 -718 1000
1-E0  8.02E+01 0.011      1   -3    3 1000
1-Gn  5.09E-02 3.8       16   18   20   -2 1000
1-Gg  8.60E-02 15.4      -7   -9   -6  -70 -553 1000
2-E0  1.51E+02 0.025      0    0    0   -1   -2    0 1000
2-Gn  4.17E-02 4.8        5   11    6    6   11    7 -302 1000
2-Gg  8.60E-02 16.0      -2   -2   -3   -3   -3   -3  359 -612 1000
```

Parameter	This work[%]	Mughabghab and Chrien [%]
$E(1)$	0.012	0.006
$\Gamma_n(1)$	4.0	13
$\Gamma_\gamma(1)$	7.8	10
$E(2)$	0.011	0.009
$\Gamma_n(2)$	3.8	15
$\Gamma_\gamma(2)$	15.4	(10)
$E(3)$	0.025	1.1
$\Gamma_n(3)$	4.8	29
$\Gamma_\gamma(3)$	16.0	(10)

Covariance Generation with SAMMY

- This study was carried out with Kawano's RM/MLBW code and the KALMAN code.
- Numerical derivative technique was used.
- Our goal is to use the SAMMY code, and repeat this:
  - SAMMY calculates derivatives ($\partial\sigma/\partial p$) analytically.
  - SAMMY generates resonance parameter covariances in the existing ENDF-6 format or "compact format."
  - Test of the resonance covariance with ERRORJ is straightforward.

Data processing (Resonance Part)

- ERRORJ (Go Chiba, JNC)
  - The ERRORJ code that processes Reich-Moore covariance data can be used with NJOY, AMPX, and PUFF-2 data processing systems.
  - ERRORJ can read the compact covariance format generated by SAMMY.
  - The code has been distributed to Sumitomo Atomic Energy Industries, JAERI Nuclear Data Center, JAERI ADS Project, Toshiba, ORNL, ANL, LANL, NEA Dababank, and IPPE.
- NJOY (R.E. MacFarlane, LANL)
  - Larson provided a subroutine that calculates derivatives of R-matrix theory (not numerical but analytical). This subroutine will be incorporated into NJOY to process resonance covariances.
- SAMMY (N. Larsoon, ORNL)
  - (SAMMY is not a processing code !) but it also has a capability to generate group-averaged cross sections and their covariance. This would help us to check the generated group constant covariance.

Concluding Remarks

- Covariance evaluation tools available
  - KALMAN — Bayesian parameter estimation
    - The KALMAN code can be combined with Hauser-Feshbach statistical codes — CoH, GNASH, EMPIRE, TALYS
  - SOK — Least-squares fitting
  - GMA, GLUCS
  - SAMMY
    - Retroactive method to estimate covariances of resonance parameters
- Processing code
  - NJOY (LANL)
  - ERRORJ (JNC)