IAEA 60 Years
Atoms for Peace and Development

Covariance methodology for the FENDL project

Georg Schnabel

Nuclear Data Section
Division of Physical and Chemical Sciences NAPC
Department for Nuclear Sciences and Applications
IAEA, Vienna

CM on Further Development of FENDL

30 October 2023

Outline

- Motivation for covariance determination
- What is a covariance matrix?
- Examples from major nuclear libraries
- How to determine a covariance matrix?

Situation in neutron sublibrary

- 192 materials in neutron sublibrary
- Only ~1/3 of the files contain covariance info in MF33
- Missing for important structural materials (e.g. Cr, Ni, Fe, Cu)
- Further: V, Ta, Pb, etc.

Consistent evaluations

Nuclear data evaluation with Bayesian networks

Georg Schnabel,[1,*] Roberto Capote,[1] Arjan Koning,[1] and David Brown[2]

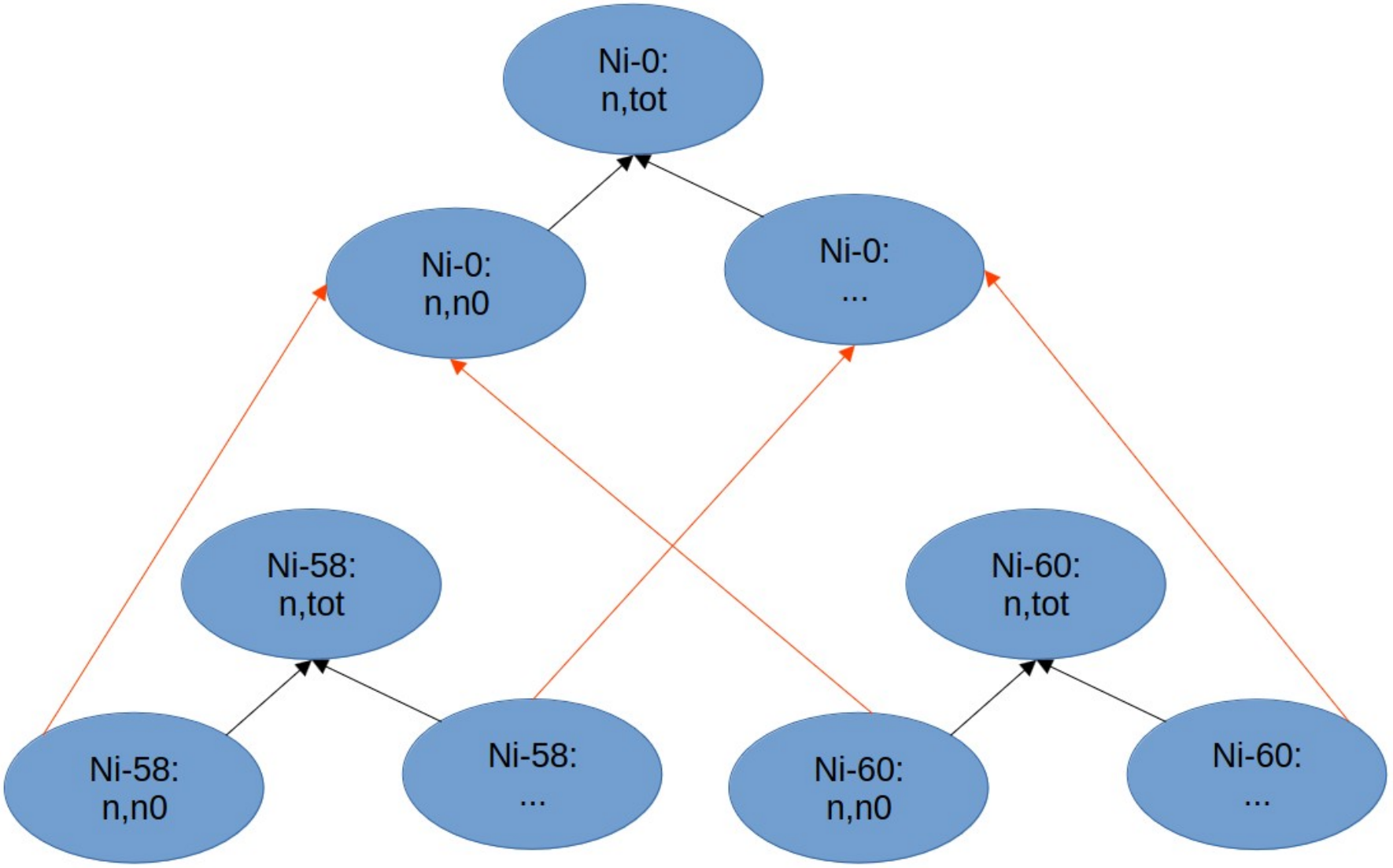
[1] *NAPC–Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria*
[2] *National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973-5000, USA*

(Dated: October 22, 2021)

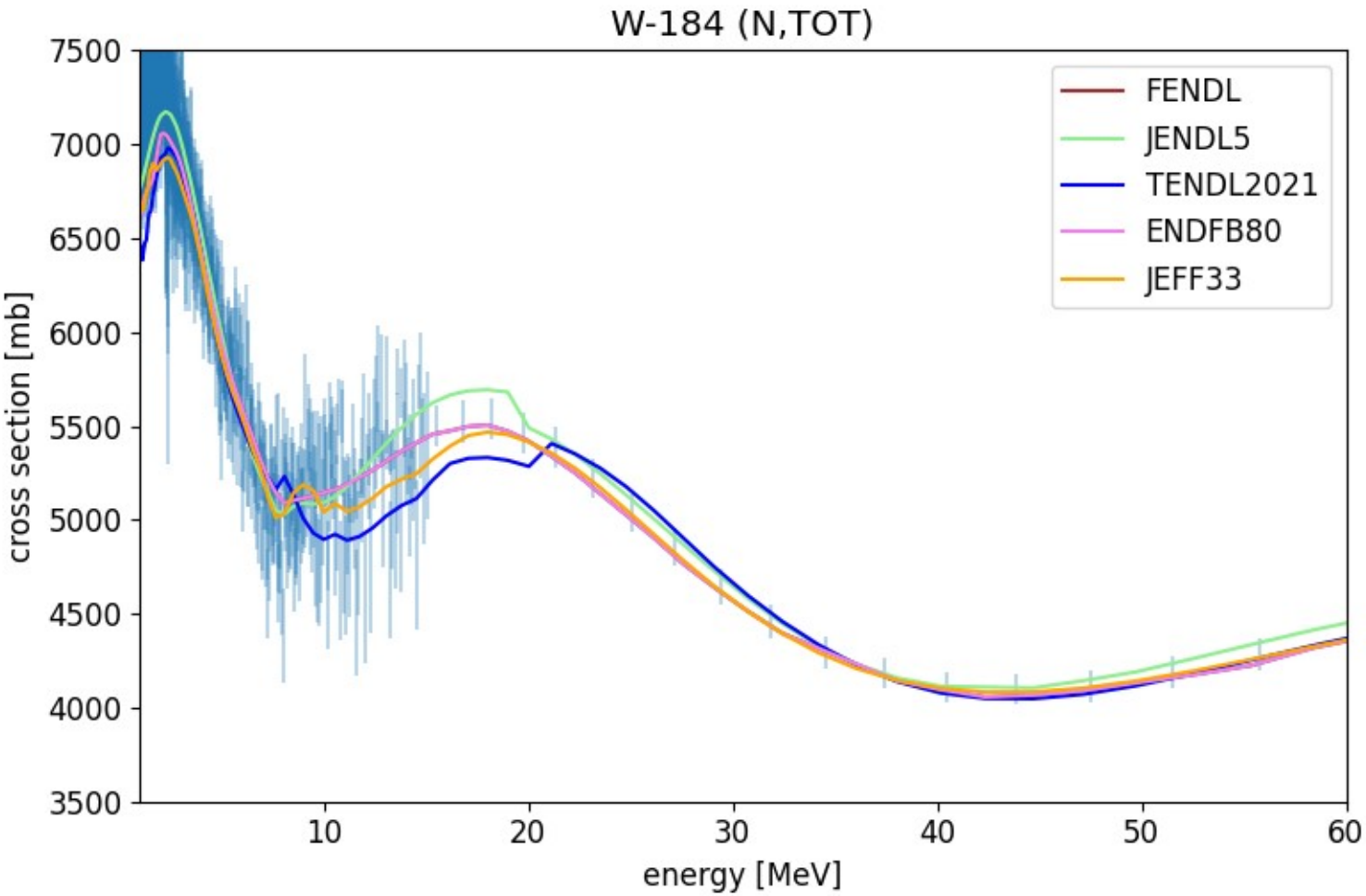
Bayesian networks are graphical models to represent the deterministic and probabilistic relationships between variables within the Bayesian framework. The knowledge of all variables can be updated using new information about some of the variables. The Bayesian Generalized Linear Least Squares method can be regarded as an inference method for Bayesian networks of variables with multivariate normal priors and linear relationships between them. We show that relying explicitly on the Bayesian network interpretation enables large scale inference and gives more flexibility in incorporating prior assumptions and constraints into the nuclear data evaluation process, such as the constraints that some cross sections equal linear combinations of other cross sections and that all cross sections must be non-negative. The latter constraint is accounted for by a non-linear transformation and therefore we also discuss inference in Bayesian networks with non-linear relationships between variables. Using Bayesian networks, the evaluation process yields more detailed information, such as posterior estimates and uncertainties of all statistical and systematic errors associated with the experiments. We further elaborate on a sparse Gaussian process construction that can be well integrated into the Bayesian network framework and applied to, e.g., the modeling of energy-dependent model parameters, model deficiencies of the physics model or energy-dependent systematic errors of experiments. We present three proof-of-concept examples that emerged in the context of the neutron data standards project and in the ongoing international evaluation efforts of ^{56}Fe. In the first example we demonstrate the modelization and explicit estimation of relative energy-dependent error components associated with experimental datasets. Then we show that Bayesian networks in combination with the outlined Gaussian process construction may be applied to an evaluation of ^{56}Fe in the energy range between one and two MeV, where it is difficult to obtain satisfactory evaluations by R-Matrix and nuclear model fits. Finally, we present a model-based evaluation of ^{56}Fe between 5 MeV and 30 MeV with a consistent and statistically sound treatment of model deficiencies. The R scripts to reproduce the Bayesian network examples and the *nucdataBaynet* package for Bayesian network modeling and inference have been made publicly available.

https://arxiv.org/abs/2110.10322

Example application to Ni isotopes



Cross sections



Multivariate normal distribution (MVN)

$$\rho(\vec{x}) = \frac{1}{\sqrt{(2\pi)^N |\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^T \boldsymbol{\Sigma}^{-1}(\vec{x}-\vec{\mu})\right)$$

center vector
(evaluated cross sections)

covariance matrix

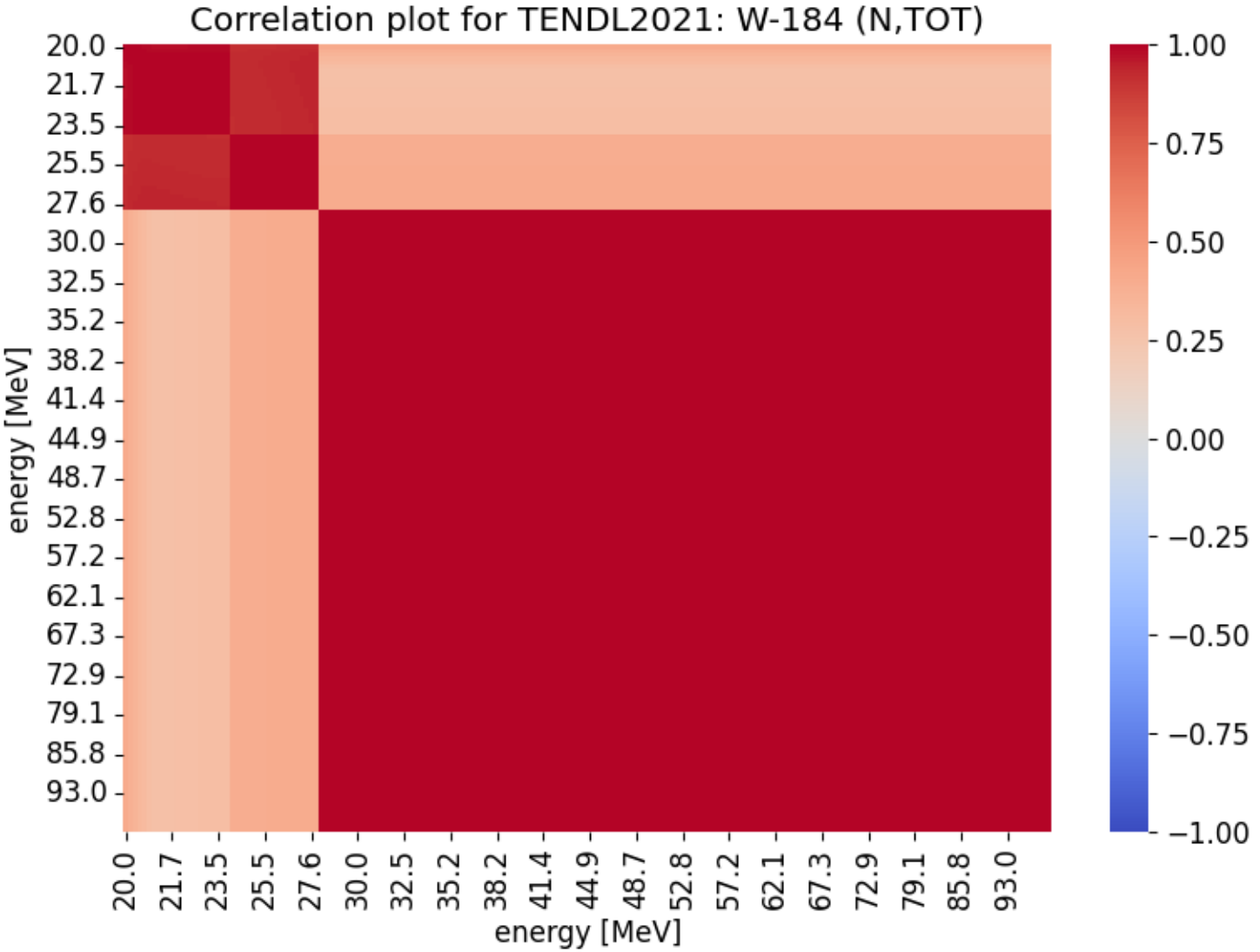
MVN as probability distribution for functions

$$\sigma(E') = \text{Interpolate}[(E_1, \sigma_1), \ldots, (E_i, \sigma_i), \ldots (E_N, \sigma_N)](E')$$

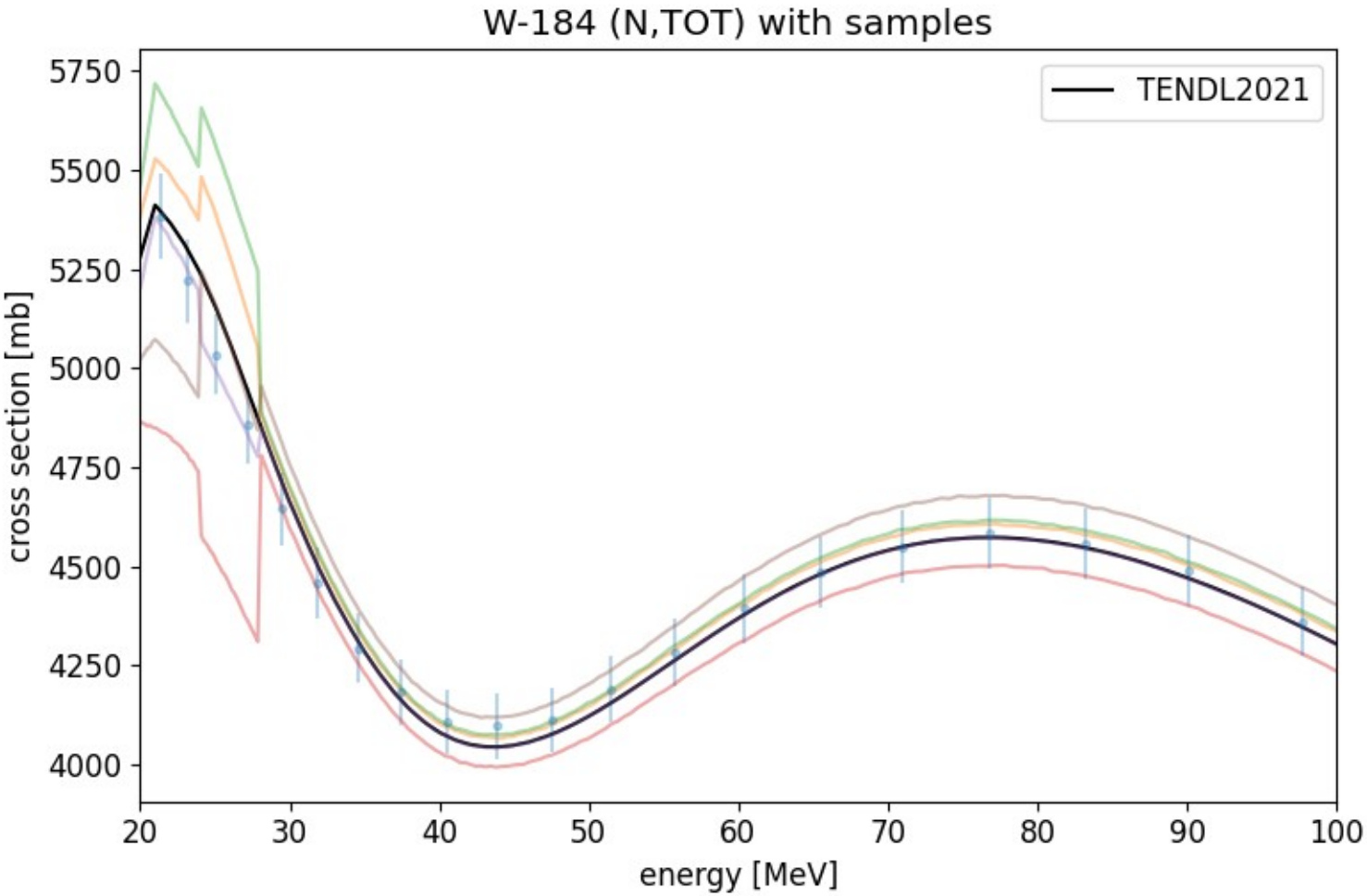
$$\vec{\mu} = \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \vdots \\ \sigma_i \\ \vdots \\ \sigma_N \end{pmatrix} \qquad \mathbf{\Sigma} = \begin{pmatrix} \delta_1^2 & \text{cov}_{12} & \cdots \\ \text{cov}_{12} & \delta_2^2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

$$\text{cor}_{12} = \text{cov}_{12}/(\delta_1 \delta_2)$$

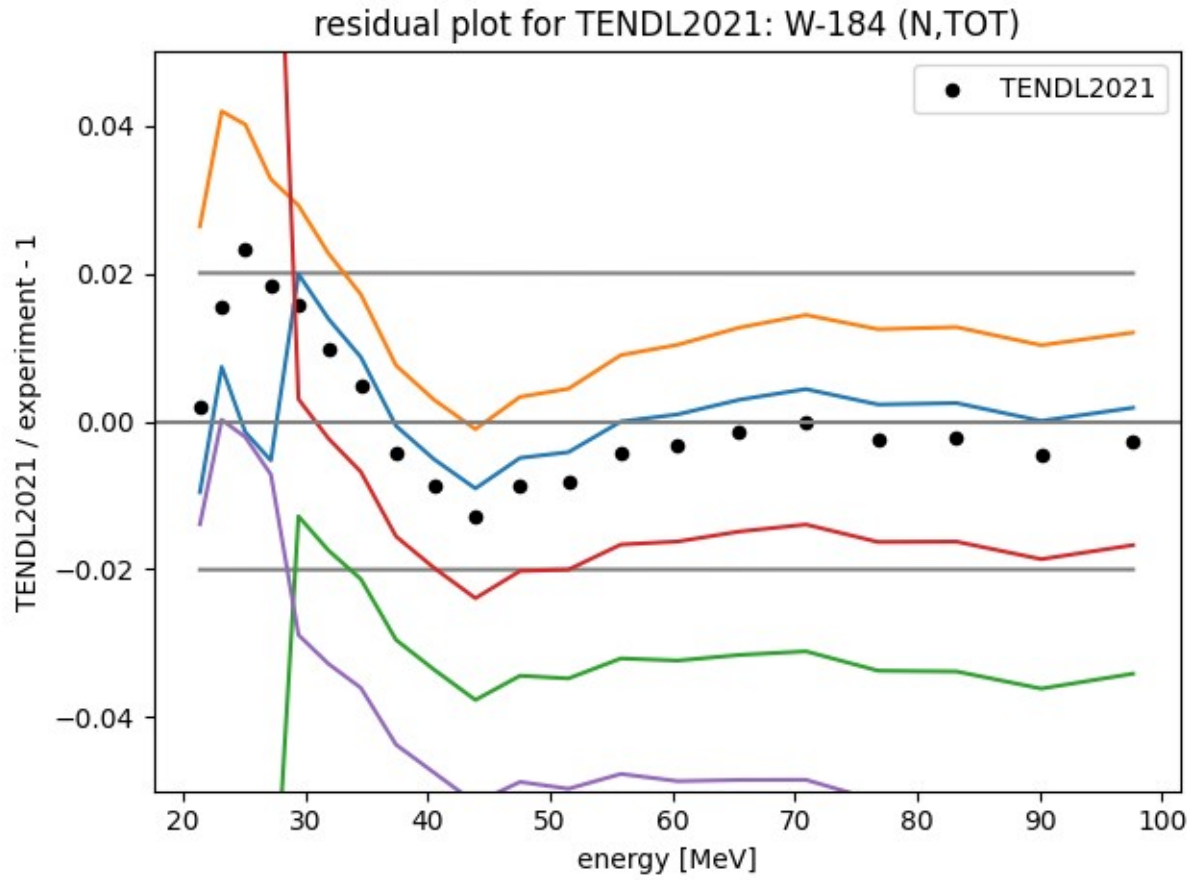
Correlation plot (TENDL2021)



Samples (TENDL covariance matrix)

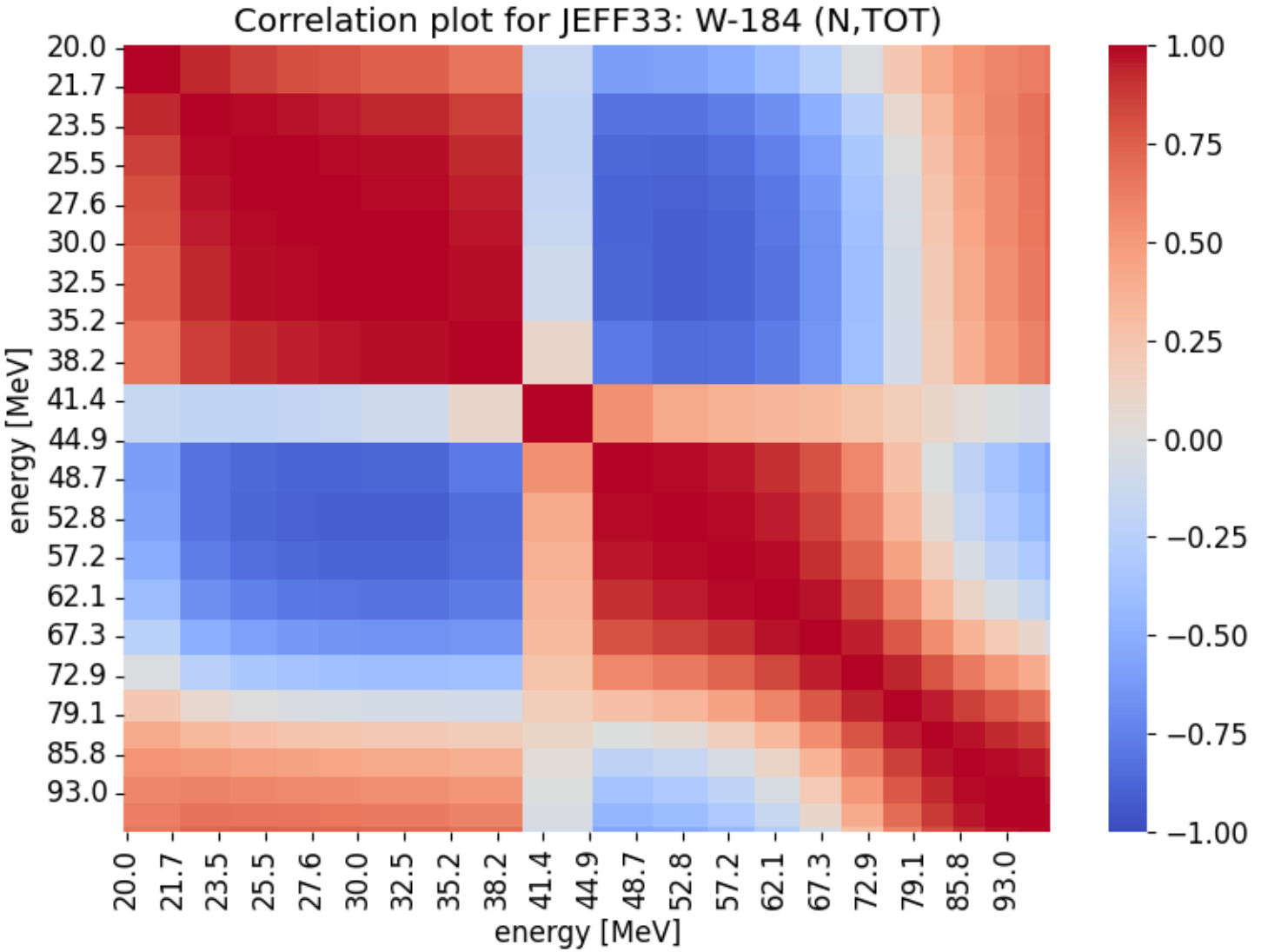


Samples (TENDL covariance matrix)

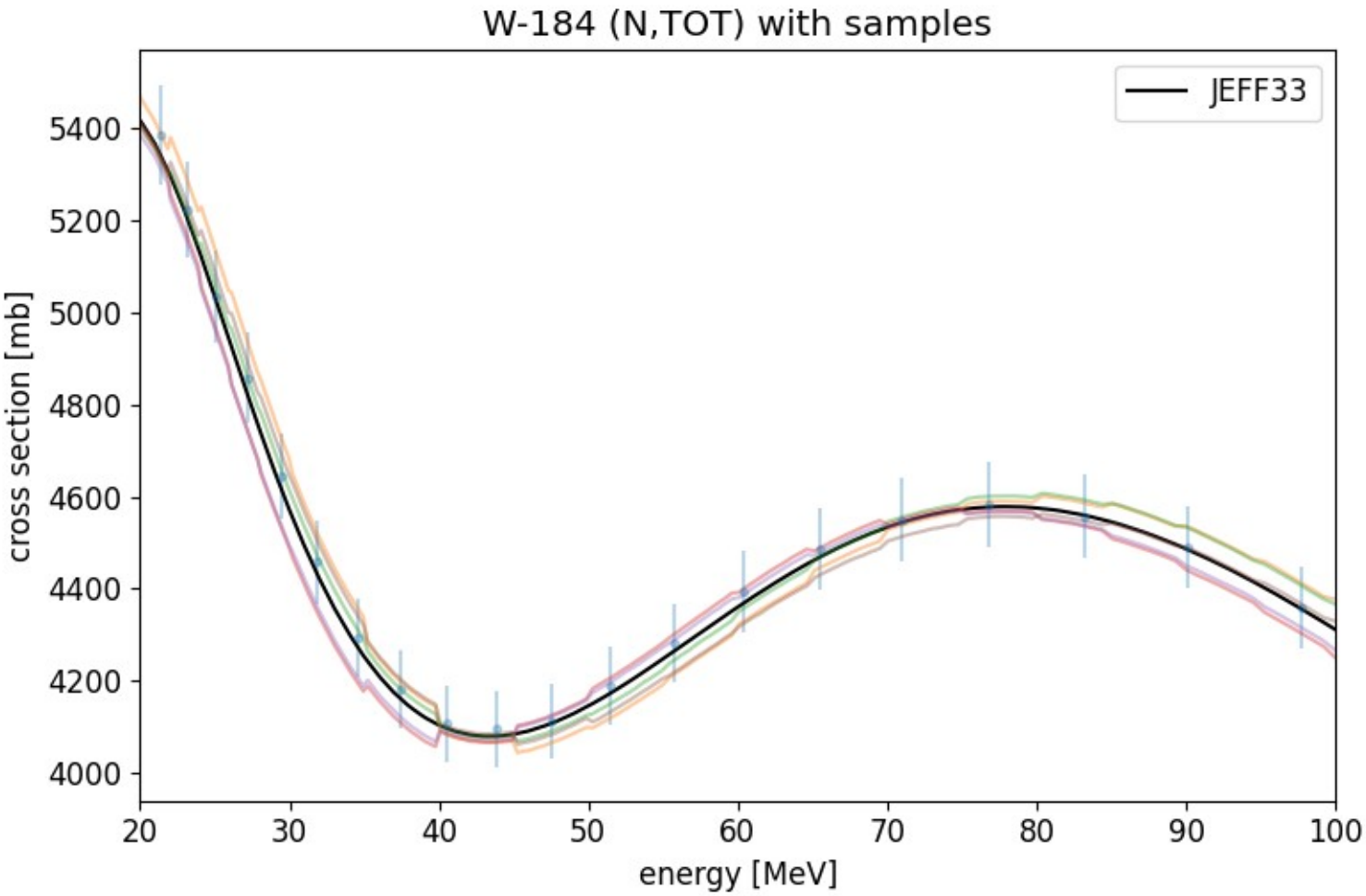


median uncertainty of sample distribution: 3.1%

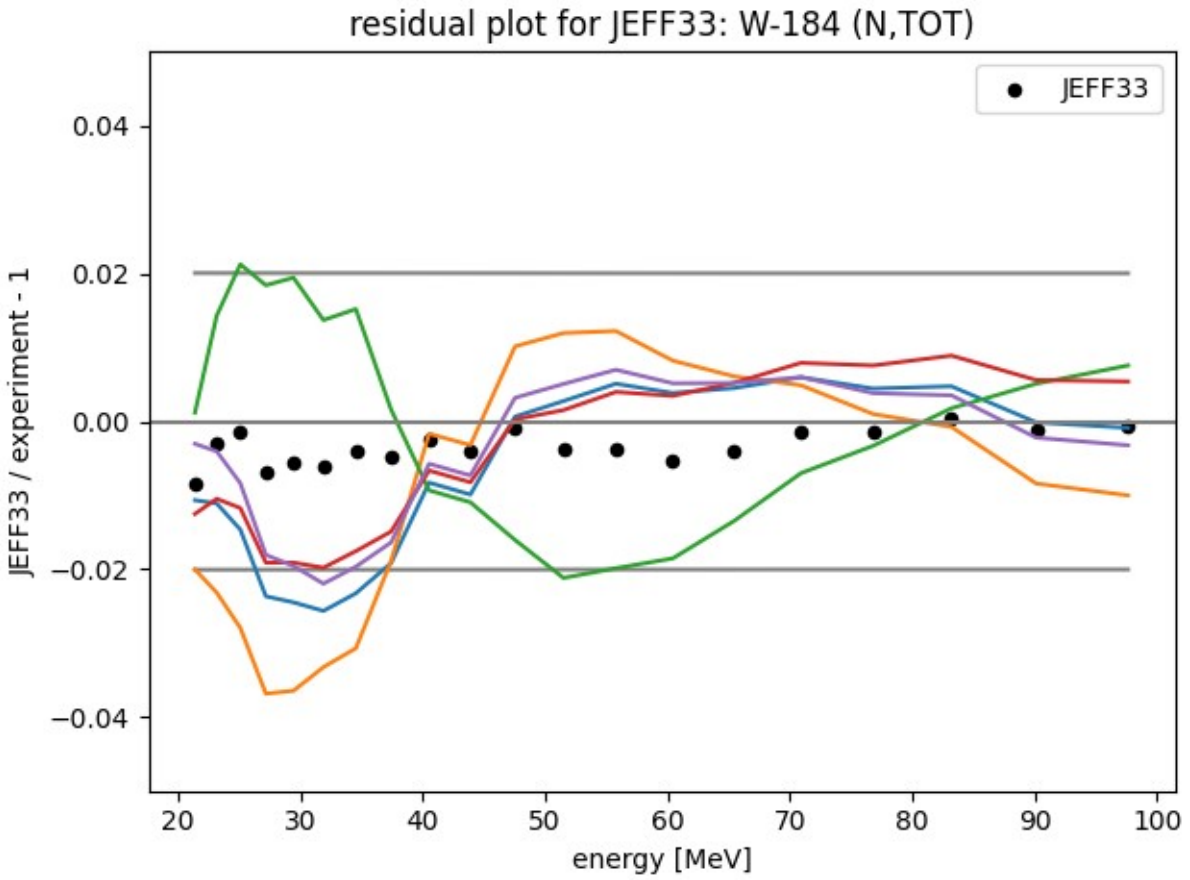
Correlation plot (JEFF33)



Samples (JEFF covariance matrix)

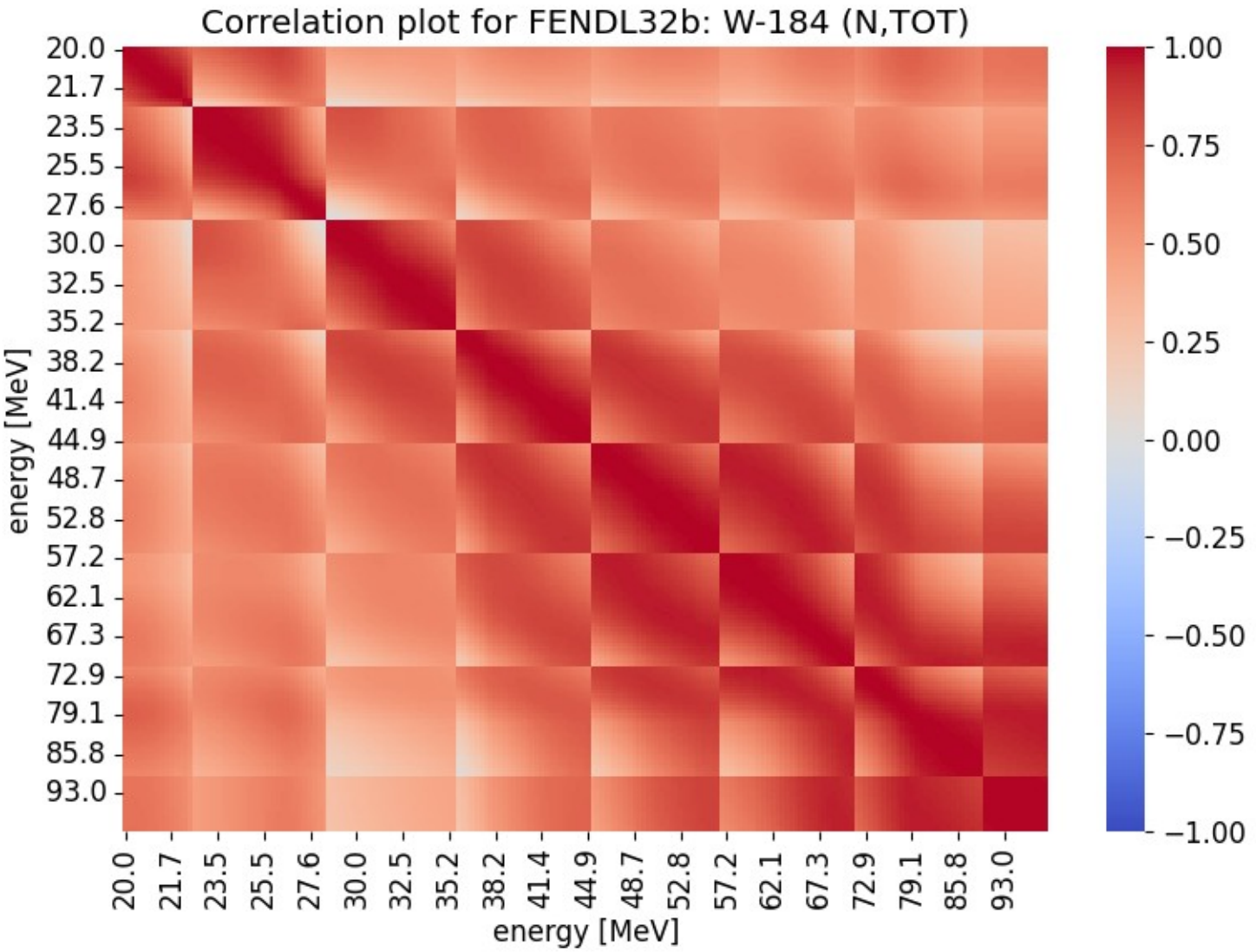


Samples (JEFF covariance matrix)

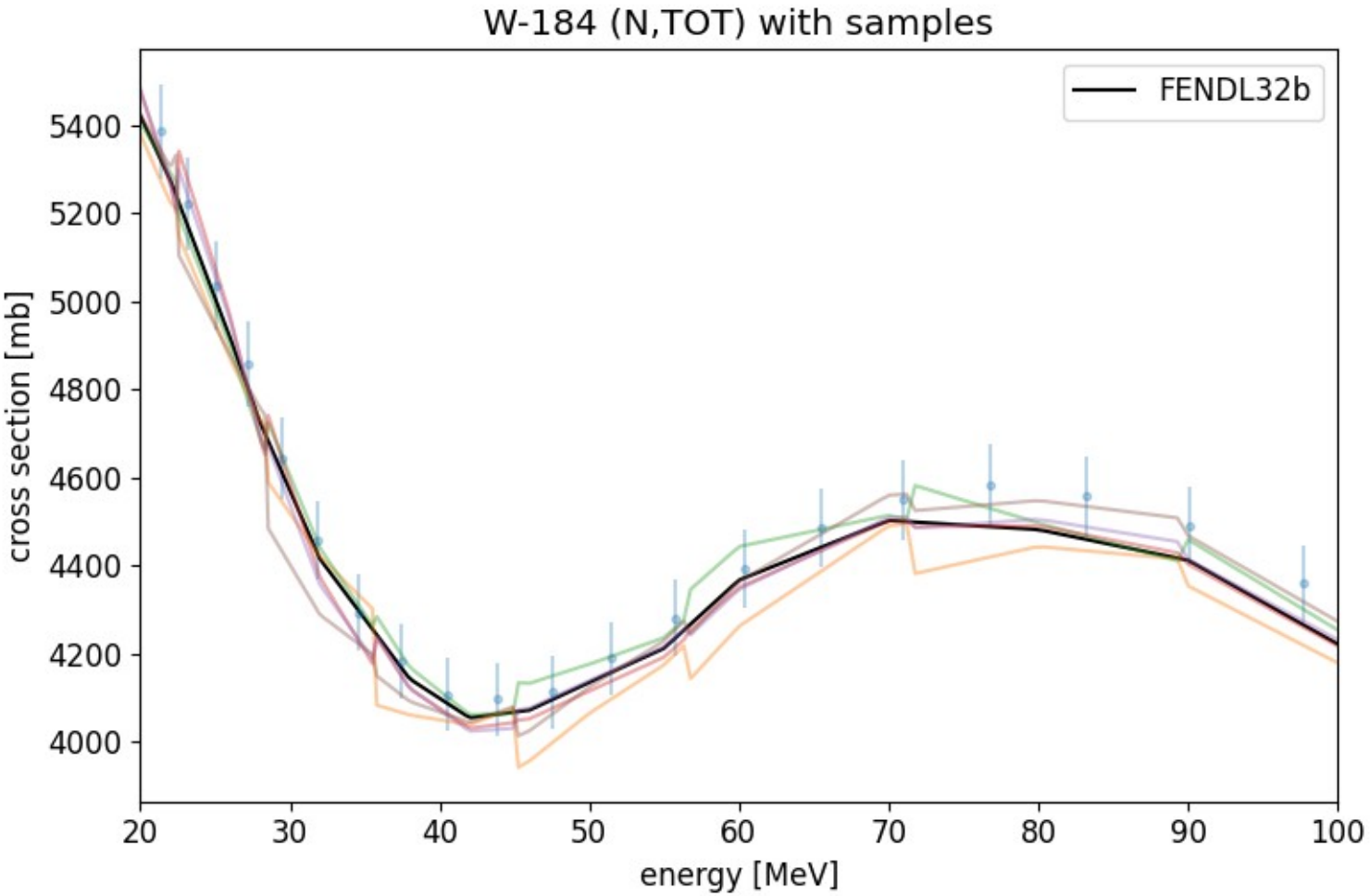


median uncertainty of sample distribution: 1.2%

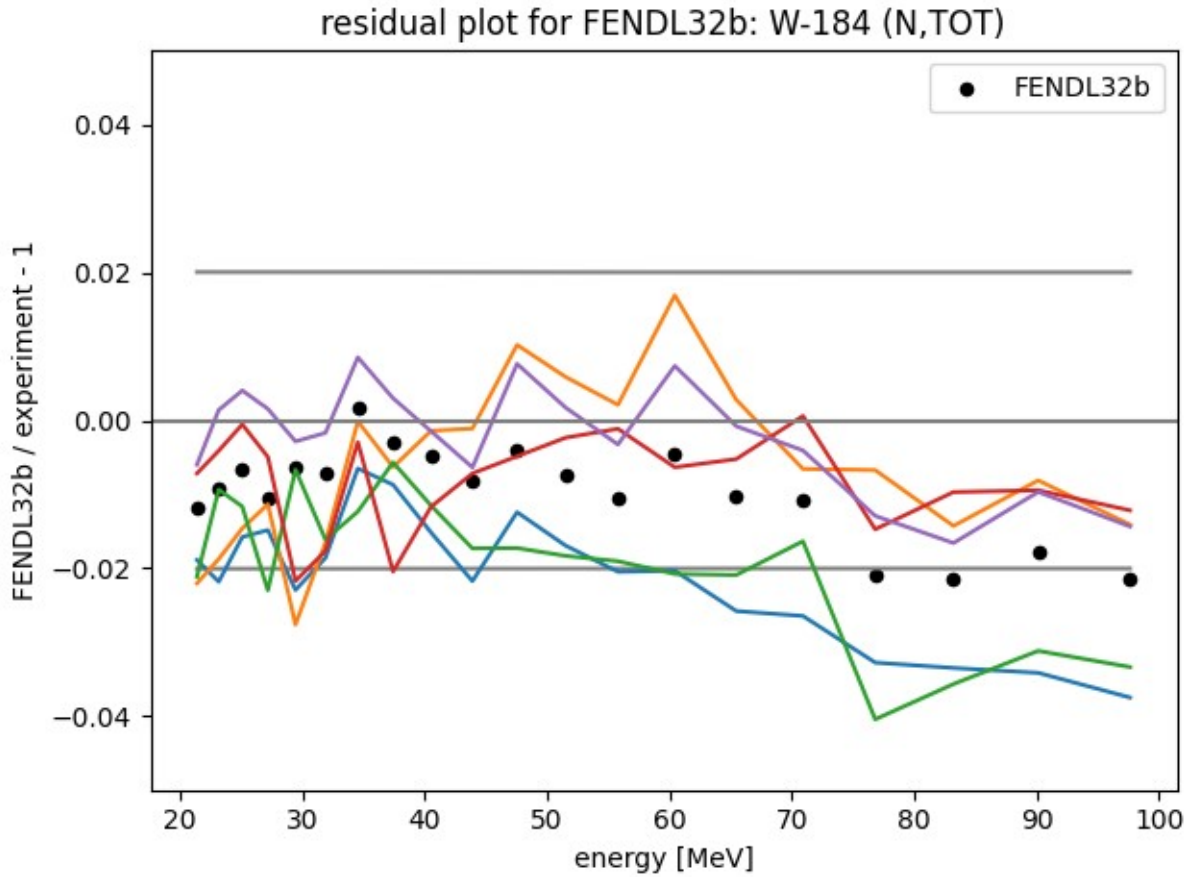
Correlation plot (ENDFB80=FENDL32b)



Samples (FENDL covariance matrix)



Samples (FENDL covariance matrix)



median uncertainty of sample distribution: 1.2%

Construction of covariance matrix

Situation

- Original covariance matrix missing or incomplete
- Don’t want to change cross sections (no re-evaluation)

Desiderata

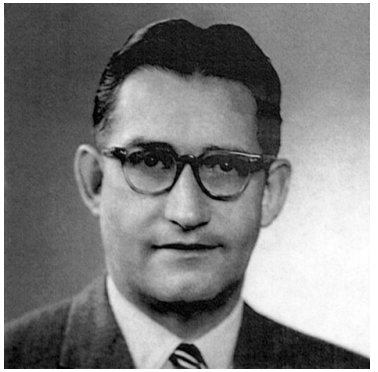
- Mathematically sound procedure
- Account for measured values and their uncertainty information

Kullback-Leibler Divergence

Solomon Kullback

KL divergence for continuous distributions:

$$D_{\mathrm{KL}}(P \parallel Q) = \int_{\mathcal{X}} \log\left(\frac{P(dx)}{Q(dx)}\right) P(dx),$$



Richard Leibler

"Distance" between two distributions

KL divergence = 0: distributions are identical

Specialized to case of two MVN distributions:

$$D_{\mathrm{KL}}(\mathcal{N}_0 \parallel \mathcal{N}_1) = \frac{1}{2}\left\{\operatorname{tr}\left(\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\Sigma}_0\right) + (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^{\mathrm{T}}\boldsymbol{\Sigma}_1^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) - k + \ln\frac{|\boldsymbol{\Sigma}_1|}{|\boldsymbol{\Sigma}_0|}\right\},$$

Nuclear data case

$$\mathcal{N}\left(\vec{\mu}_{lib}, \boldsymbol{\Sigma}_{lib}\right)$$

$$\mathcal{N}\left(\vec{\mu}_{exp}, \boldsymbol{\Sigma}_{exp}\right)$$

Adjust $\boldsymbol{\Sigma}_{lib}$ to make distributions as similar as possible measured by KL divergence

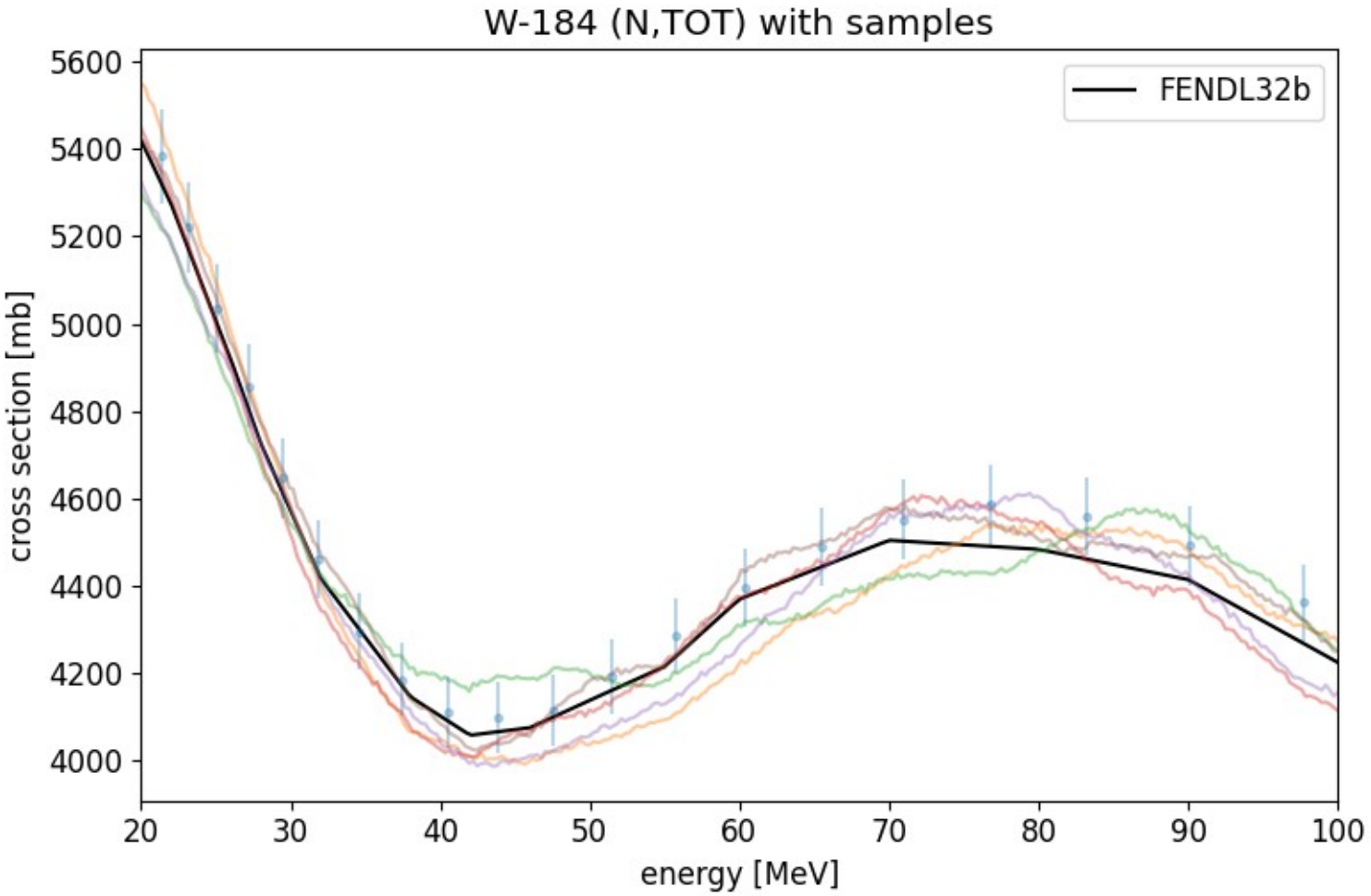
Structure of Σ_{lib}

- A lot of possible reasonable choices (to be explored more)
- Here for (n,tot) between 20 and 100:
  - Smooth cross section
  - Simple parametrization: amplitude σ and length scale ρ

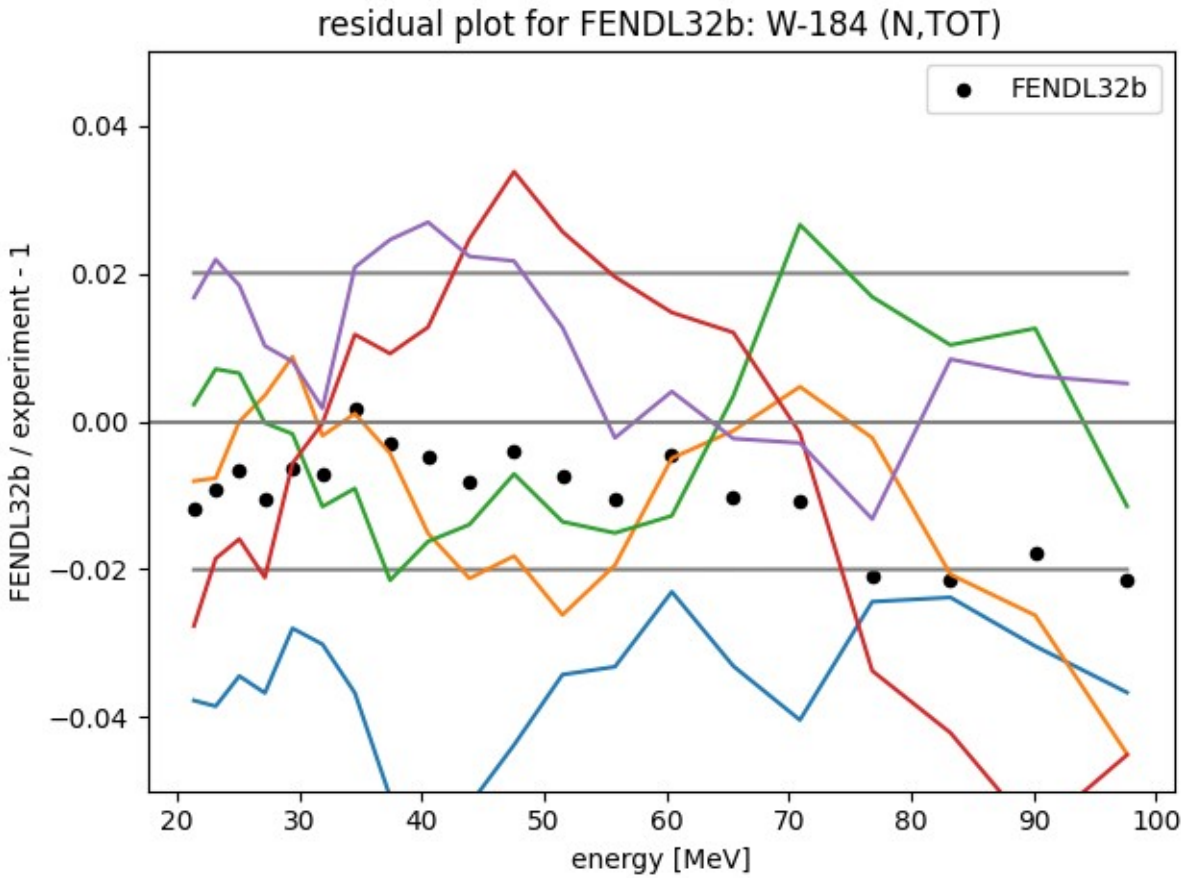
$$C_{3/2}(d) = \sigma^2 \left(1 + \frac{\sqrt{3}d}{\rho}\right) \exp\left(-\frac{\sqrt{3}d}{\rho}\right)$$

Matern covariance function
($d = E_i - E_j$)

Samples (FENDL) with optimized Matern covmat

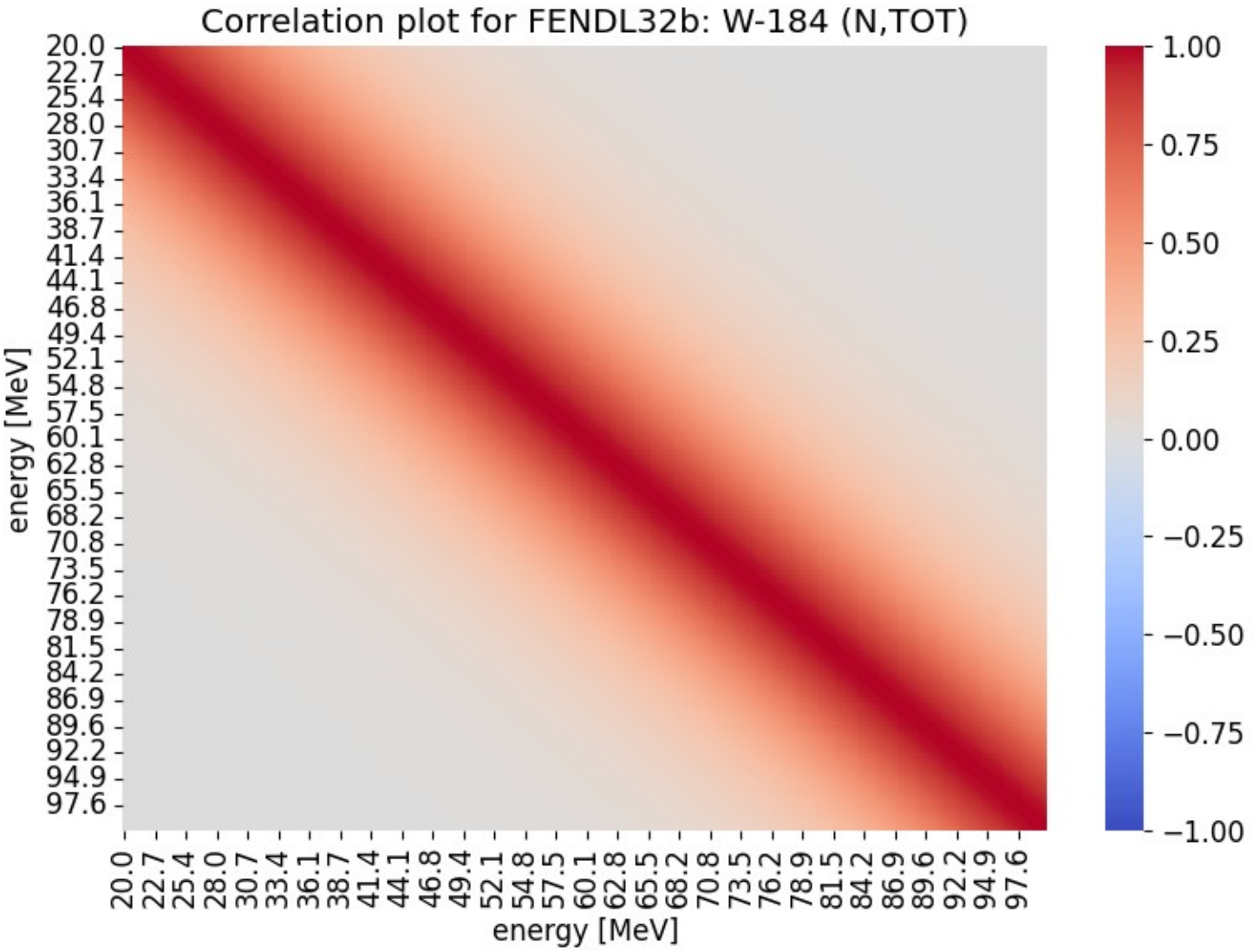


Samples (FENDL) with optimized Matern covmat

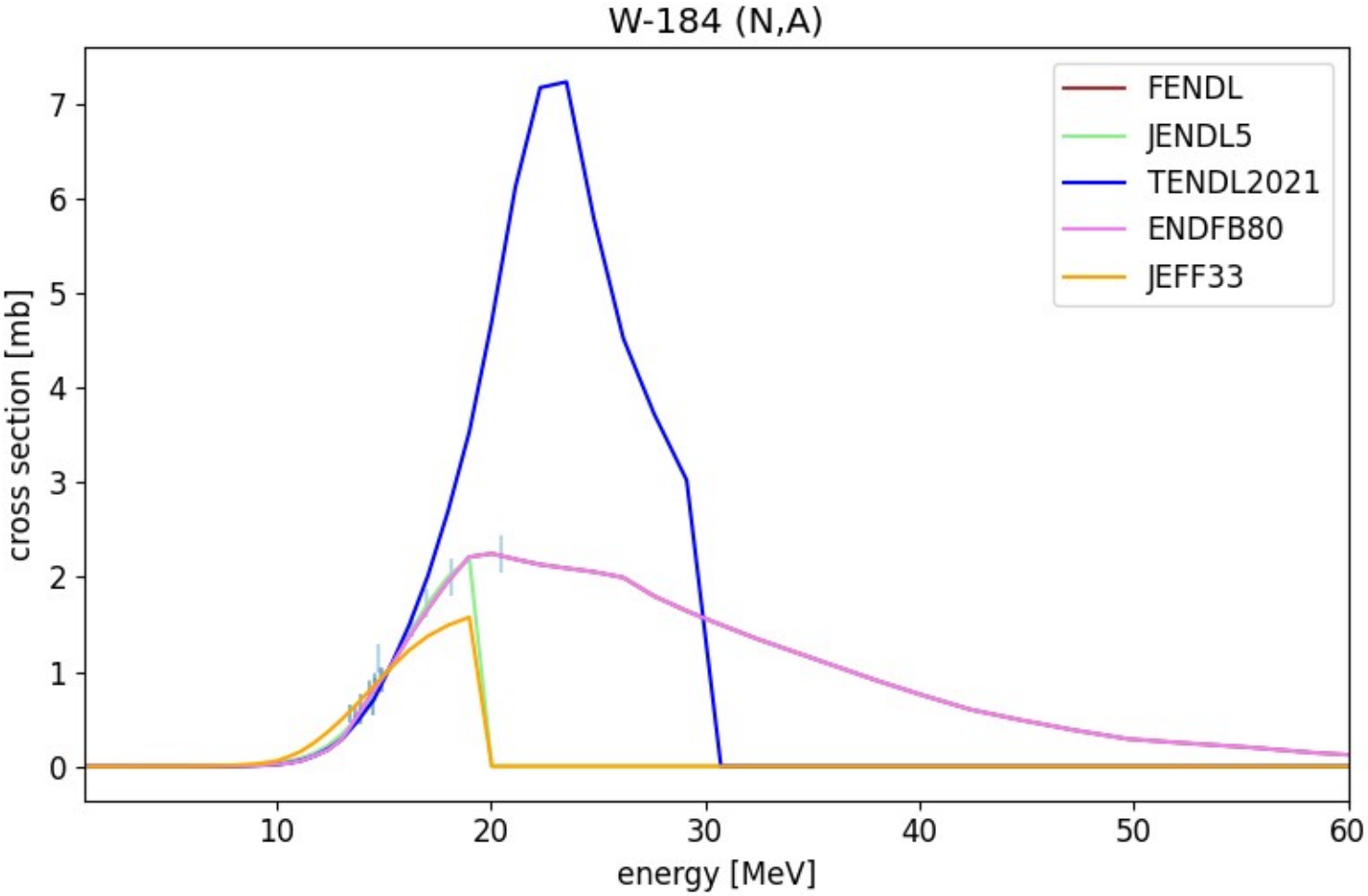


median uncertainty of sample distribution: 2.1%

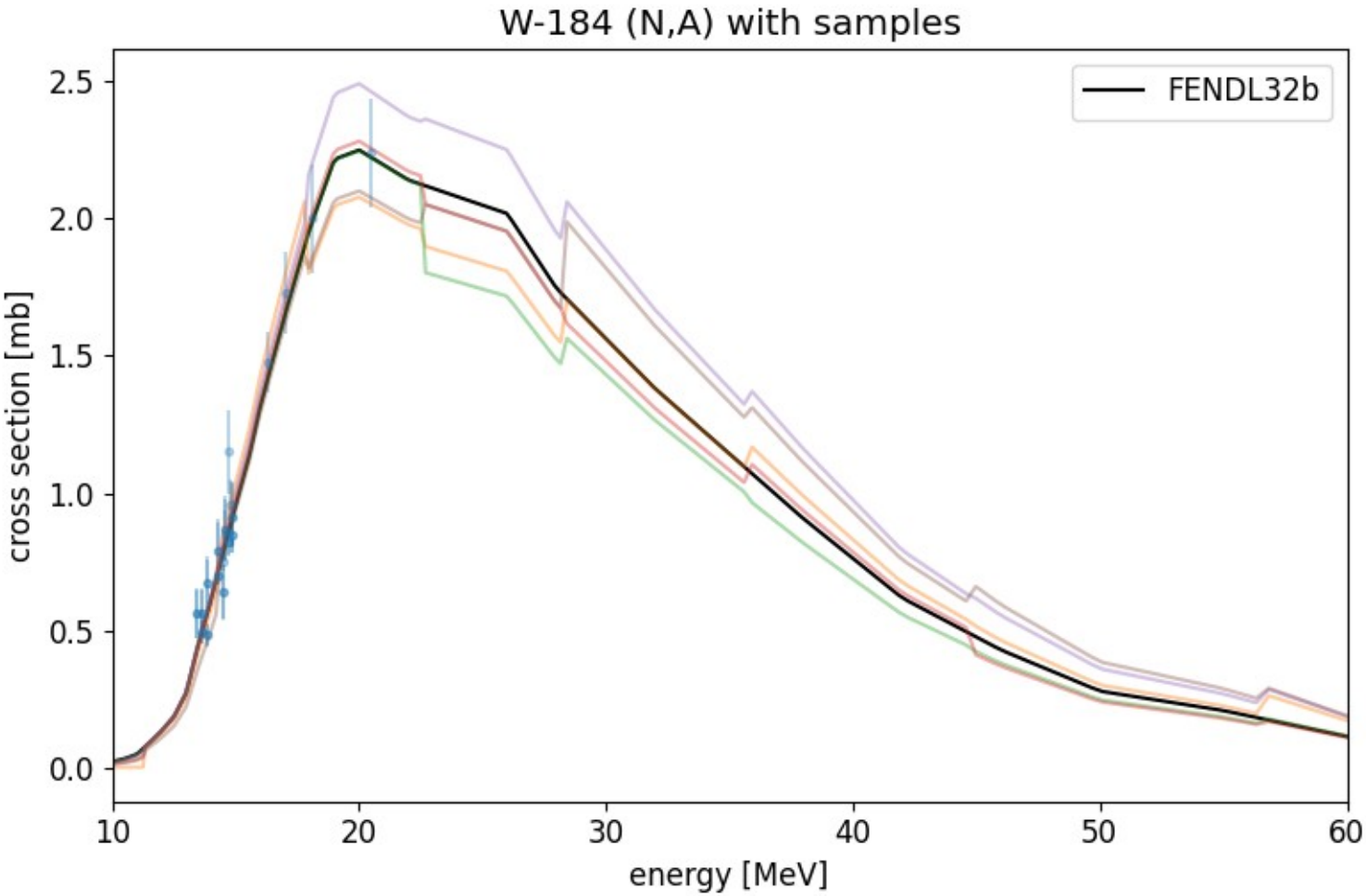
Optimized Matern covariance matrix



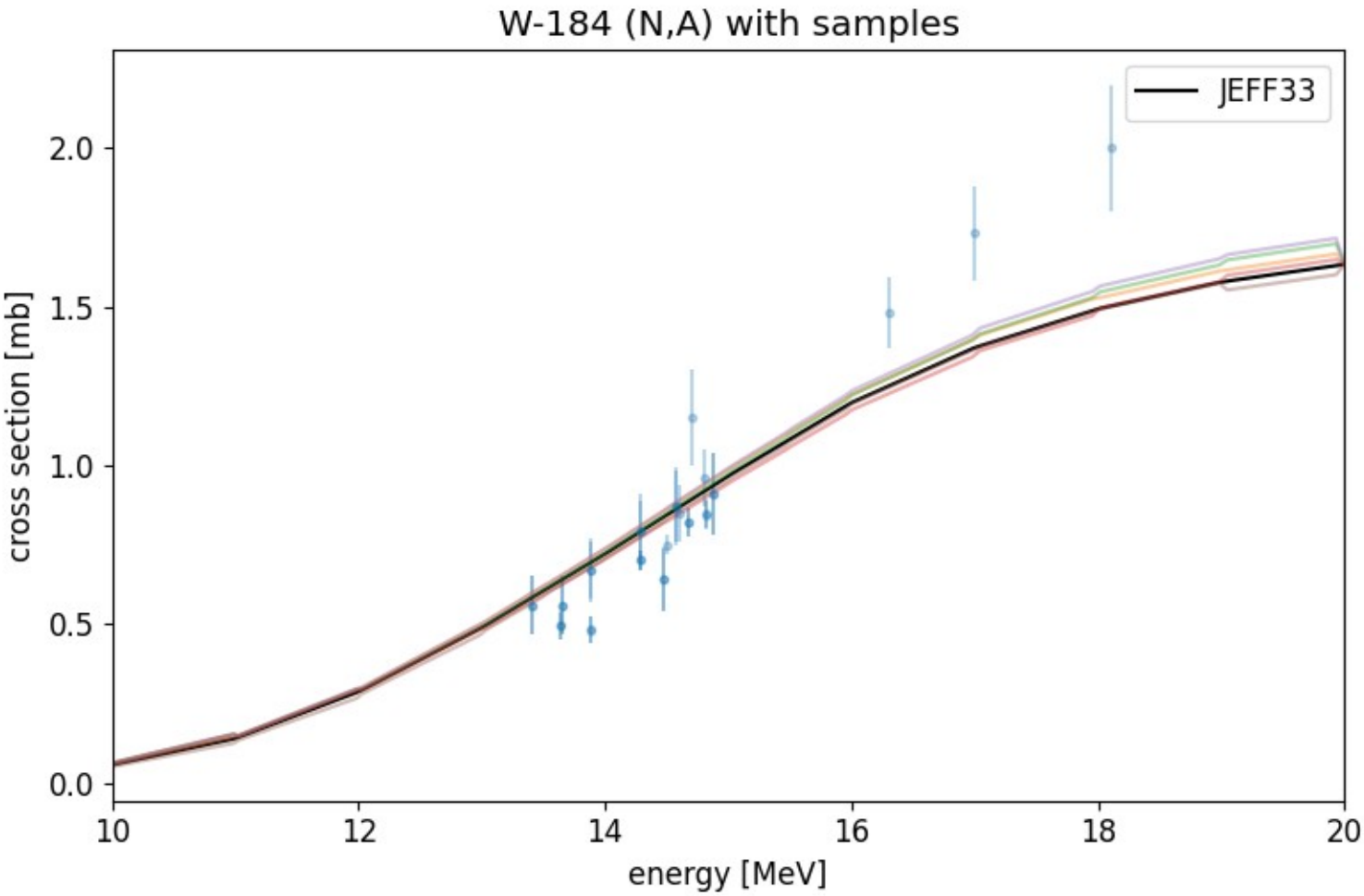
Challenging modeling cases



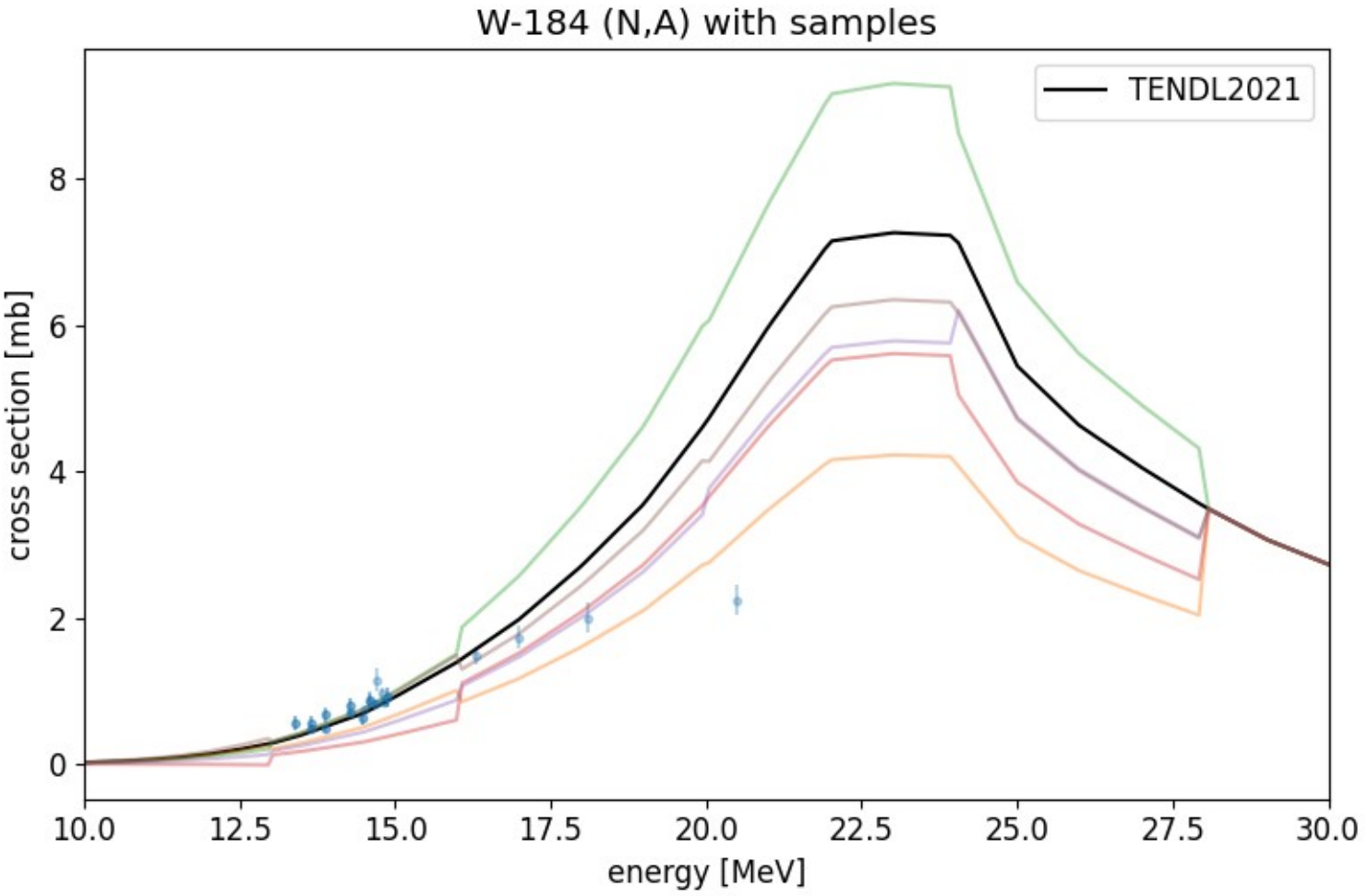
Sampling using FENDL32b



Sampling using JEFF33



Sampling using TENDL2021



Summary

- Meaning of covariance matrix (e.g., as pdf on function space)
- Proposed Kullback-Leibler divergence for estimating covariance matrices without re-evaluation of mean values
- Maximizing “compatibility with experimental data”
- Proof-of-concept application to W-184 (n,tot)
- Many open questions for further exploration:
  - Structure of covariance matrix
  - Especially if experimental data scarce
  - Incorporation of model constraints
  - Sum rules
- Such covariance matrix estimation capability especially attractive in FENDL project where parts of evaluation may come from different libraries or evaluators (with/without uncertainty information)

Discussion points

- Do all isotopes need uncertainty information?
- How data users are using uncertainties?
- Any isotopes that should be prioritized?