Status of the n + 239Pu evaluation effort

1) GMA analysis of new fission-TPC data

2) New optical model fit

A. Sieverding, S. Quaglioni, G. Potel Aguilar, M.A. Descalle, K. Kravvaris, W.E. Ormand,
B. Beck, C. Mattoon, I.J. Thompson, K.A. Wendt, R. Casperson, L. Snyder

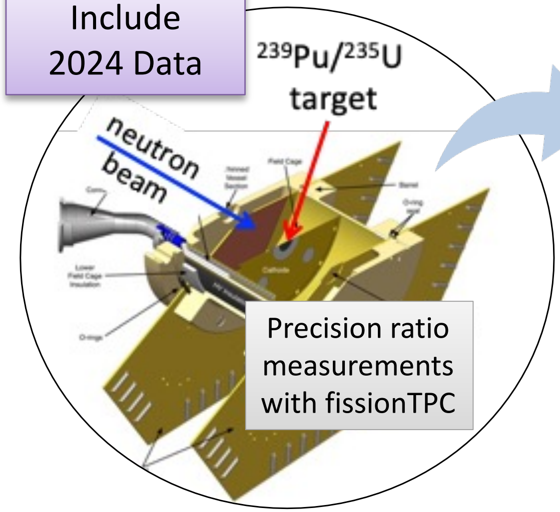
November 07, 2024

LLNL-PRES-871119

Lawrence Livermore National Laboratory

Components of the evaluation of n+^{239}Pu

Include 2024 Data



Expt.: neutron standards + fissionTPC ^{239}Pu(n,f)/^{235}U(n,f) shape

Fission properties from ENDF/B-VIII.1

Generalized Least-Squares Fit (GMA)

^{239}Pu(n,f)

Optical + statistical models (YAHFC)

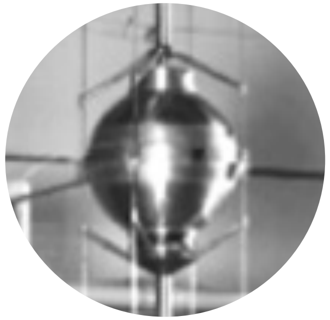
n+^{239}Pu evaluation

Processing (FUDGE)

GNDS Library

V&V (METIS)

Ex: Jezebel assembly



Expt.: all reaction channels except fission, $E_n \geq$ ~0.1 MeV

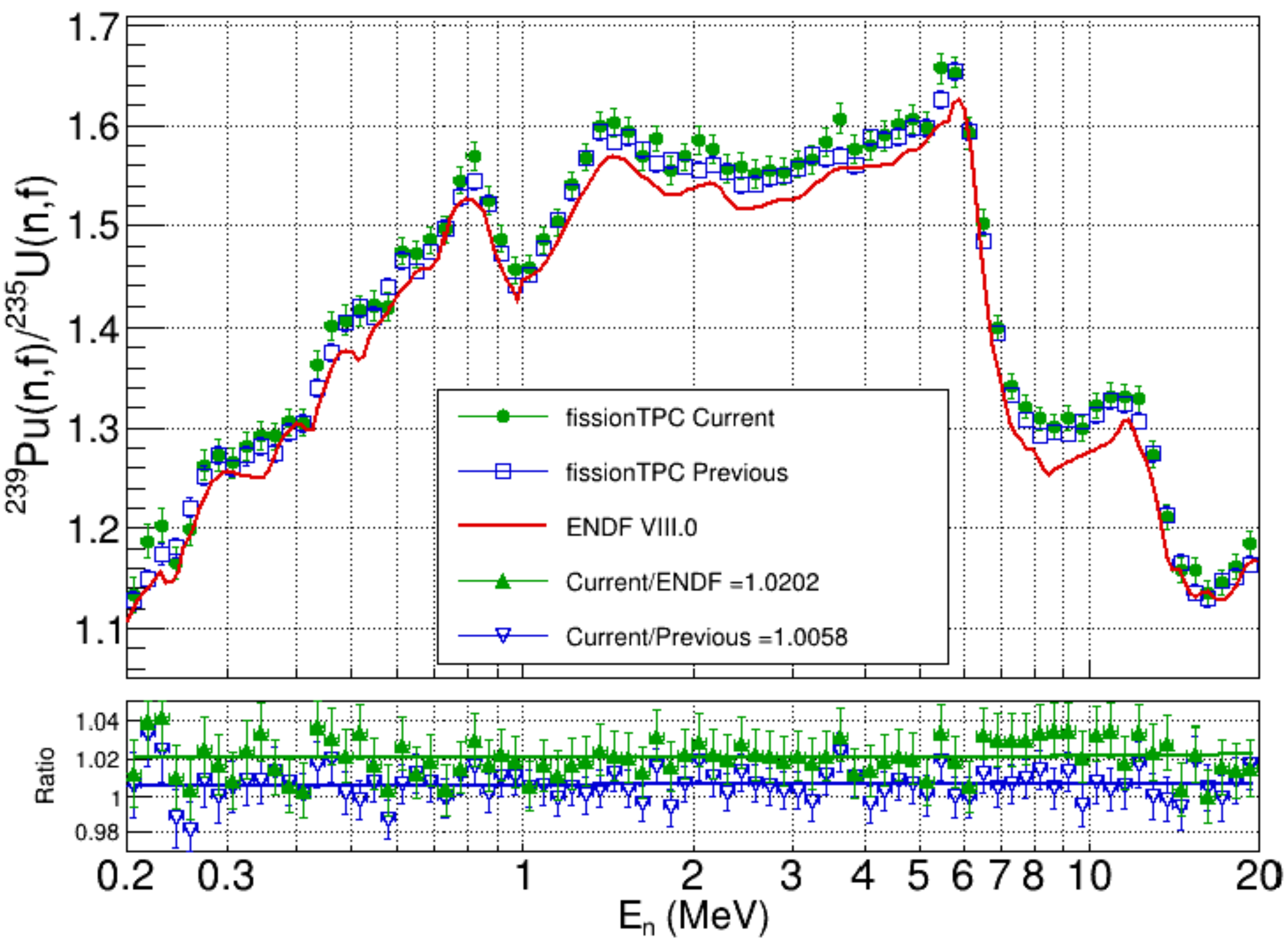
Resonance Region from ENDF/B-VIII.1

Update I

Including of new fission-TPC measurements

2021 Fission-TPC results

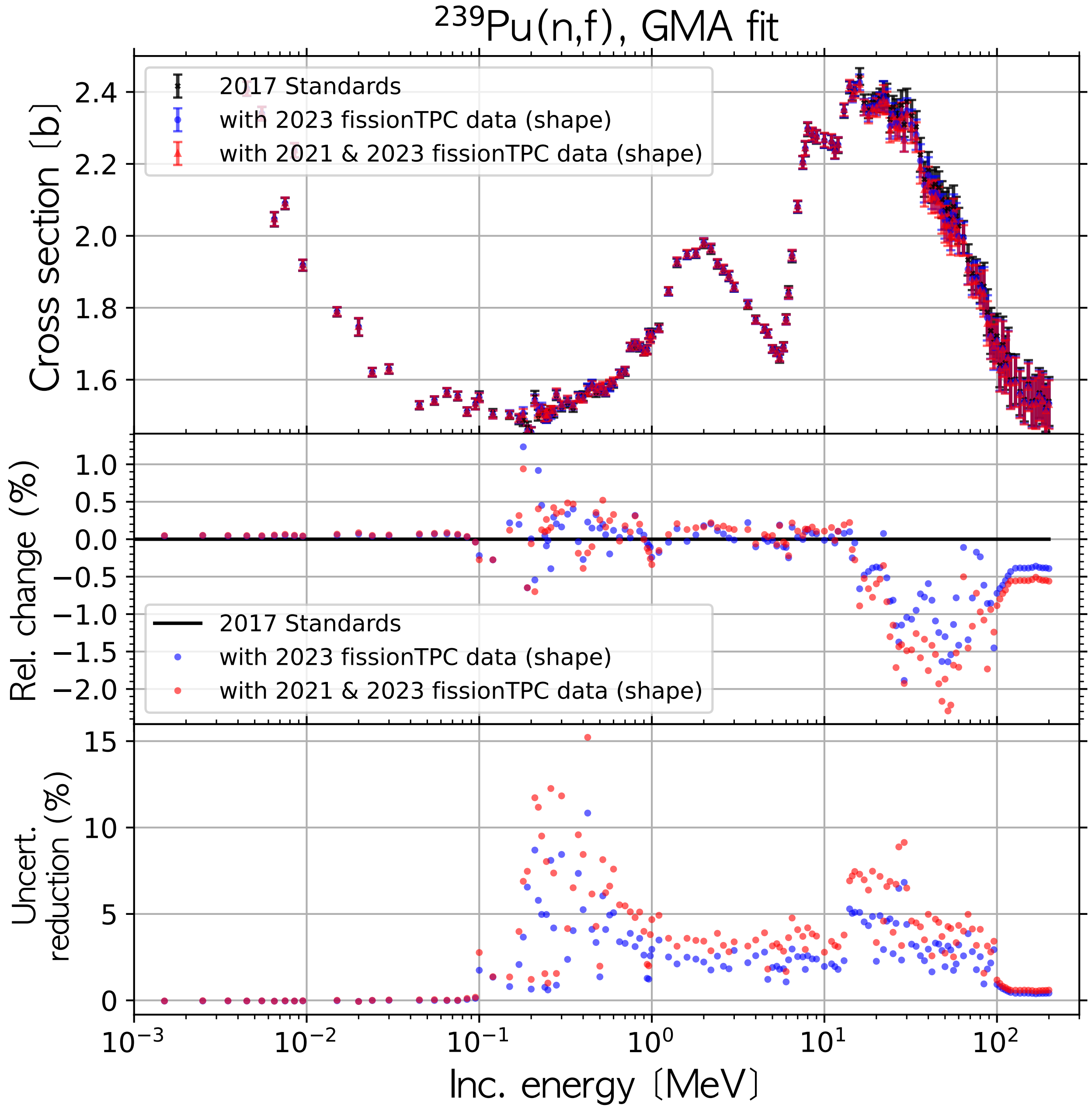
L. Snyder, et al. **NDS 178 (2021) 1-40,** *M. Monterial, et al.* **NIM A 1021 (2022) 165864**



- Almost 2% systematic offset from ENDF
- Confirmed by 2023 measurement with new target [arXiv:2409.18279v1, see presentation by L. Snyder on Tuesday]
- We use the GMAP code together with the 2017 neutron standards for the evaluation
- Inclusion in the GMA analysis:
  - Combined 2021 and 2024 datasets

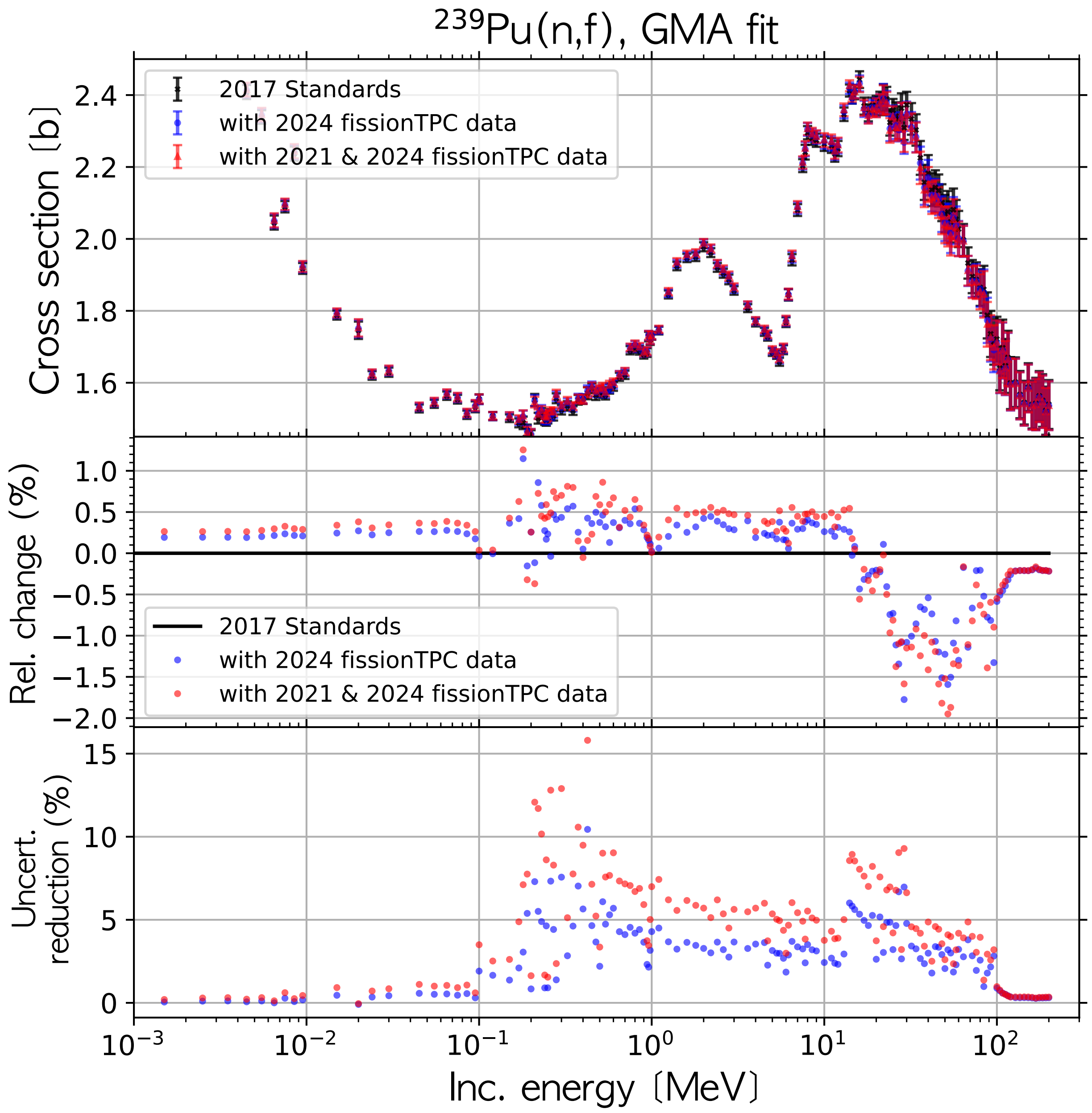
Impact of the new data I: Ratio shape

- Taking the 2021 measurements as cross-section ratio shape, i.e., with unknown normalization
- The impact of the new data on the GMA evaluation of the $^{239}Pu(n,f)$ cross section is less than 1%
- Consistent with D. Neudecker's analysis *[LA-UR-21-24093]*



Impact of the new data II: Absolute ratio

- Systematic increase is reflected in the GMAP result
- Normalization uncertainty (0.8%) limits the impact of the new measurement in the combined analysis
- Including the 2021 and 2024 experiments as separate experiments increases the impact and reduces the uncertainty



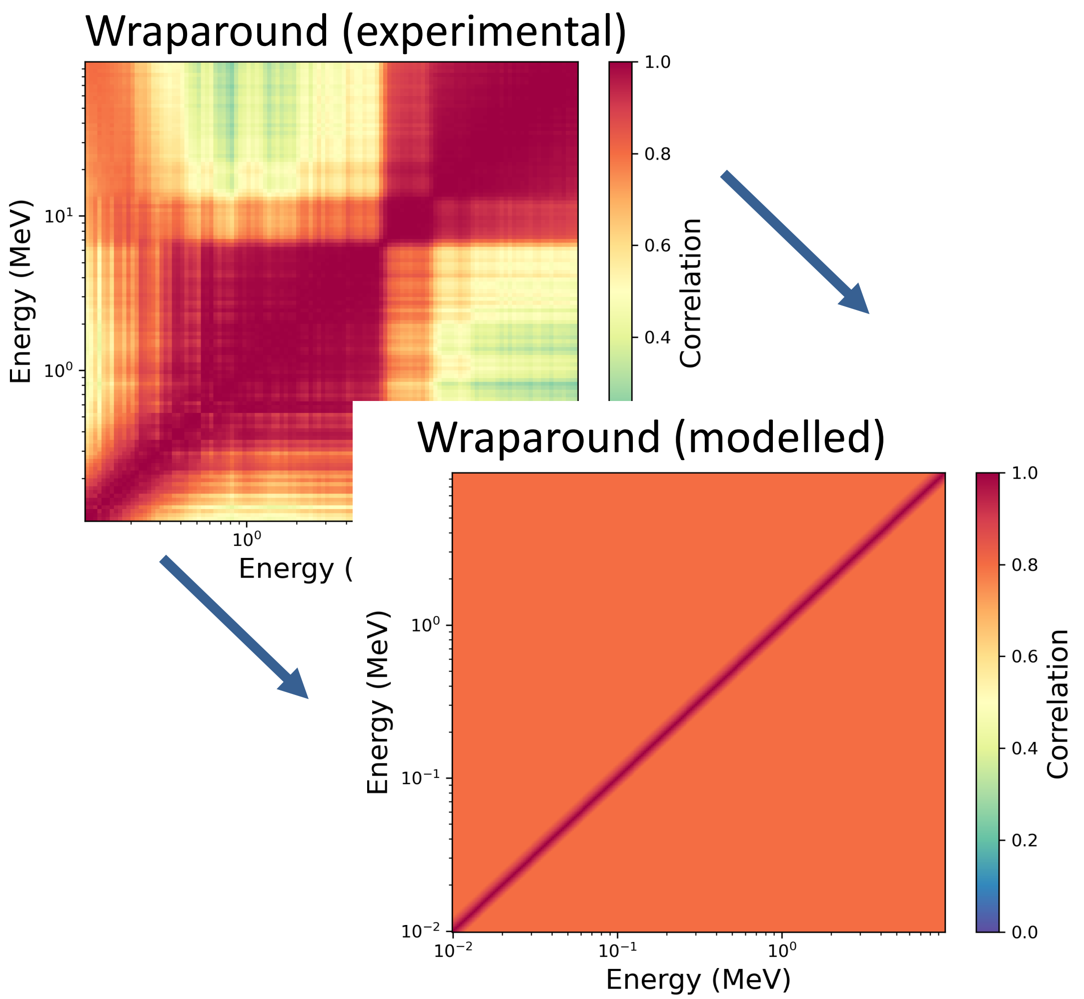
Measurement uncertainties and modelling of correlations

- The GMAP code allows to parameterize correlations due to energy-dependent uncertainties

- Correlations did not change in the re-measurement

Source of uncertainty	Shape of covariance
Variational (Particle-ID)	Diagonal
Wraparound	Diagonal+ 0.8 average
Efficiency	Diagonal
Impurity	Diagonal + 0.35 average
Beam-target Overlap	Diagonal

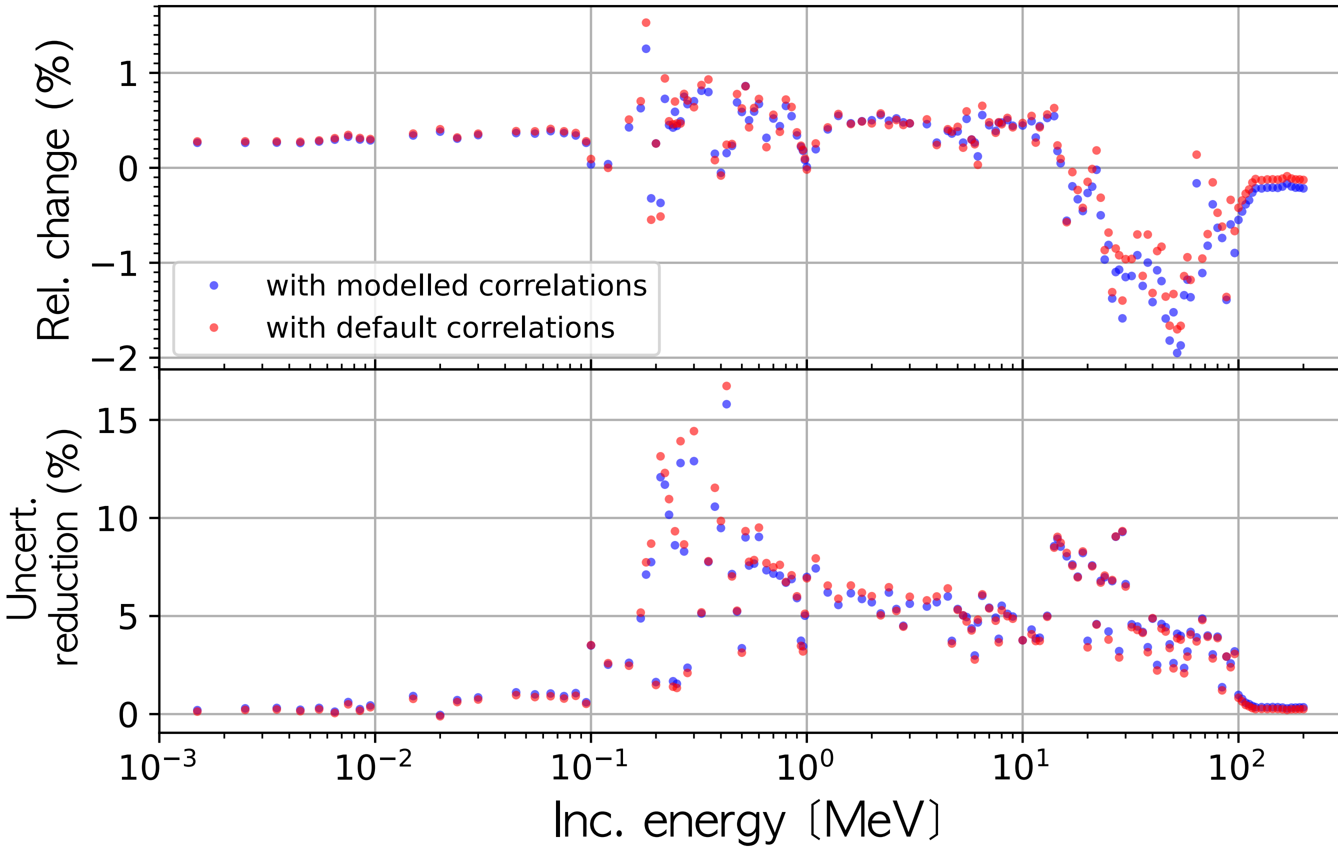
- Following D. Neudecker's evaluation of the 2021 shape data



Measurement uncertainties and modelling of correlations

- The GMA code allows to parameterize correlations due to energy-dependent uncertainties

Source of uncertainty	Shape of covariance
Variational (Particle-ID)	Diagonal
Wraparound	Diagonal+ 0.8 average
Efficiency	Diagonal
Impurity	Diagonal + 0.35 average
Beam-target Overlap	Diagonal



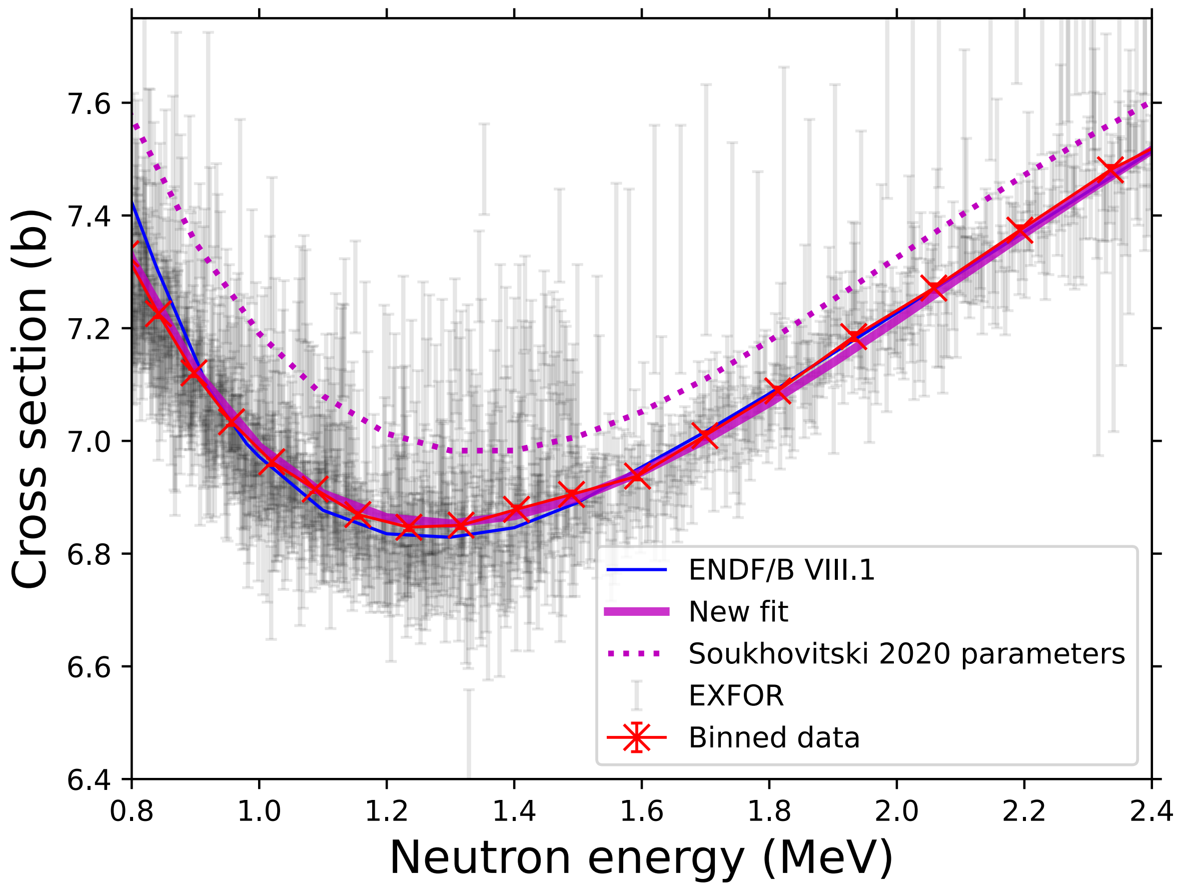
- Taken from D. Neudecker's evaluation

Update II

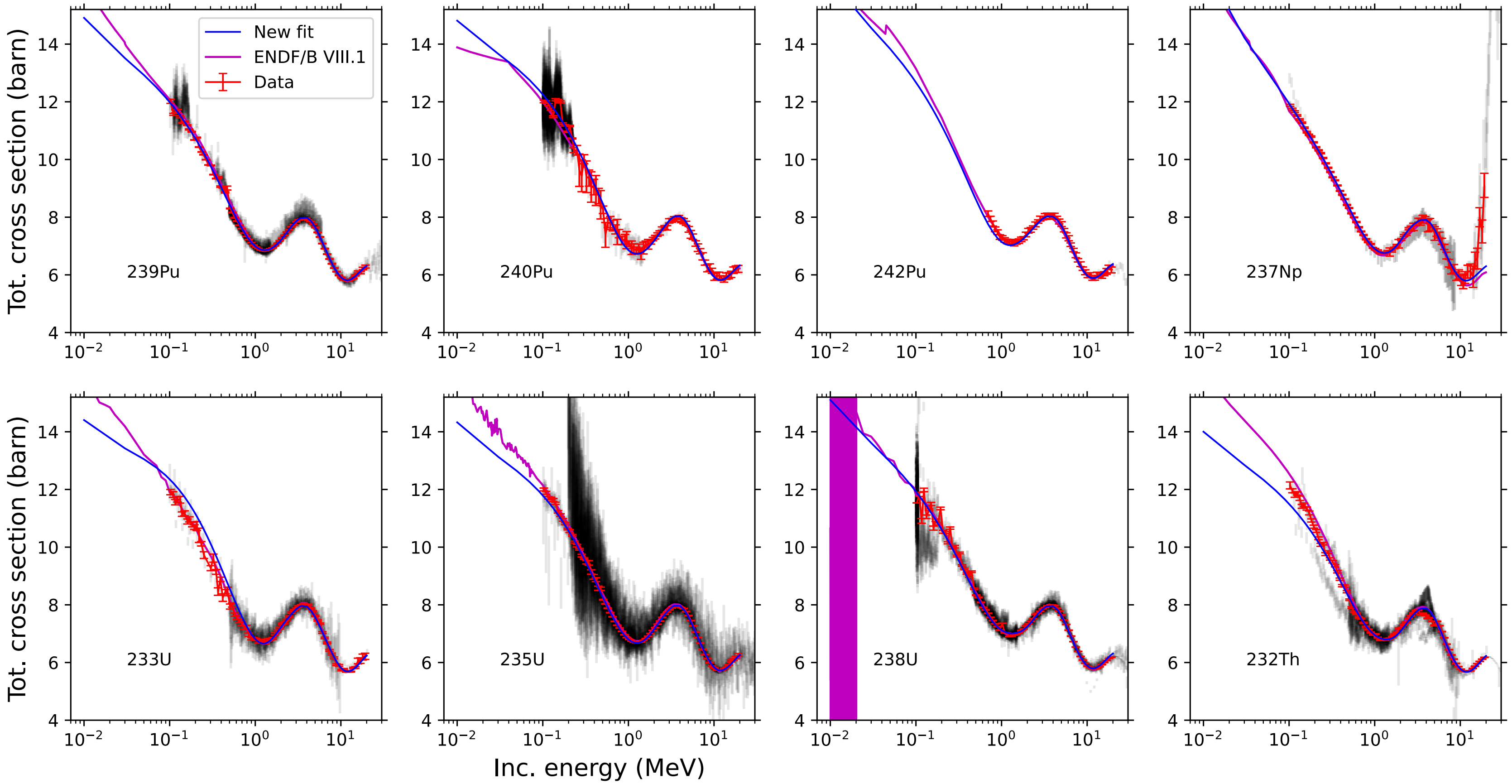
New fit of optical model parameters

Re-fitting the optical model potential

- Coupled-Channels calculations with FRESCO *[I. Thompson]*) with a phenomenological, dispersive optical potential (OMP) by Soukhovitskiĩ (2016,2020)
- Re-fitting of the OMP parameters (~30) to ensure a good reproduction of the total cross section within the model *[lead by K. Kravvaris]*
- Re-fitting also allows to evaluate the uncertainties and covariances
- For our binning of the exp data:
  - $\chi^2_{Fit} = 0.49$ ($\chi^2_{ENDF} = 1.29$)



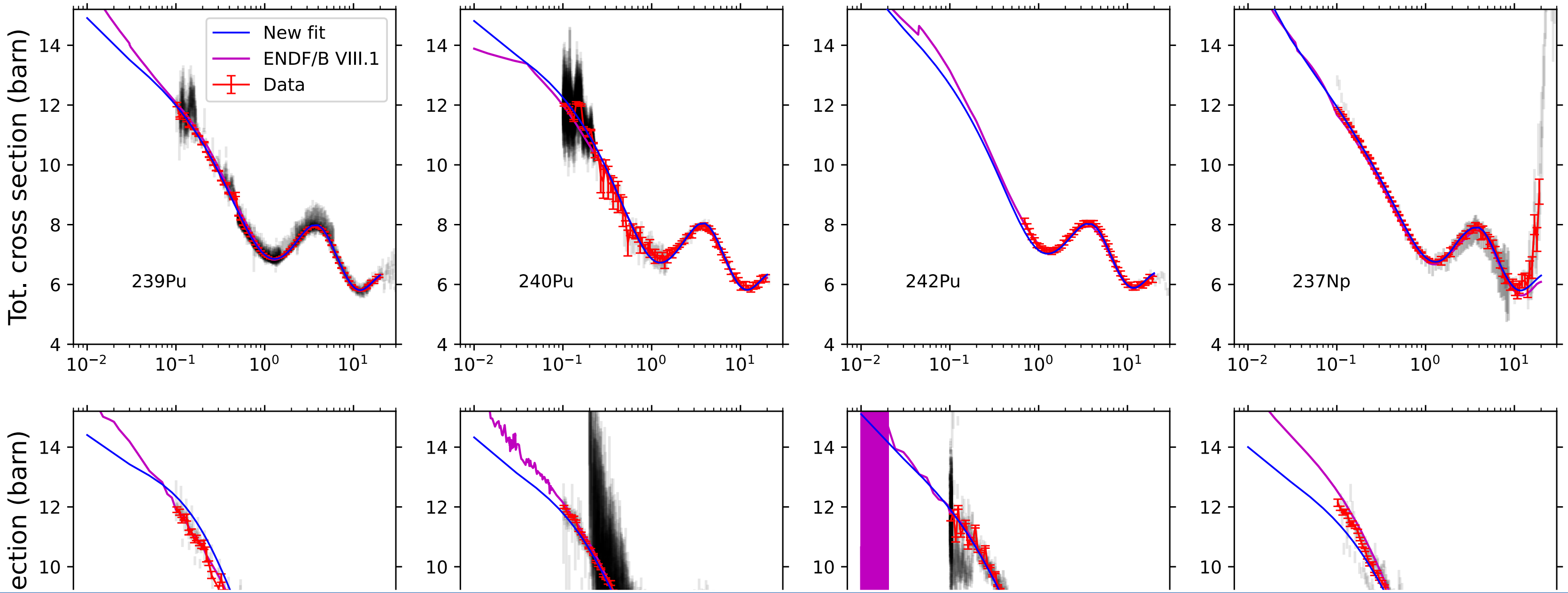
Global fit to the OMP + deformation parameters



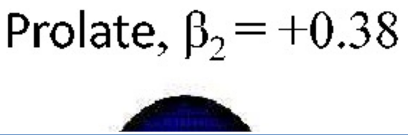
- Fit OMP parameters to data for 8 actinides
- Include deformation parameters simultaneously
- Very good agreement can be achieved

Prolate, $\beta_2 = +0.38$

Global fit to the OMP + deformation parameters



- Fit OMP parameters + deformation parameters simultaneously
- Very good agreement can be achieved

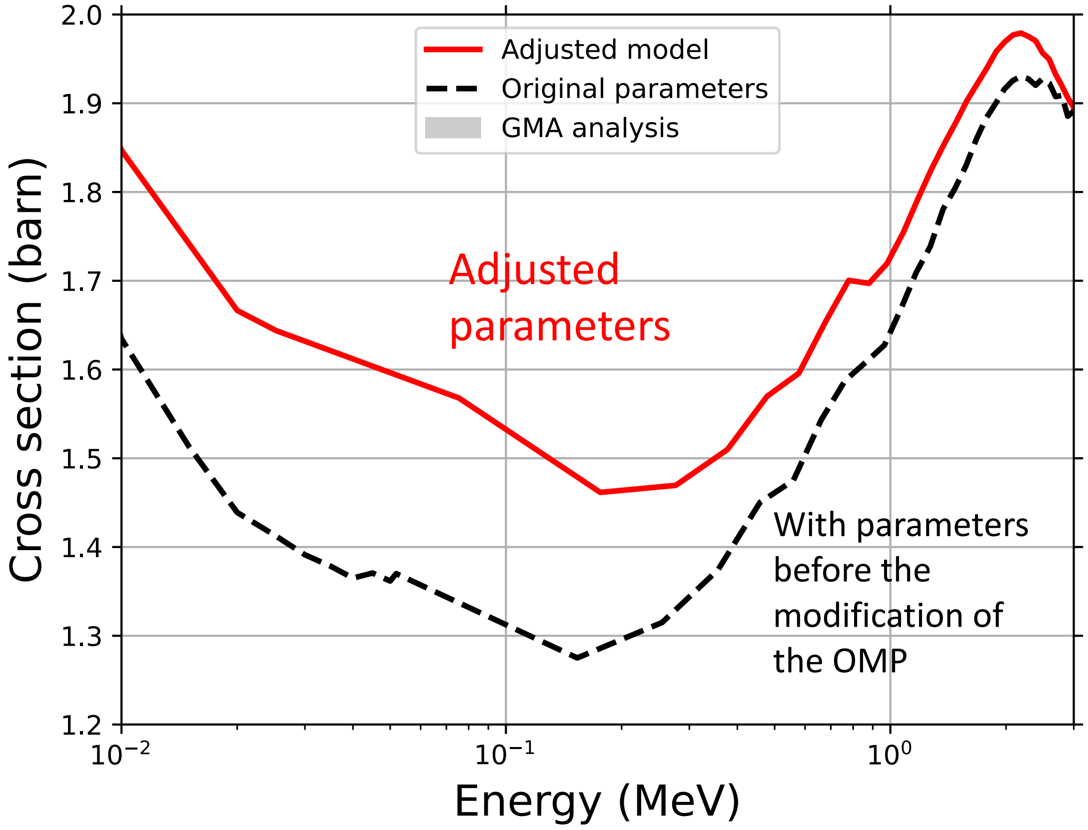


Deformation parameter β_2								
	232Th	233U	235U	238U	237Np	239Pu	240Pu	242Pu
New Fit	0.209	0.172	0.199	0.223	0.231	0.206	0.196	0.228
FRDM12	0.205	0.206	0.215	0.236	0.226	0.236	0.237	0.237
Soukhovitskiĩ et al. (2020)	0.201	0.181	0.220	0.223		0.226		

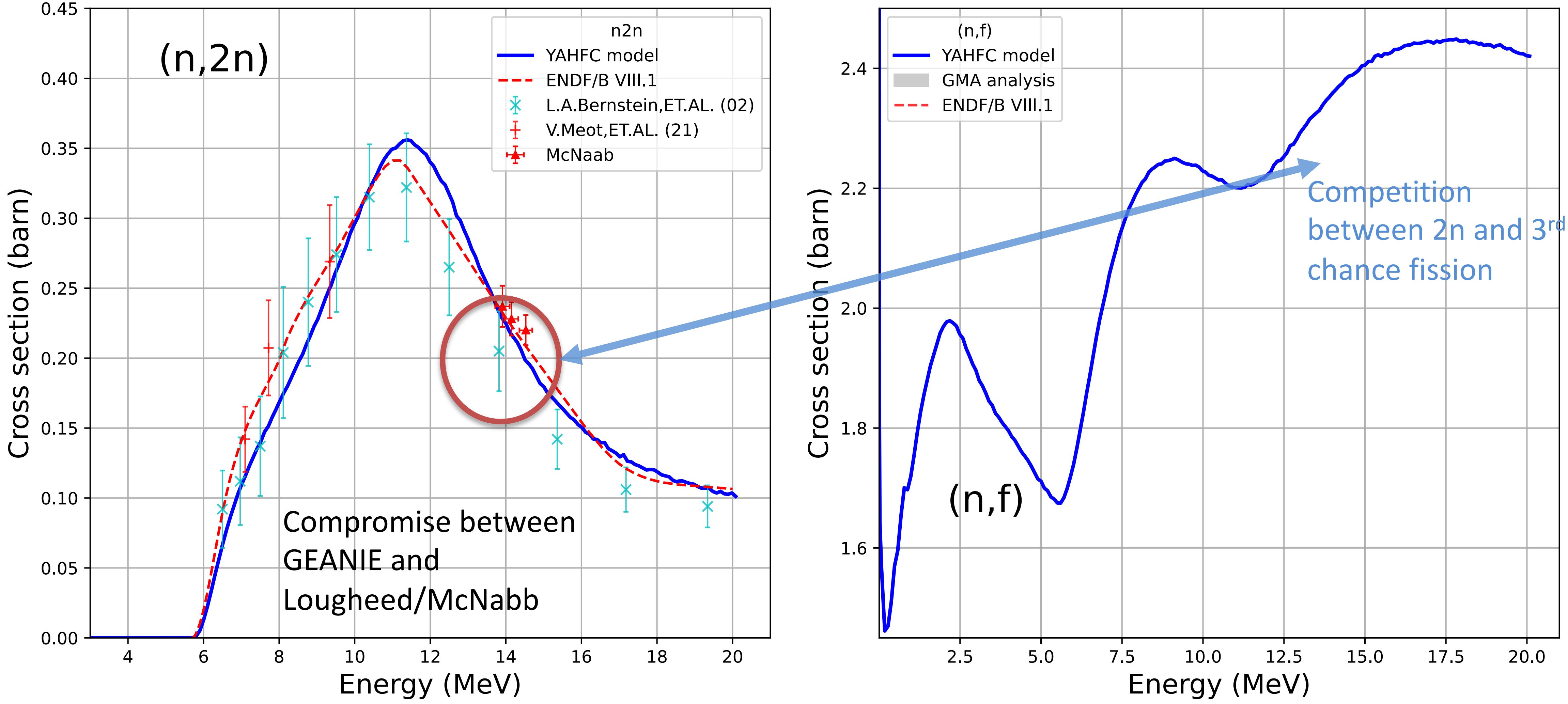
Hauser-Feshbach (YAHFC) model parameters

- New total cross section leads to a need for an adjustment of the reaction model parameters

- In the evaluation:
  - We will use the GMAP result for (n,f)
  - Differences in the (n,f) cross sections are compensated by adjustments of the elastic channel -> aim to make the residual as small as possible
- Aspects of using a reaction model:
  - Model uncertainties and covariances
  - Including cross-channel correlations

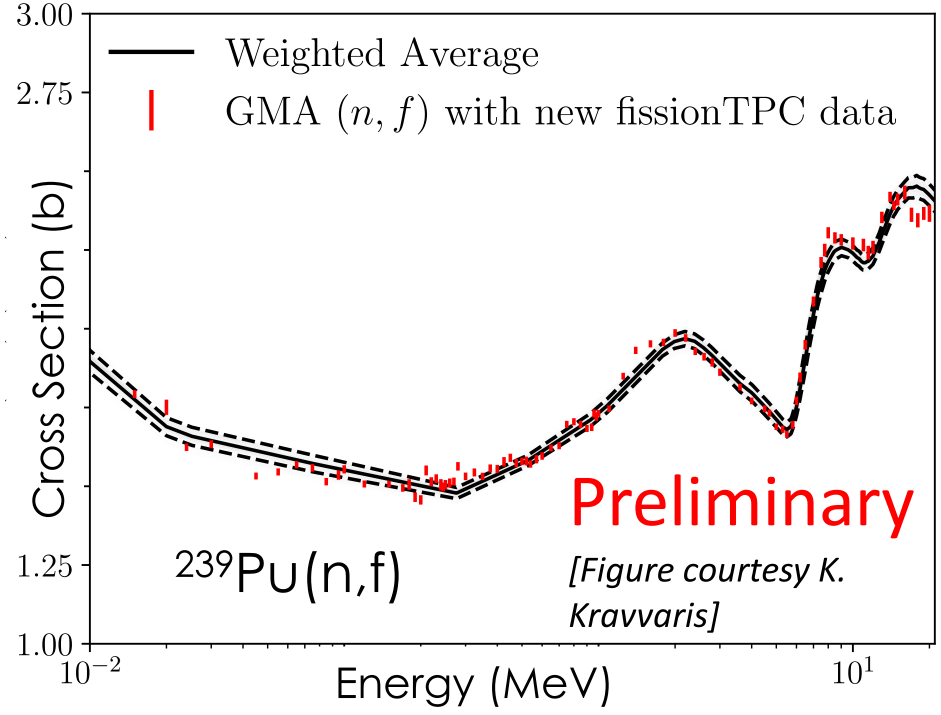


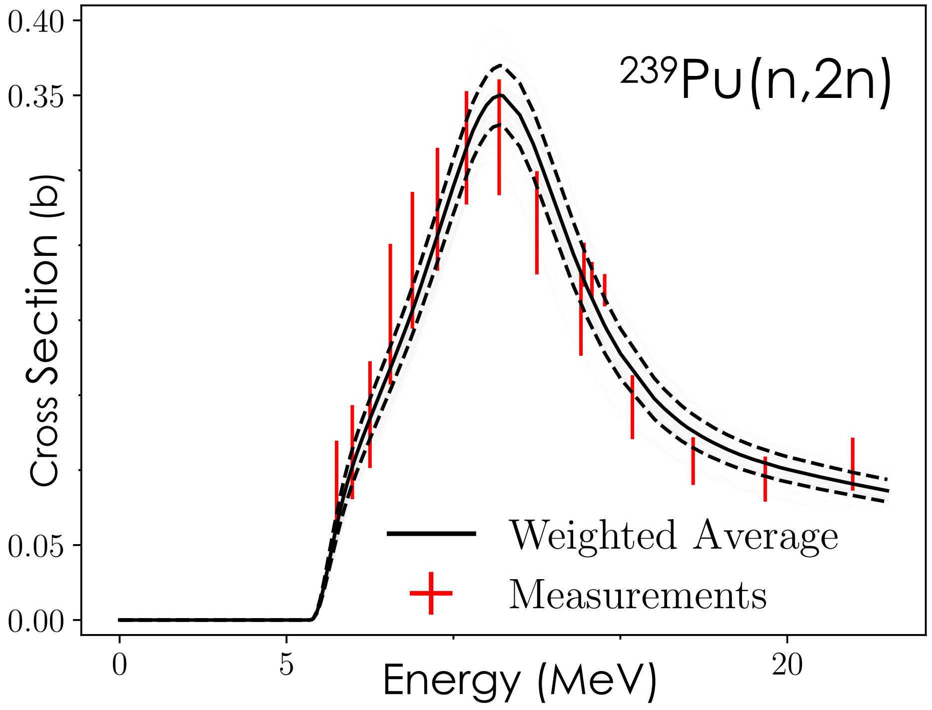
Cross-check with (n,2n)



Refinement and covariances with Backward-Forward Monte-Carlo

- After the initial fit "by eye" reaction model parameters are adjusted to data by a BFMC approach *[Bauge et al. 2007]*
- From this sampling, **covariances** are obtained that take the experimental uncertainties and model uncertainties into account.





Next steps

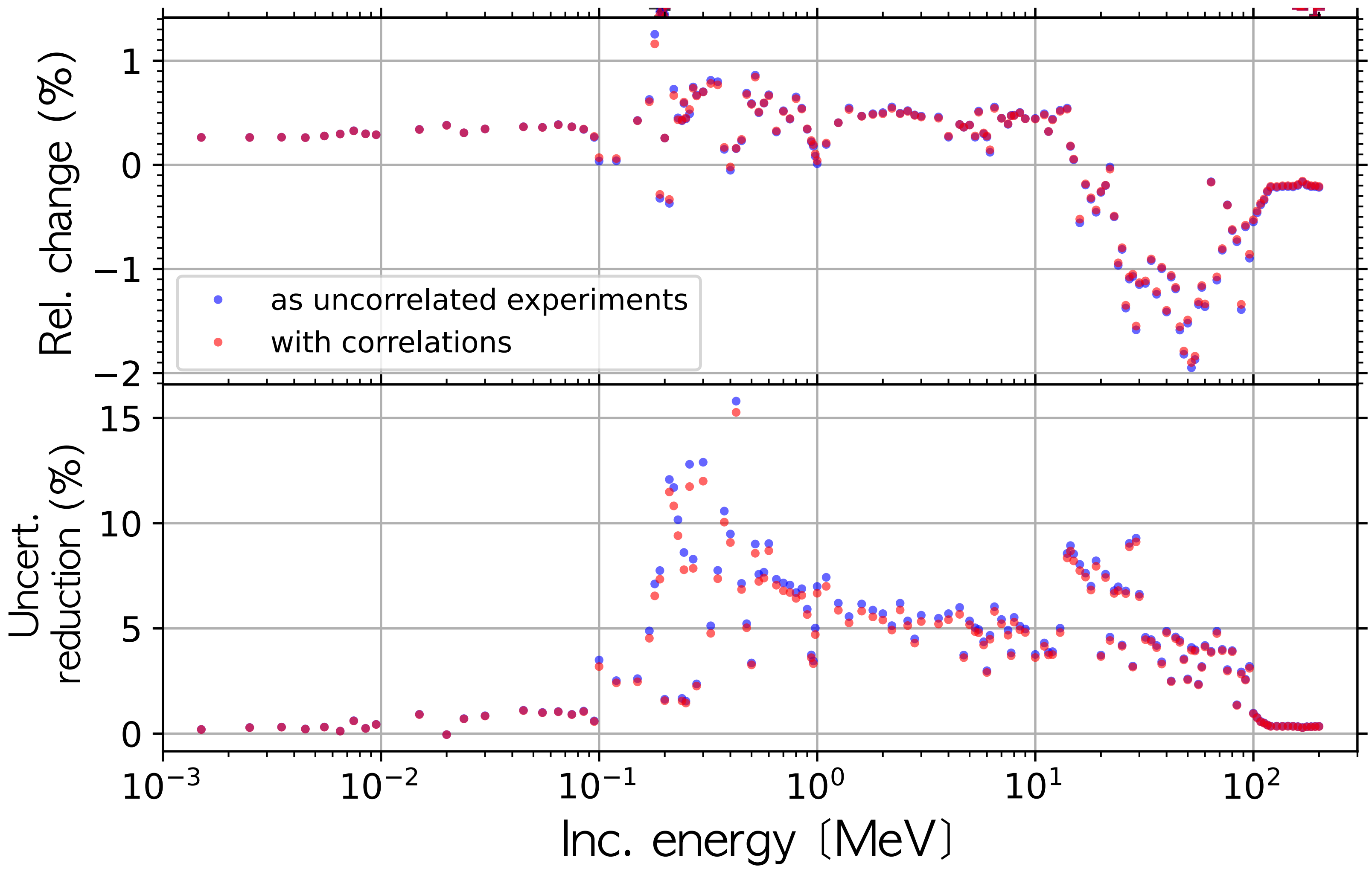
- Estimate uncertainties and covariances
- Replace modelled (n,f) cross-section with GMA result
- Add resonances and yield data from ENDF/B VIII.1 to obtain a full evaluation dataset
- Translate and process in GNDS format -> V&V

Lawrence Livermore National Laboratory

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Impact of correlation between experiments

- Correlation between experiments are difficult to estimate
- In our analysis, including correlations between some of the major uncertainties does not have a large impact



GMA (Gauss-Markov-Aitken)

- Generalized least squares (“non-model”) fit
- Gives maximum likelihood values and covariances

- Implementation:
  - GMAP: Fortran 77 code (Poenitz 1980’s, ANL)
  - gmapy: recently python version: G. Schnabel (IAEA)
- Combined with neutron standards database

GMA equations

- Generalized least-squares.
- Assumes normal distribution of random variables.
- Linearization close to most probable value.
- Linear algebra problem, good numerical implementation.

$$p = (A^T V_y^{-1} A)^{-1} A^T V_y^{-1} \mathbf{y}$$

$$V_p = (A^T V_y^{-1} A)^{-1}$$

measured covariances

measured parameters

design matrix

evaluation

best parameters

best covariances