OAK RIDGE National Laboratory

Progress on Light Water Covariance for ENDF/B-IX

Chris W. Chapman, Jordan McDonnell, Goran Arbanas, Iyad Al-Qasir

Oak Ridge National Laboratory

CSEWG meeting – 6 November 2024

ORNL is managed by UT-Battelle LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

Outline

- Previous Work
- Proposed Plan
- Current Progress
- Future Work

Previous Work

- Several different attempts to quantify TSL uncertainties:
  - Fitting LEAPR parameters of light water to total cross sections [1]
  - Fitting molecular dynamics (MD) parameters to light water double differential scattering cross sections [2]
  - Studying effect of phonon density of states (PDOS) covariance on $S(\alpha, \beta)$ covariance [3]
- Each have various pros and cons

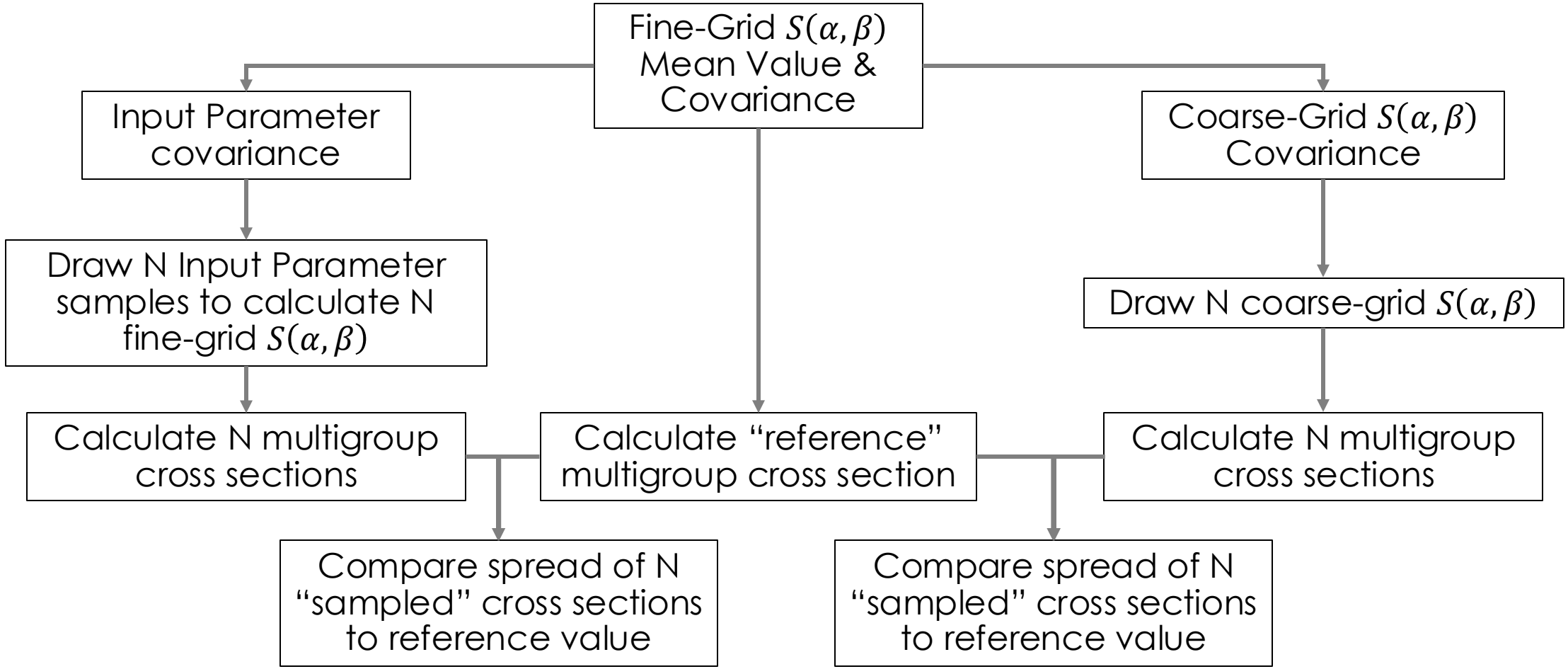
Previous Work

- Previous work:
  - Varied parameters of molecular dynamics potential
  - Fit to experimental double differential scattering cross sections (DDXS) measured at SNS
  - Calculated mean value and covariance using UMC-G method (Bayesian Monte Carlo method)
- Pitfalls
  - Varied parameters didn't include nuclear cross section
  - Didn't fit to total cross sections
  - UMC-G on large experimental datasets

Proposed Plan

- Re-generate mean value and covariance
  - Vary parameters of LEAPR input based on work from [1]
    - Simpler than MD parameters,
    - Quicker to calculate, so more samples
  - Fit to smaller subset of DDXS data from SNS as well as collection of total cross section measurements
  - Focus on generating covariance of both input parameters & $S(\alpha, \beta)$
- How to test efficacy of these two covariances?

Proposed Plan – Validating Coarse-grid Covariance



Proposed Plan – DNCSH Task

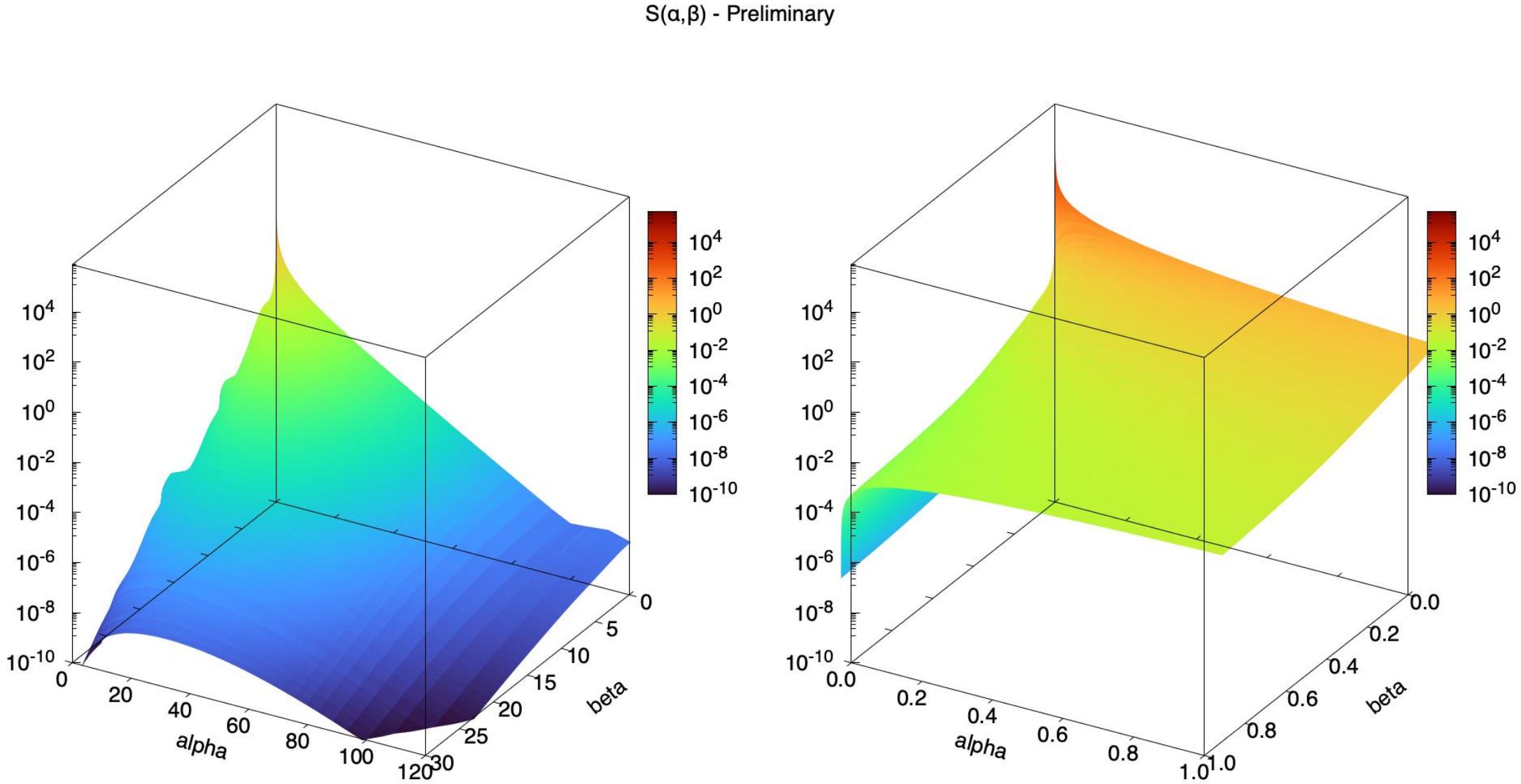
- Once we have a covariance, it's time to use it!
- Convert $S(\alpha, \beta)$ covariance to DDXS covariance
  - Requires DDXS covariance format for transport code; work underway on constructing COVERX format for SCALE
- Modify SAMPLER to draw samples from DDXS covariance
- Confirm spread of results gives consistent results compared to spread of results from independently sampled $S(\alpha, \beta)$

Current Progress

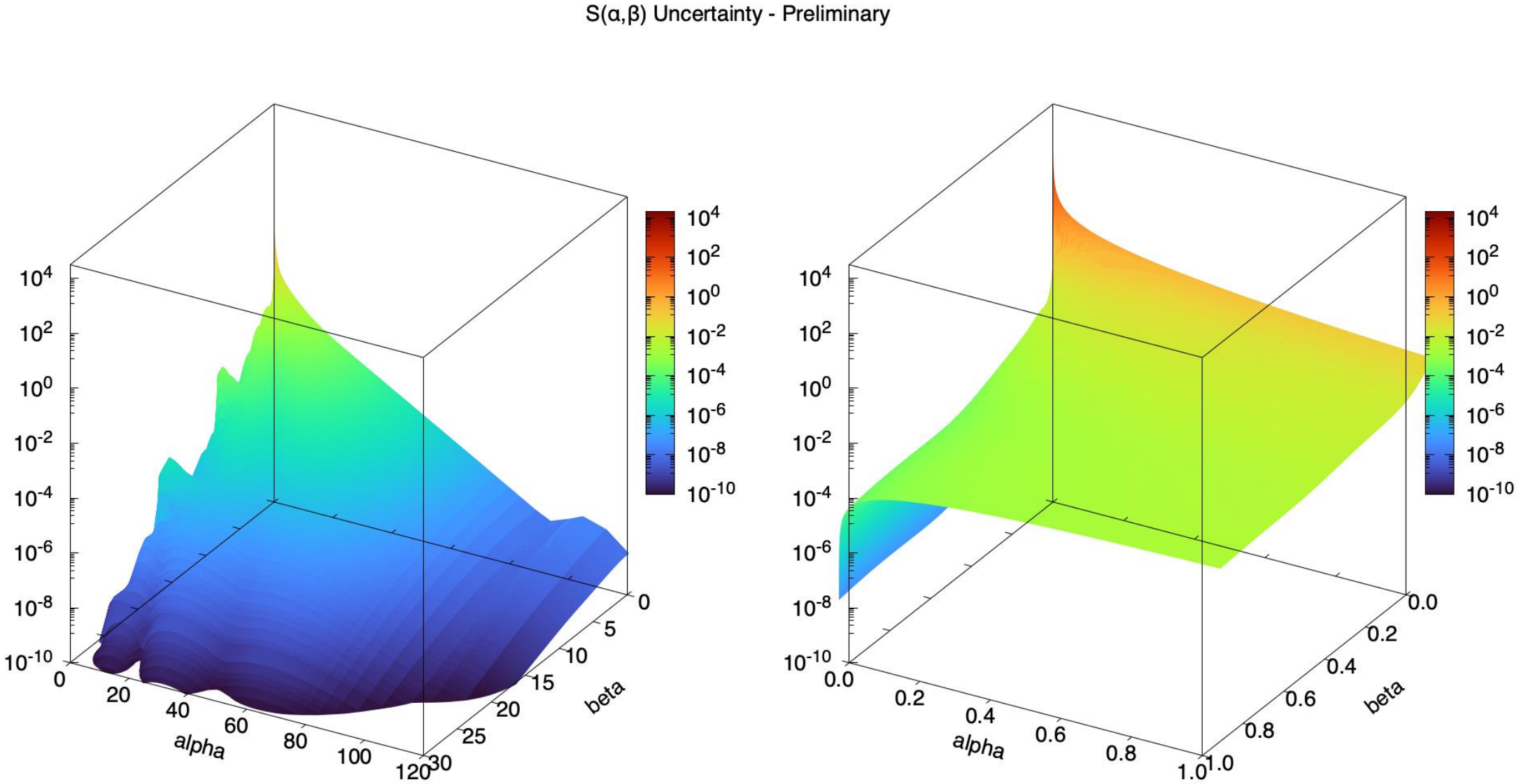
- Mean values & covariances calculated using basis of 2500 input samples
  - Only 250 were used in previous study
- Matrix reduction underway using:
  - Coarse (α, β) grid (every other α & β point)
  - Removal of zero-variance values

Covariance Algorithm	File Size [GB]
Full Matrix	36.8
Coarse-grid	2.32
Coarse-grid (zeros removed)	1.01

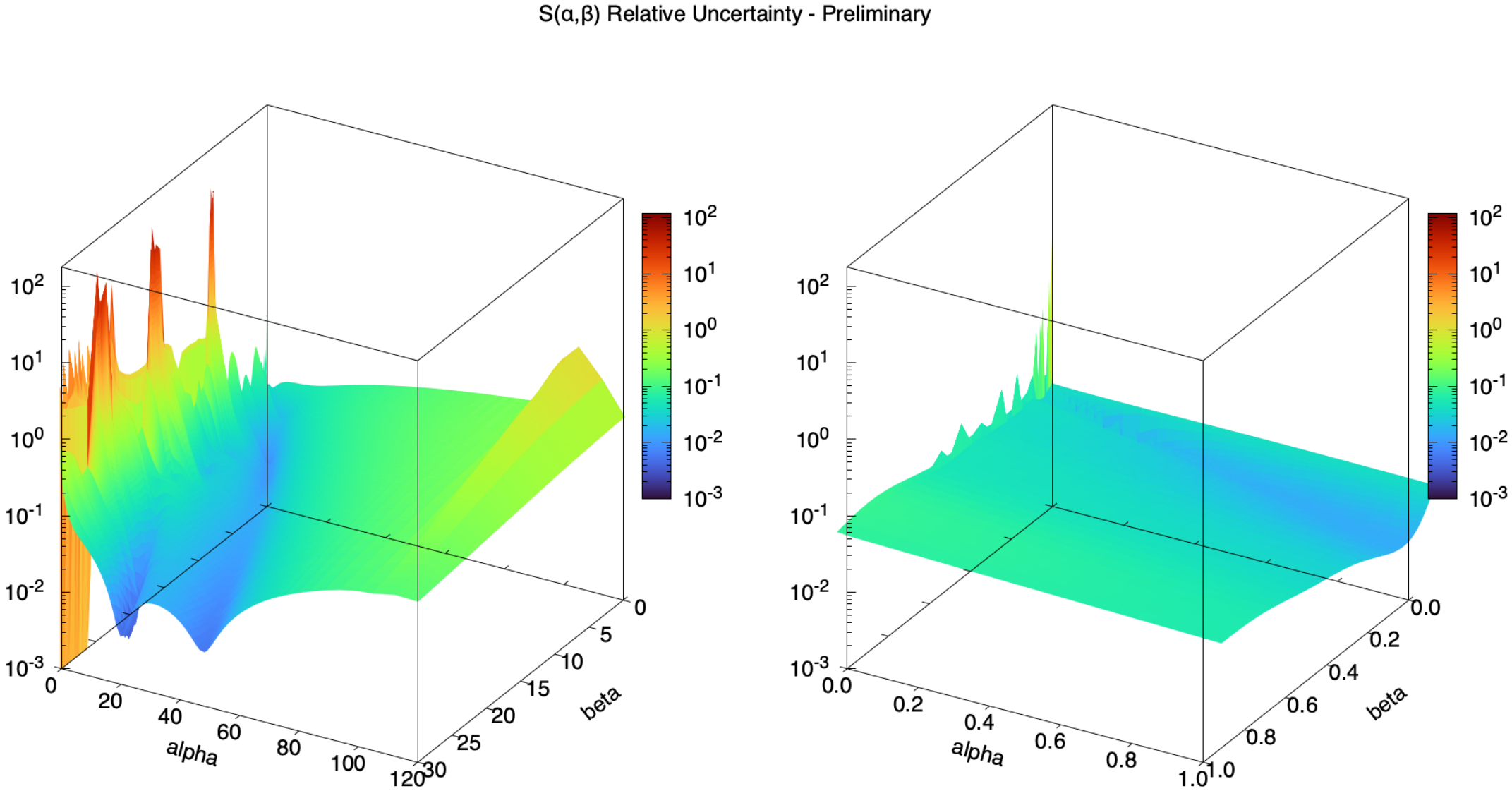
Current Progress – $S(\alpha, \beta)$



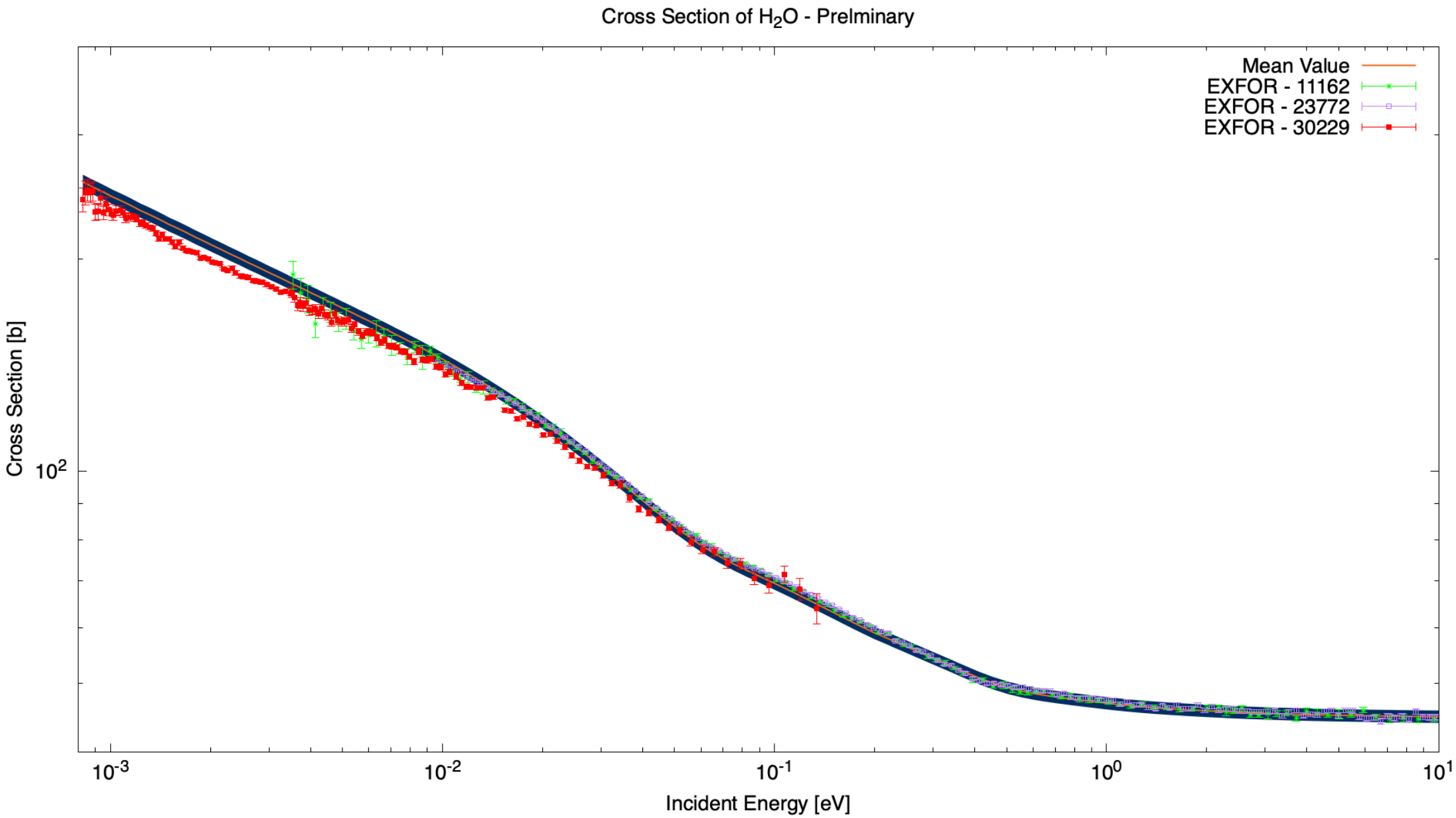
Current Progress – $S(\alpha, \beta)$ Uncertainty



Current Progress – $S(\alpha, \beta)$ Relative Uncertainty



Current Progress – Total XS



Future Work

- TSL covariance
  - Finalize framework
  - Determine best format for storing & disseminating covariance
- SCALE implementation
  - Finalization of COVERX format
  - Implementation of sampling routine within SAMPLER

Acknowledgements

- This work is supported under the framework of DOE / US Nuclear Regulatory Commission (NRC) collaboration for Criticality Safety support for commercial-scale HALEU fuel cycles project (DNCSH)
- The entire Nuclear Data team at ORNL (J. Brown, K. Guber, L. Leal, M. Pigni, K. Ramić, D. Wiarda)

References

- [1] L. Maul, J. I. M. Damián, G. Braoudakis, M. Ho, and G. H. Yeoh, "Perturbation scheme for estimating uncertainties in thermal scattering cross sections of water," *Ann. Nuc. Eng.* Vol. 121 pp. 232-249, 2018, https://doi.org/10.1016/j.anucene.2018.07.020
- [2] C. W. Chapman, G. Arbanas, A. I. Kolesnikov, L. Leal, Y. Danon, C. Wendorff, K. Ramić, L. Liu, and F. Rahnema, "Methodology for Generating Covariance Data of Thermal Neutron Scattering Cross Sections," *Nuc. Sci. Eng.* Vol. 195, no. 1, pp. 13-32, 2021, https://doi.org/10.1080/00295639.2020.1792716
- [3] J. C. Holmes, A. I. Hawari, M. L. Zerkle, "A Phonon-Based Covariance Methodology for ENDF S(α,β) and Thermal Neutron Inelastic Scattering Cross Sections," *Nuc. Sci. Eng.* Vol. 184, No. 1, pp 84-113, 2016, https://doi.org/10.13182/NSE15-89

Questions?