Bayesian Monte-Carlo Evaluation Framework of Differential and Integral Data

Goran Arbanas, Andrew Holcomb, Jesse Brown, and Dorothea Wiarda

Nuclear Data and Criticality Safety Group

Reactor and Nuclear Systems Division

Oak Ridge National Laboratory

Cross Section Evaluation Working Group (CSEWG) Meeting, Nuclear Data Week, BNL, Nov. 4 – 8, 2019

Presentation Outline

- Extant methods (linear approximation)
- Bayes theorem for generalized data
- Schematic diagram
- Framework Demonstration on U-233 integral and differential data
  - Comparison to linear approximation
- Summary and outlook

Summary of conventional evaluation of diff. and integral data:

- Extant *R*-matrix resolved resonance range (RRR) evaluations assume normal probability density functions (PDFs) and use Newton-Raphson method to minimize chi^2 of R-matrix and differential data only.
- *R*-matrix parameters are subsequently further optimized to improve the fit of neutron transport simulations of integral benchmark experiments (IBEs), by a generalized linear least squares (GLLS) of the SAMINT module of SAMMY.
- The 2 methods above are based on Bayes theorem but assume all PDFs are normal (Gaussian) and use a linear approximation for IBEs.
- The proposed framework would remove both approximations
- Similar MC methods exist for optimization of TENDL optical model cross sections
  - P. Helgesson, H. Sjostrang, A.J. Koning, J. Ryden, D. Rochman, E. Alhassan, S. Pomp, Prog. Nucl. Ener. 96 (2017) 76-98
- MC method for fitting RRR to diff. data alone announced in the AZURE *R*-mat. Code
- SAMPLER module in SCALE randomly perturbs c.s.'s and geometry of IBEs

A general form of Bayes theorem

- Model parameters, data, and any model defect treated on the same footing:
  - G. Arbanas et al., “Bayesian Optimization of Generalized Data”, CW2017, EPJ-N, 4 (2018) 30, https://doi.org/10.1051/epjn/2018038
- Uses *posterior* expectation values of constraints relating model, data, and any defect
- Its likelihood function is an exponential function of constraints; prior may be any PDF.
  - Sergio Davis, “*Exponential Family Models from Bayes’ Theorem under Expectation Constraints*” (2016) https://arxiv.org/abs/1503.03451
- Constraints could be imposed selectively on posterior expectation values of
  - 1st moment i.e. mean values of $T(P) - D - \delta$
  - 2nd moment i.e. covariances of the above
  - Conventional Bayes’ theorems is a special case where both constraints are set to 0 (next slide)
- *cf.* conventional Bayes’ theorem: posterior exp. values determined by priors & model
- Conventional form of Bayes’ assumes normal PDFs: *chi*^{2}-minimization
  - Demonstrated to be inferior to using MCMC: G.B. King et al. Phys. Rev. Lett. 122, 232502 (2019)
  - https://doi.org/10.1103/PhysRevLett.122.232502

Linear approx. in the RRR is used is used twice: for $\Delta\sigma$ *and* Δk_{eff}

- $\Delta\sigma$ from R-matrix resonance parameter cov. matrix in ENDF File 32 (e.g. SAMMY):

$$\left\langle \delta\sigma_i \, \delta\sigma_j \right\rangle = \sum_{n,m} \frac{\partial \sigma_i}{\partial u_n} M_{nm} \frac{\partial \sigma_j}{\partial u_m}$$

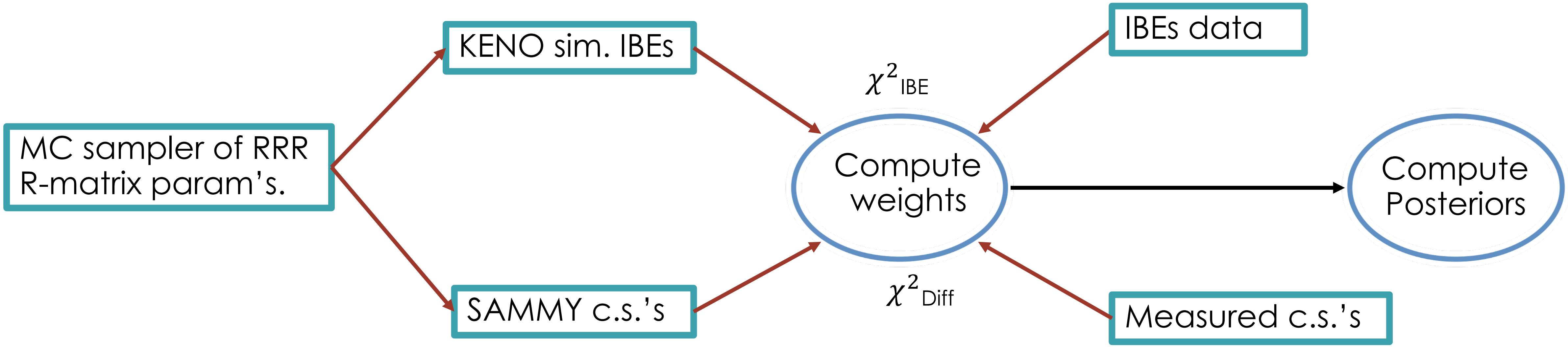
- Δk_{eff} from the covariance matrix of cross sections computed above (e.g. TSURFER)

$$\mathbf{C_{kk}} = \mathbf{S_{k\alpha} C_{\alpha\alpha} S_{k\alpha}^T} \qquad \mathrm{S}_\alpha = \frac{\alpha}{\mathrm{R}} \frac{\partial \mathrm{R}}{\partial \alpha}$$

- Both linear approximations need to be accurate to obtain accurate results

Bayesian MC optimization framework overview

- Flexible: IBEs or Diff. Data alone could be analyzed independently or simultaneously



- MC sample weight takes into account agreement with differential and IBE data
  - Initially assuming normal PDFs:

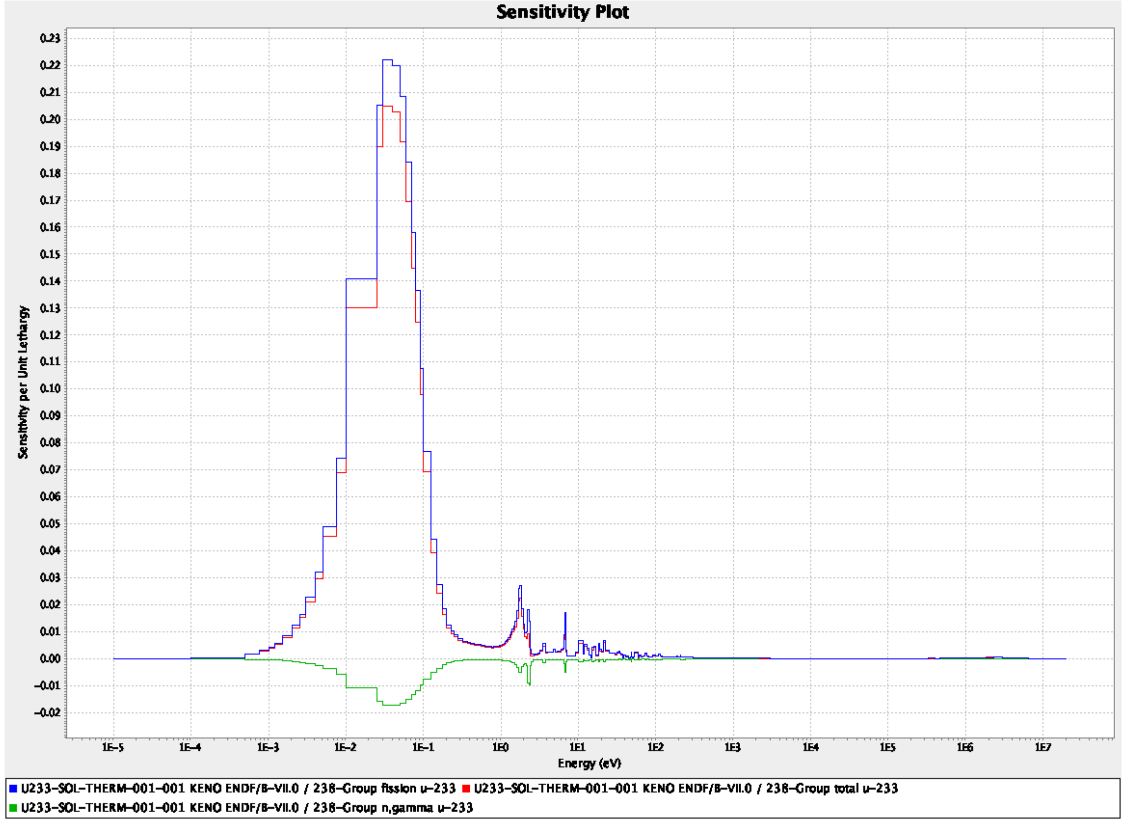
$$w = \exp[-\chi^2/2] \qquad \chi^2 = \chi^2_{\text{IBE}} + \chi^2_{\text{Diff}}$$

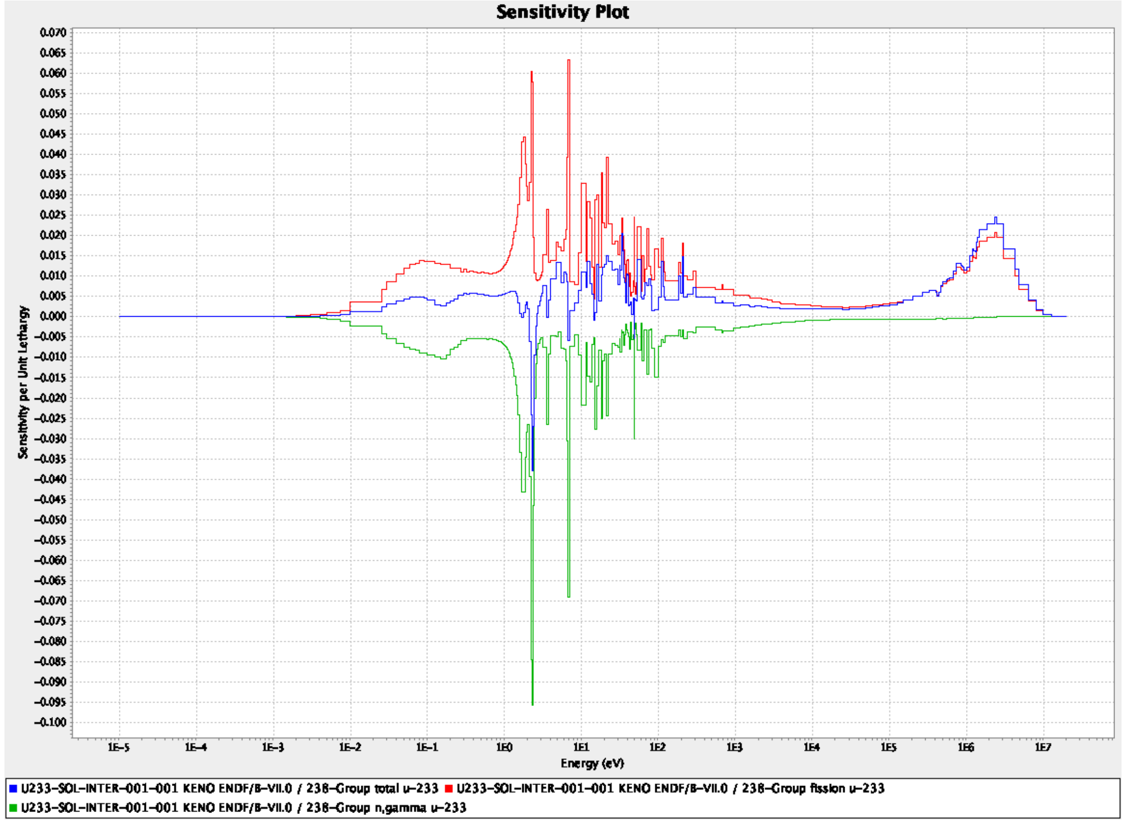
- Large number of R-matrix param's. requires Metropolis-Hastings MCMC method
  - For MC random sampling to arrive at the posterior PDFs of parameters

Application to U-233

- 1000 randomly perturbed resonance parameter sets created by sampling File 32
- For each set calculate k_{eff} for U233-SOL-{THERM, INTER}-001-001 (KENO code), and then calculate k_{eff} mean values and uncertainties,
  - compare to corresponding TSUNAMI-IP's
  - Compare to measured IBE data
- For each set calculate differential cross sections using the SAMMY and then calculate mean values and uncertainties (transmission, fission)
  - Compare to SAMMY File 32 calculation, assuming it can be done
  - Compare to differential data (transmission, total, fission) by K. Guber (ORNL)

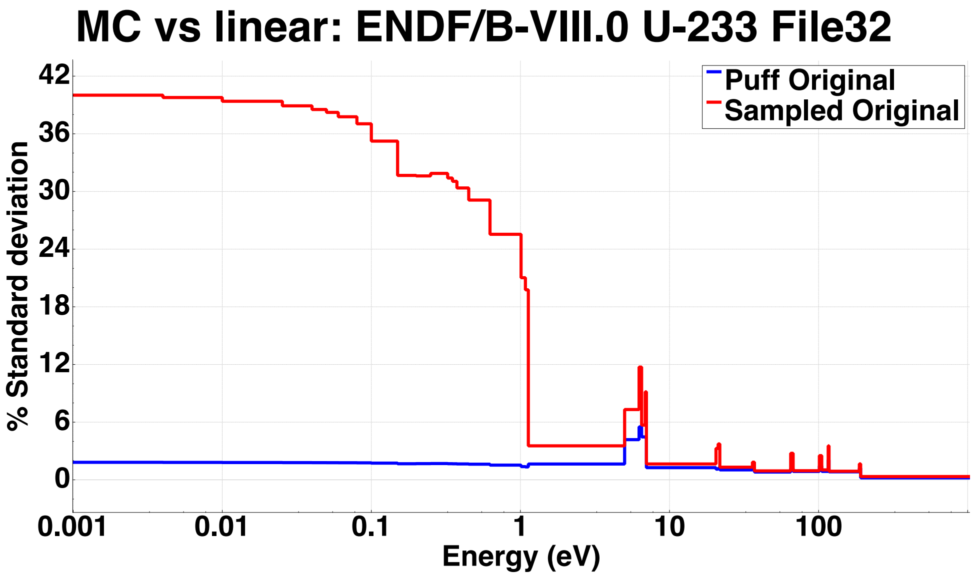
Cross Section Sensitivity of U233-SOL-{THERM, INTER}-001-001

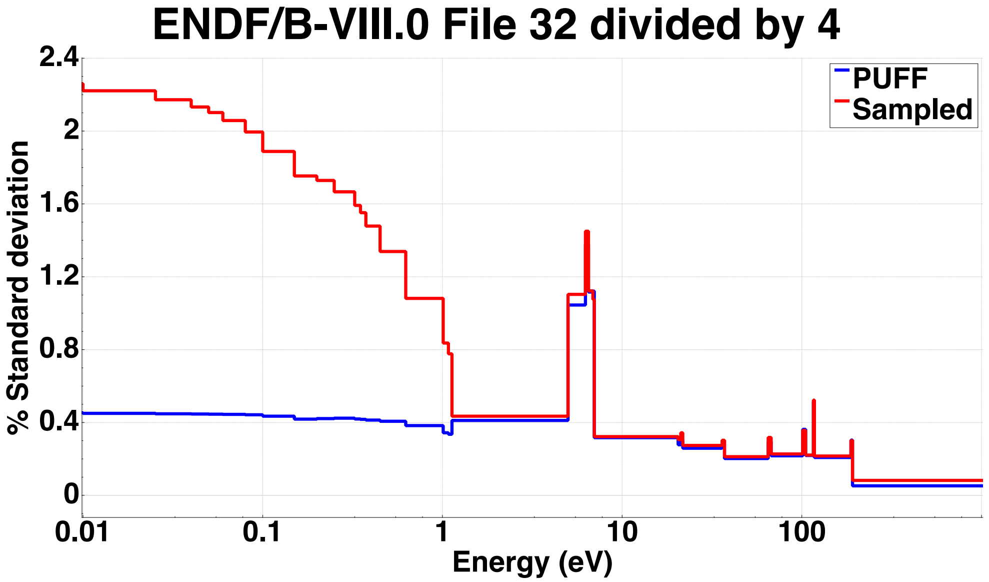




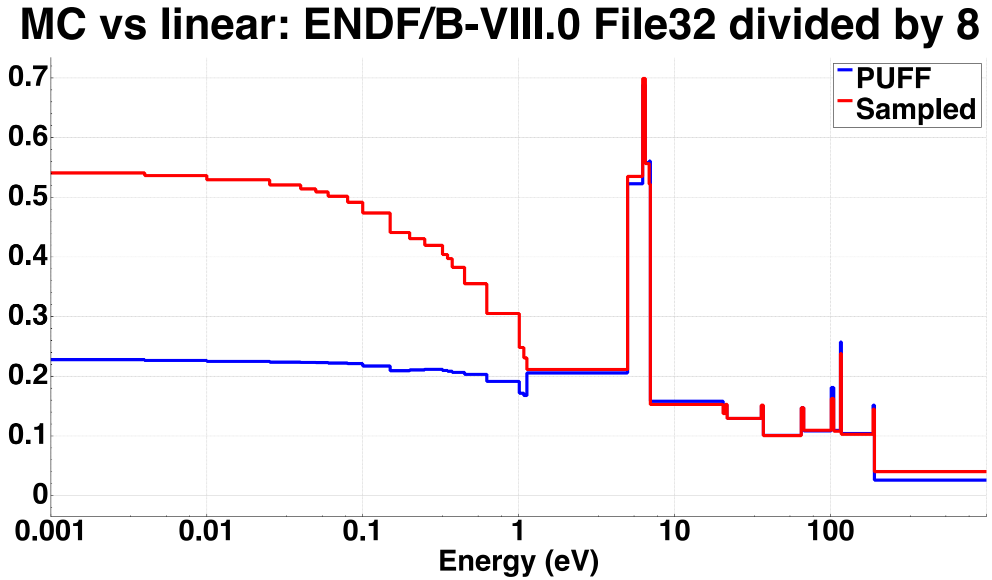
Uncertainties from MC *vs.* lin. approx. of ENDF/VIII.0 U-233 File 32

- Linear approximation significantly underestimates uncertainties encoded in File 32





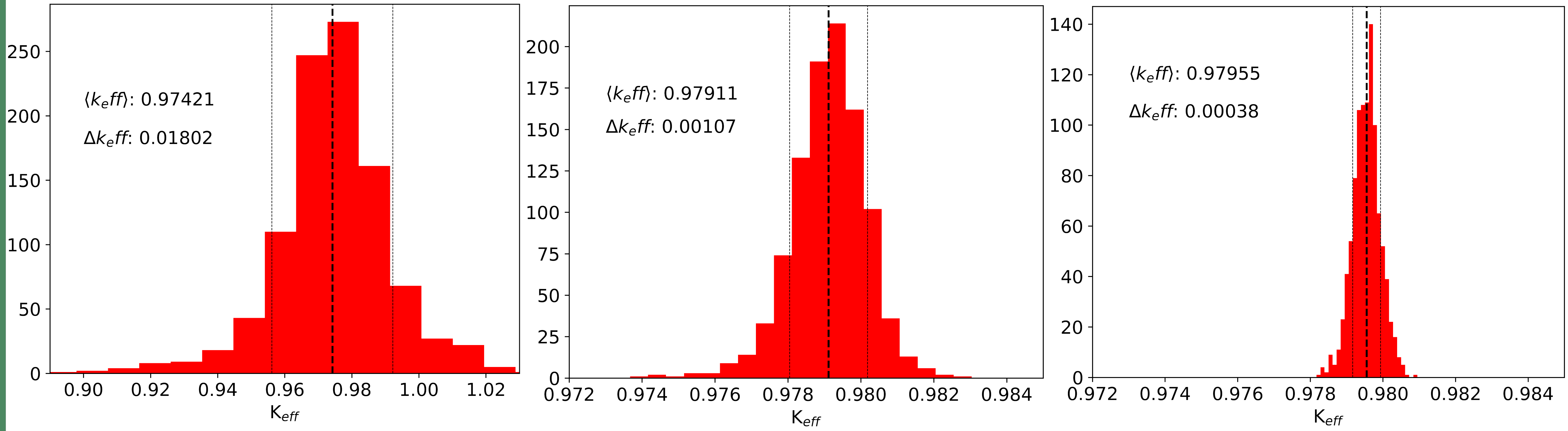
- → Δk_{eff} (MC) >> Δk_{eff} (linear approx.)
- MC and linear approx. reach similar uncertainty in the RRR for File 32/8
- The effect of large uncertainty on sub-threshold resonance seen below 1 eV



MC vs. linear approx.: Δk_{eff} of U233-SOL-INTER-001

- For U233-SOL-INTER-001 consistency between MC and linear approx. is achieved after dividing the U-233 ENDF/B-VIII.0 File 32 by 8

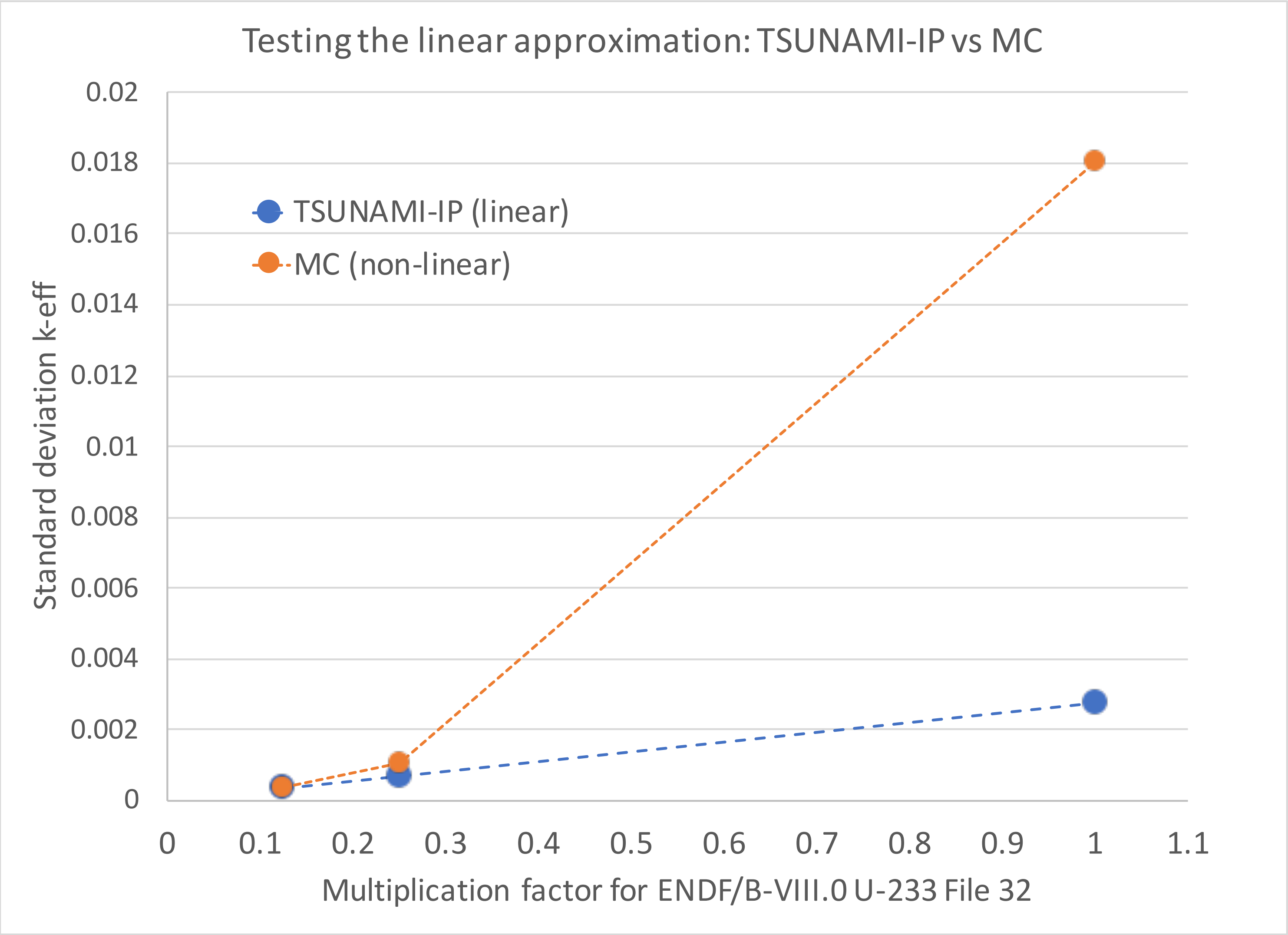
MC samples from: ENDF/B-VIII.0 File 32, File 32 divided by 4, File 32 divided by 8



- k_{eff} uncertainty is decreasing significantly faster than linear scaling would imply

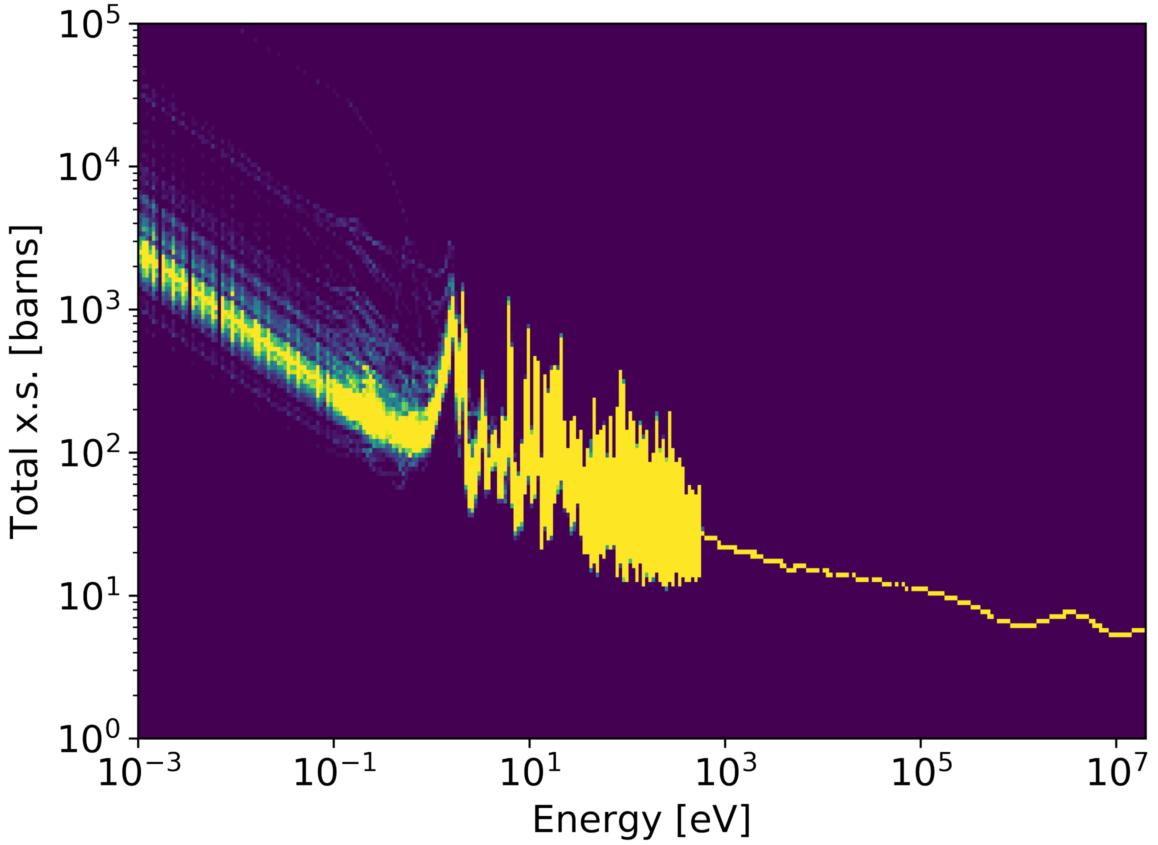
MC *vs.* linear approx. for Δk_{eff} of U233-SOL-INTER-001-001

- MC reveals large deviation from non-linearity for ENDF/B-VIII.0 U-233 File 32



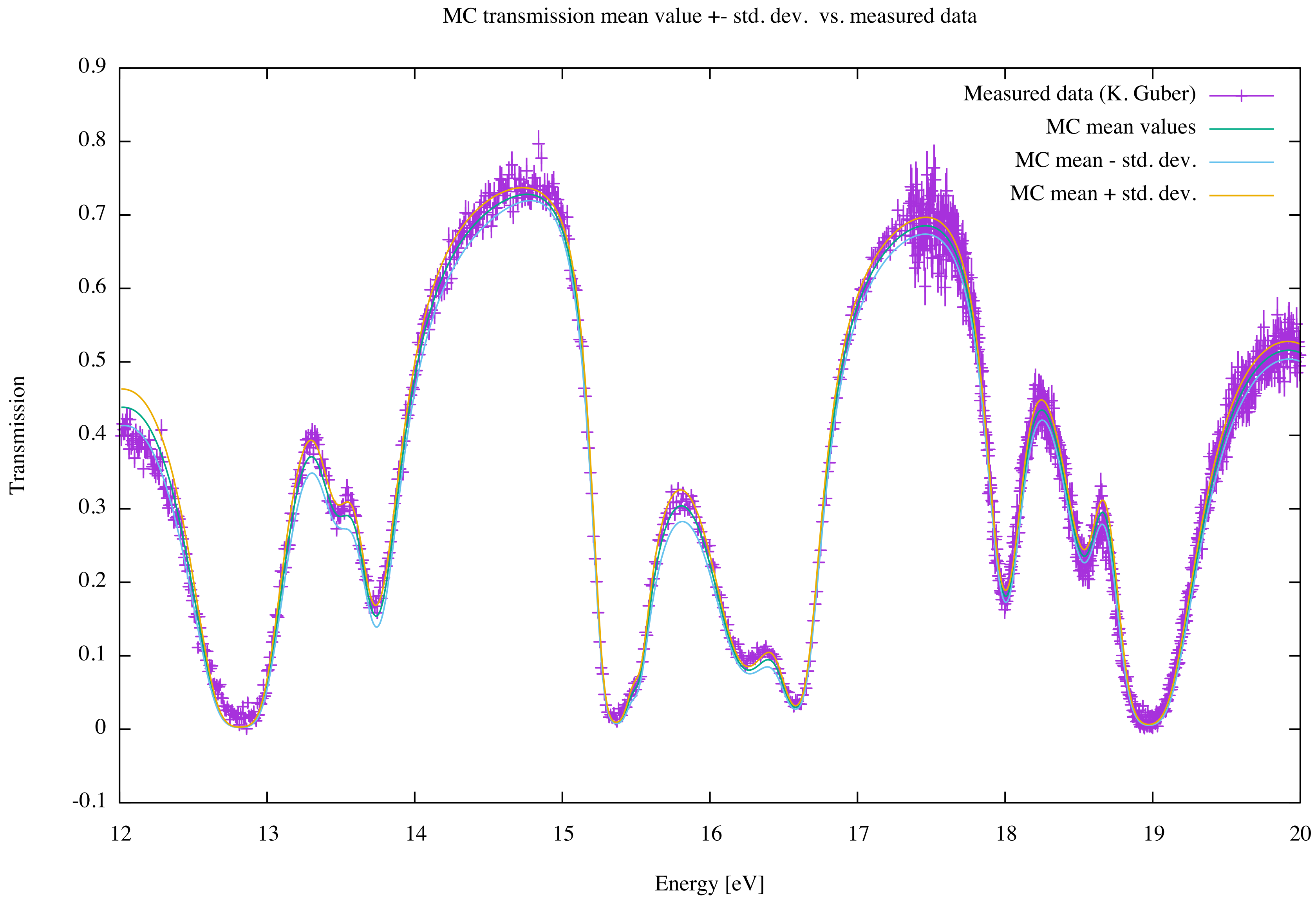
MC total cross section heat map: large variation below 1 eV

- Extremely large thermal cross sections can occur when MC random perturbations of subthreshold resonance energy fall near 0 eV
  - Due to large uncertainty of subthreshold resonance in the ENDF/B-VIII.0 U233 File 32.



Transmission measured data vs. MC ensemble

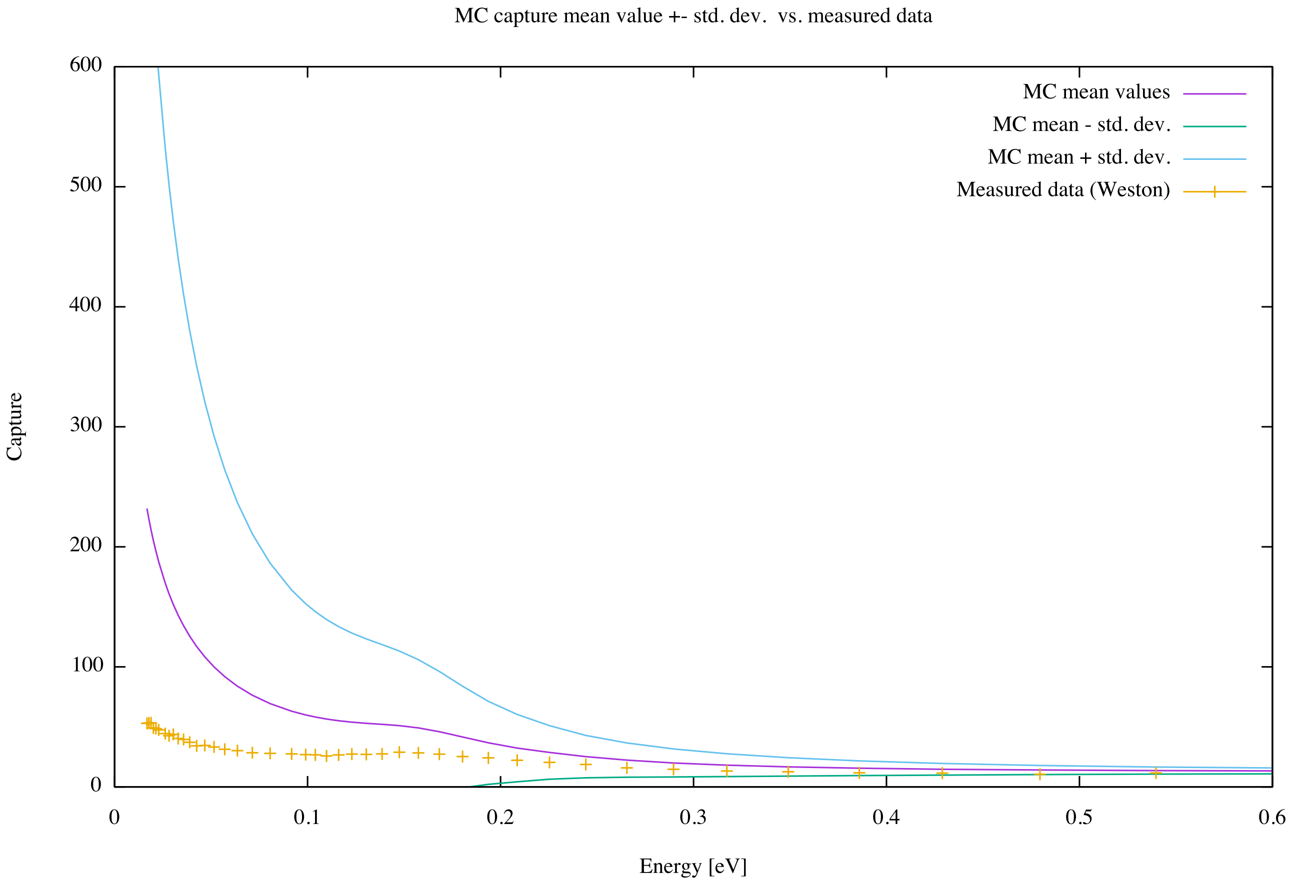
- Agreement above 12 eV is consistent with agreement seen with PUFF on slide 10

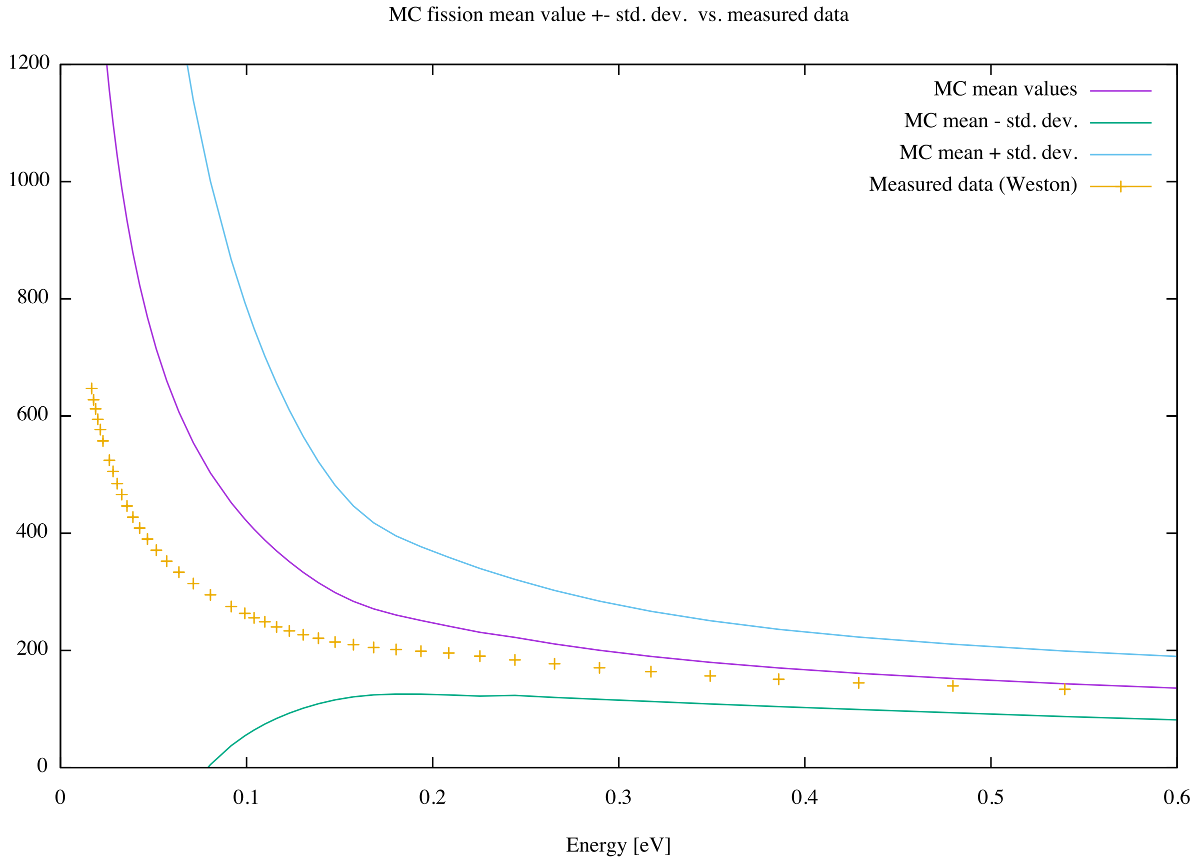


OAK RIDGE National Laboratory

Large variance of MC cross sections below 0.6 eV

- Comparison to Weston capture and fission data:





Conclusions and outlook

- Basic components of the MC evaluation framework of differential and integral data
  - Computation of random MC ensemble from ENDF File 32
  - Simulation of IBEs and R-matrix cross section compared to experimental data
  - Computation of weighted averages
- Application to U-233 indicates deviation from the conventional linear approximation
  - IBEs: U233-SOL-{INTER,THERM}-001-001
  - Diff. data: transmission and fission
- Evaluation framework will require MCMC method e.g. Metropolis-Hastings (M.-H.)
  - Computational burden of IBEs makes this more realistic for differential data evaluation
  - Currently surveying parallelized generalizations of the M.-H. method

Special thanks to ORNL contributors:

- Marco T. Pigni:
  - U-233 SAMMY input files
- Klaus Guber:
  - U-233 transmission and fission data
- B.J. Marshall:
  - Guidance with IBEs and SAMPLER
- Vladimir Sobes:
  - Analytically solvable neutron transport problem for testing

This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.

Auxiliary slides

Overview of generalized form of Bayes' Theorem

- Generalized data = (parameters, data, model defect): $z \equiv (P, D, \delta)$
- Generalized data covariance matrix $\mathrm{C} \equiv \langle (z - \langle z \rangle)(z - \langle z \rangle)^{\intercal} \rangle$
- Constraint on the posterior expectation values define the evaluation:

$$\omega \equiv T(P) - D - \delta$$

$$\langle \omega \rangle' = \omega'_f$$
$$\mathbf{\Omega}' \equiv \langle (\omega - \langle \omega \rangle')(\omega - \langle \omega \rangle')^{\intercal} \rangle' = \mathbf{\Omega}'_f,$$

- Posterior PDF; model T(P) appears only in the the likelihood function via constraints:

$$p(z|\langle z \rangle, \mathbf{C}, f) \propto p(z|\langle z \rangle, \mathbf{C}) \times p(f|z, \langle z \rangle, \mathbf{C})$$

- Exponential likelihood function

$$p(f|z, \langle z \rangle, \mathbf{C}) = e^{-\sum_i \lambda_i \omega_i - \sum_{ij} \Lambda_{ij} (\omega - \langle \omega \rangle')_i (\omega - \langle \omega \rangle')_j}$$

- Extant evaluations impose constraints $\omega'_f = 0$ $\mathbf{\Omega}'_f = 0$ leading to:

$$p(f_0|z, \langle z \rangle, \mathbf{C}) = \delta_{\mathrm{Dirac}}(\omega)$$